Use of Simulation for Optimum Performance of Hydro-desulfurization Unit with ULSD Regulations

An Industry White Paper

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Overview

The European Union 10-ppm sulfur fuel regulations present various challenges for operating and controlling refinery desulfurization units. Repsol-YPF has been using simulation to mitigate some of these challenges.

In a joint project with AspenTech, the two companies developed a rigorous steady-state and dynamic Aspen HYSYS® model of Repsol's Puertollano refinery's hydrodesulfurization (HDS) unit. This model was further integrated with the unit multivariable predictive controller (MPC), Aspen DMCplus®, which helped investigations of reactor conditions and operations to establish better control strategies. This paper presents an account of the project and some lessons learned.

Fuel Specifications and Regulations

In 2009 the European Union introduced environmental fuel specifications and regulations, such as the requirement for refiners to make sulfur-free fuels available in order to reduce pollution from transport emissions and to improve the environmental quality of diesel fuel. The terms "zero sulfur" and "sulfur-free" fuels refer to gasoline and diesel products with less than 10 ppm of sulfur.

Such sulfur specifications severely affect process units dedicated to producing these fuels: It forced refineries to improve the quality of blend stocks through investment in desulfurization and dearomatization technologies and through operational changes.

In general, the European specification has required not only a revamp of several HDS units but also the review of the control philosophy. A more accurate control strategy for HDS units improves profit margins, pushing operating conditions tighter to constraints and specifications, and reducing quality giveaways in the HDS process.

To achieve these ultralow sulfur specifications, Repsol and AspenTech explored how process models may help to evaluate different advance control strategies and achieve a more accurate control strategy.

The companies initiated an R&D project[2,3] to develop a first-principles HDS simulation model integrated with the MPC. The project focused on an HDS unit in Repsol's high-complexity refinery at Puertollano.

Research

Repsol has dedicated considerable effort and R&D resources to understand the ultralow sulfur diesel process. This knowledge, acquired through pilot plant experiments and industrial unit monitoring, has been used to develop a rigorous HDS reaction model including thermodynamic and kinetic mechanisms. The model is based on MS Excel and provides a simple and fast way to calculate all relevant information to predict HDS reaction behavior and performance.

A critical step in the project was to implement Repsol's proprietary technology as a standard unit operation in Aspen HYSYS, the simulator platform. In addition, implementation of the HDS unit operation was to enable its use in both steady-state and dynamic mode.

A multi-disciplinary team from Repsol's technology center and the advanced control departments, collaborated with AspenTech. This team represented combined knowledge in process simulation, HDS process, and advanced control to develop a complete HDS unit simulation and an integrated solution with the Aspen DMCplus multivariable predictive controller (Figure 1).

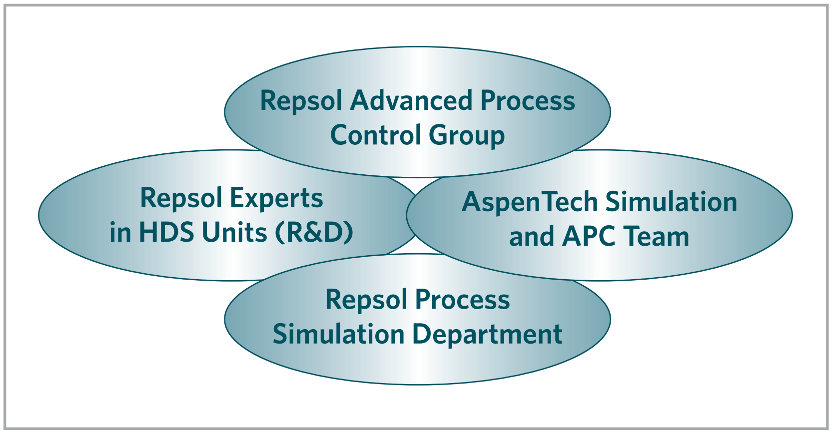


Figure 1. Multidisciplinary project team

The project team had to tackle many challenges during the project:

1. Migrating the HDS Repsol reactor from its Excel Visual Basic for Applications (VBA) format to the Aspen HYSYS simulation platform: The Repsol proprietary model is a complex application in terms of data structure and programming. In addition, the kinetic reaction model was entirely developed in steady-state conditions. A mathematical model for the dynamic behavior of the reactor would be needed.

2. Simulation of the full unit's dynamic behavior in Aspen HYSYS with sufficient accuracy including process dead-times, real proportional–integral–derivative (PID) controllers, valves responses, furnace, and all equipment dynamic behavior.

3. Integrate dynamic simulation with the existing MPC. This step required integrating Aspen HYSYS Dynamics simulation with Aspen DMCplus, with appropriate data exchange across the boundary of the two software packages.

4. Speed: It was desirable to run the entire system at a real-time factor of 10 in the dynamic simulation (10 times faster than actual unit) to be able to perform studies on control strategies and evaluate how the unit would react in a relatively fast timeframe.

To isolate each of these challenges, project execution was divided into a three-stage progression from the initial steady-state simulation to the final dynamic model linked with the Puertollano HDS unit's advanced process controller (Figure 2).

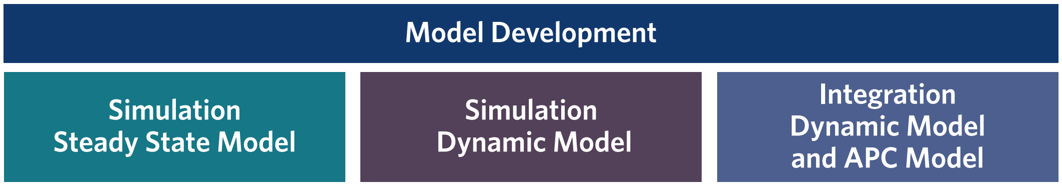


Figure 2. Project phases

First Phase

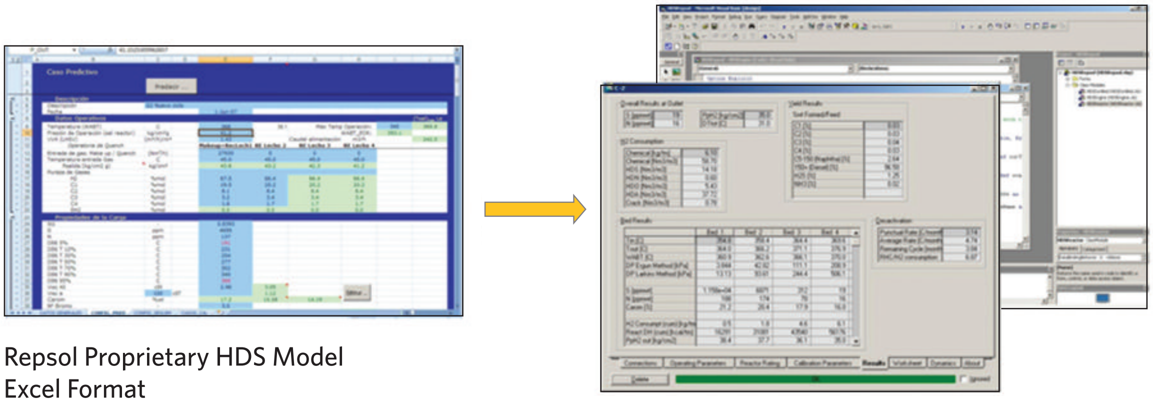
Through the following steps, the project went from an initial basic model to a well-calibrated steady-state simulation:

1. Collect engineering design and process plant data.

- Process Flow Diagrams (PFDs) and Piping and Instrumentation Diagrams (P&IDs), all design equipment datasheets (columns, pumps, compressors, heat exchangers, valves, etc.) were collected.
- A representative and stable period of time (1-3 days, 1-min samples) was selected, and all available instrument readings (pressures, temperatures, flows, levels, controller PVs, OPs, SPs) were collected. Laboratory composition analysis for feeds and products were also taken for the different operating points to be modeled. A mass-balance reconciliation was also needed for proper calibration.

2. Incorporate Repsol's proprietary technology for HDS reactor (steady state) into the simulation environment.

- This was the core activity in this phase. As mentioned earlier, Repsol's R&D technology center has a proprietary model (Figure 3) for the hydrodesulfurization reaction mechanism, developed through extensive pilot-plant data and industrial unit follow-up.[1] This model is built in MS Excel and utilizes standard VBA code and Excel spreadsheets for all its functionality.



Repsol Proprietary HDS Model
Excel Format

"Container" in AspenTech simulation platform
realized through a Visual Basic built ".dll"

Figure 3. Reactor model migration

- The entire HDS reactor's model code was transferred into a "container" (Figure 4), which can then be used as a standard unit operation in the simulation platform. The code migration involved creation of a detailed hierarchical structure of matrices to handle all information on the reactor beds (i.e., catalyst kinetic properties, catalyst physical properties, bed geometry). These matrices provide the functionalities previously realized through different Excel spreadsheets in Repsol's standalone model.

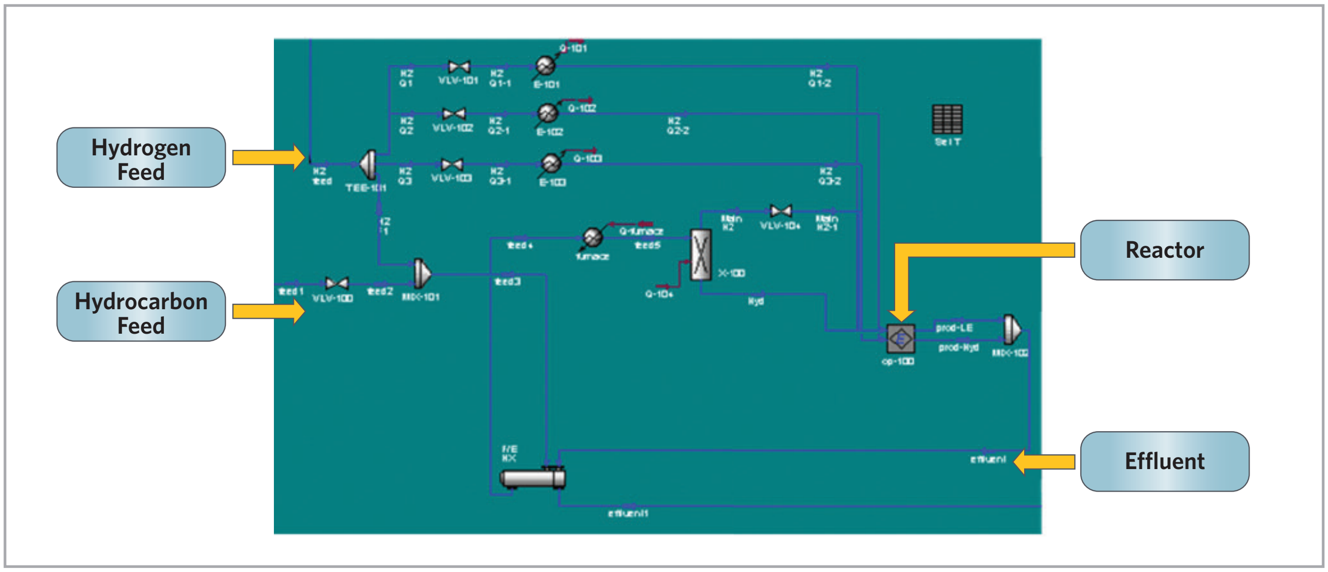


Figure 4. Reactor section in Aspen HYSYS

- The HDS reactor model thus developed can now be used by Repsol as a standard unit operation within the flowsheet simulation platform, interacting with other unit operations, automatically reading feed information and populating product information (Figure 5).

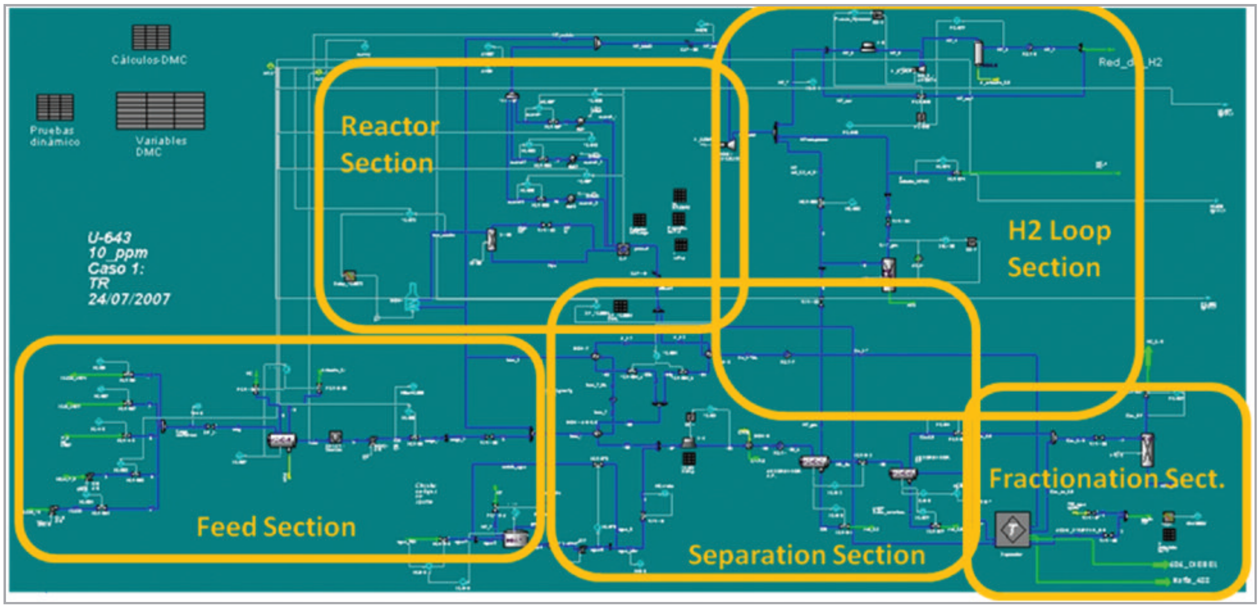


Figure 5. Aspen HYSYS model of the complete HDS unit, including dynamics

- In particular, it provides a way to translate typical output from Repsol's kinetic model (reactor effluent D86 distillation and properties) into a stream composition with pseudo-components, and populating the property distributions for these pseudo-components. As a result, a complete HDS process unit model can now be built and used.

3. Complete the fully calibrated steady-state model of Repsol's Puertollano refinery's HDS unit (feed + reactor + H2 make up/separation + fractionation sections) for a specified sulfur-level operation.

- The model was tuned and calibrated by reconciling the discrepancies with the plant data, by adjusting certain values and parameters such as boundary conditions, feed compositions, valves, and heat-exchanger pressure drops and tray efficiencies. This is a critical step to ensure the model corresponds to actual unit operation and has to be fulfilled before proceeding with further development.

Second Phase

Developing a complete dynamic model of the Puertollano HDS unit followed the steps:

1. Development of the dynamic section of the "container" representing the HDS reactor unit's operation.
    - The original Repsol reactor model was only a steady-state representation. As part of the project, the Repsol-AspenTech team developed a mathematical model to represent the dynamic behavior of the HDS reactor, with the Repsol R&D technology center sharing experiences on the phenomenon occurring in the reactor.
    - The mathematical model was then translated into code inside the "container" so that the reactor unit's operation now works in both steady-state and dynamic modes in the simulation platform. At the end of this step, the majority of the work on the "container" was done.
2. Completion of the entire dynamic model.
    - This step introduces all necessary information on existing equipment. This ranges from valve CVs to tray sizing, valve characteristics to equipment volume hold-ups, from PID controllers to equipment resistance to flow based on pressure drop. Much of this information comes from technical datasheets or plant data. (Figures 6 and 7) provide a view of the complete dynamic model.
    - At the end of the first two phases, the Repsol HDS model was ready to be used.

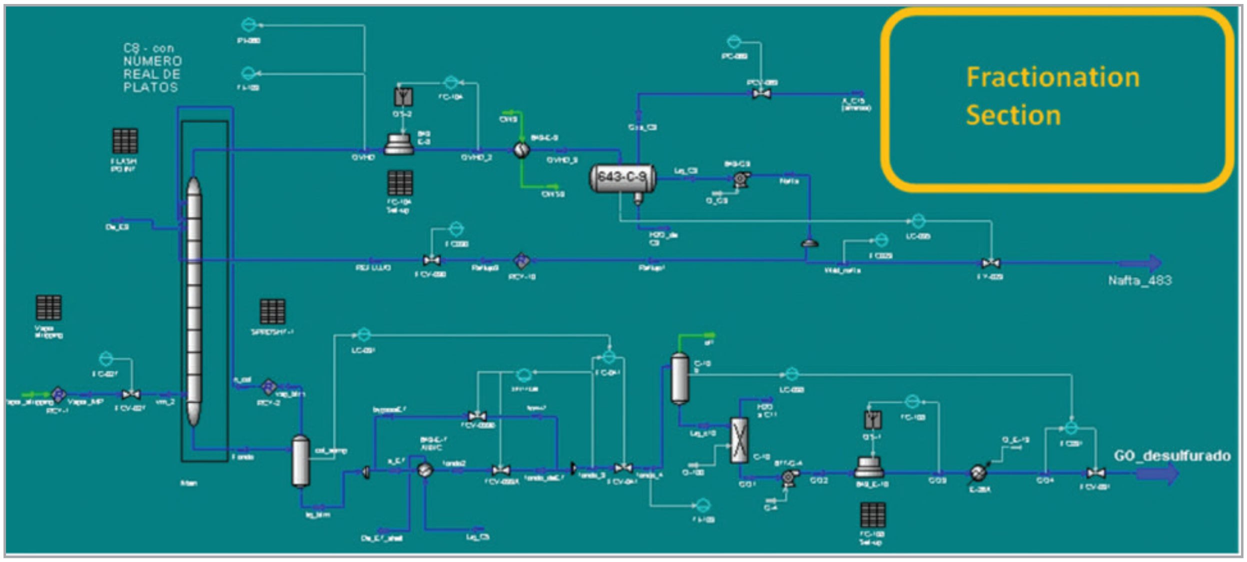


Figure 6. Fractionation section with dynamic model details

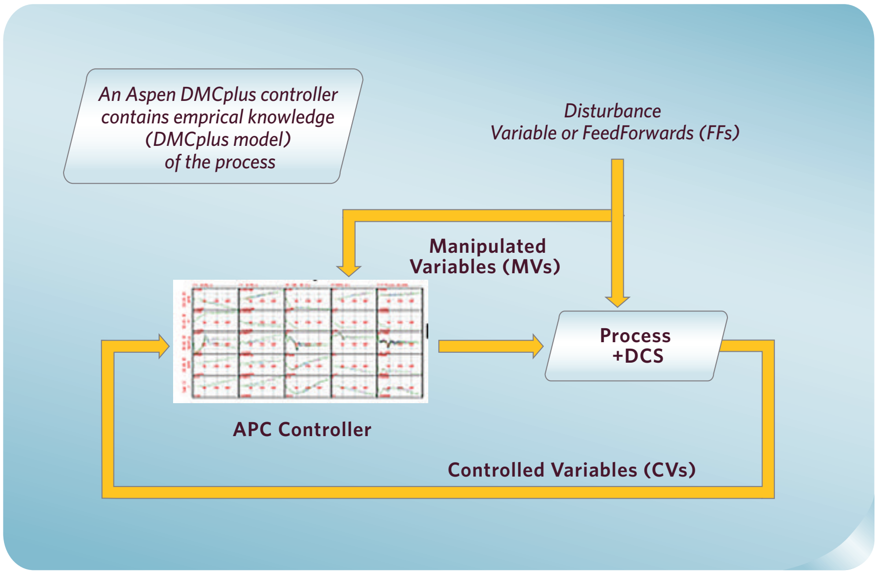


Figure 7. Dynamic Matrix Control terminology

With the previous approach, in which the reactor was modeled and used in Excel, a complicated workflow was needed to bring the results from Excel into the simulation platform and then to check the impact on the rest of the flowsheet for operational and/or catalytic changes in the reactor. The iterative convergence of the hydrogen loop was an "almost manual" procedure that involved extensive time and effort.

- At the end of the second phase, everything is integrated and represented in one environment, the Aspen HYSYS simulation platform, reducing the time to do "what-if" studies compared with the previous approach. The dynamic model also could be used as a "virtual" unit to study the dynamic behavior after operational changes (set point modifications or feed variation).
- The initial speed or real-time factor of the model (the number of times at which the model can run faster than reality) was unsatisfactory, around 1.1 only. Some modifications, especially in the way pseudo-components were managed in different sections of the model and in the number of pseudo-components, raised the time factor to 4, judged to be a good compromise.

Third Phase

The main objective of the third phase was to link the full dynamic model to the Advanced Process Control (APC) controller and test the model's accuracy vs. the real plant.

Before integration of the APC controller, the basic PID loops in the model had to reproduce the same control behavior specified by the control parameters from the distributed control system. All these parameters were introduced in the PID controller objects of the simulation platform applying the required conversion, depending on the algorithm used in each PID loop.

Dynamic matrix control (DMC) is a method of model predictive control and is especially powerful for multiple-input/multiple-output (MIMO) control systems. It is based on an empirical matrix model that predicts the behavior of the dependent process variables with respect to changes in the independent variables. Those independent variables that are available to be moved are called "manipulated variables" (MVs), typically set points or valve positions. Dependent process measurements to be maintained at a desirable point are called "controlled variables" (CVs) and are typically product qualities, process constraints, and so forth (Figure 8).

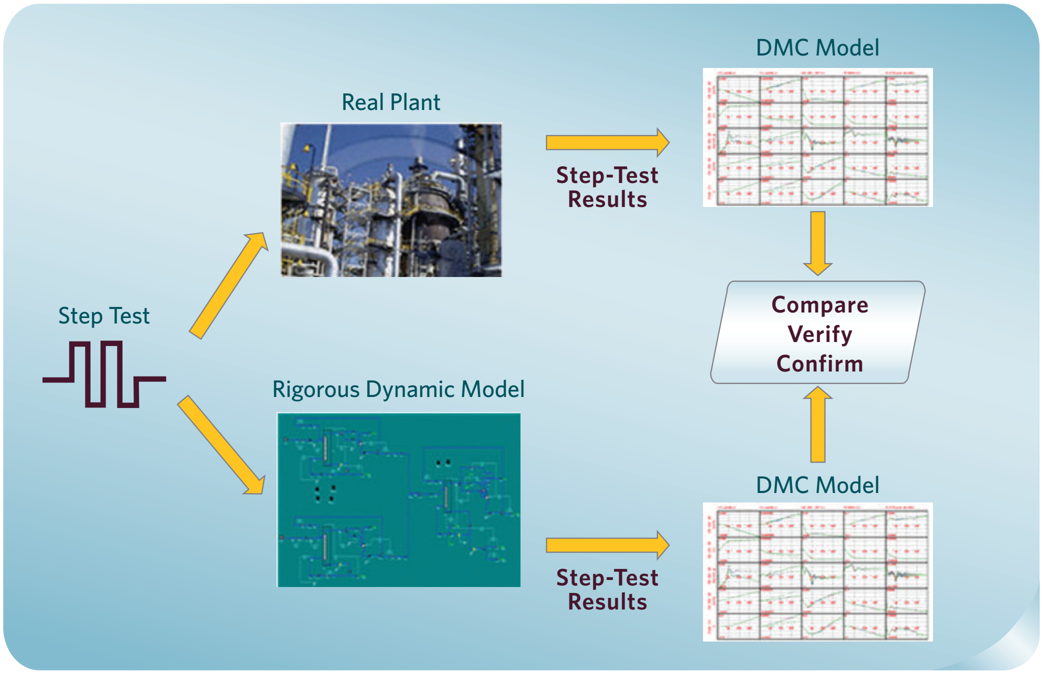


Figure 8. Aspen DMCplus model generation

The dynamic matrix control of the Puertollano HDS unit's APC controller, using Aspen DMCplus, consisted of 15 independent variables (rows) and 21 dependent variables (columns). Each cell of the matrix contains the step-response curve for each pair of independent-dependent variables.

The Aspen HYSYS Dynamics simulation platform has an object that represents the real APC controller. This object can be added to the simulation model and linked directly to the real APC controller software running on the same computer. Thus, the APC controller does not "know" that it is controlling a simulated plant.

Dynamic Validation

Once these three phases were completed, a validation stage checked how well the dynamic simulation represents the real plant.

The basic validation procedure is to obtain an Aspen DMCplus matrix model derived by step-testing the rigorous dynamic model, then compare it with the Aspen DMCplus matrix model derived from the real plant (Figure 9).

The actual plant controller, however, was designed for higher sulfur diesel operation (about 200 ppm) than the current HDS simulation for the future operating mode (10 ppm).

This change in desulfurization level affects the process variable responses. At 10 ppm operation, the residual sulfur components are much more difficult to remove than other species at 200 ppm. Therefore, the reactor severity or the hydrogen consumption required to achieve a 1 ppm decrease in sulfur content of the final product are notably different.

This issue not only affects the modeled gains matrix but also the dynamic behavior; so this procedure may introduce substantial errors if it is used in the validation process.

Therefore, comparing the dynamic model properly with a similar real HDS operation required an alternative procedure. The best option was to carry out some step tests in the real HDS plant. During a 3-day step-test period in the industrial unit, changes in the main variables were completed at a 50 ppm sulfur specification on diesel product. The resulting dynamic matrix was then used in the HYSYS dynamic validation.

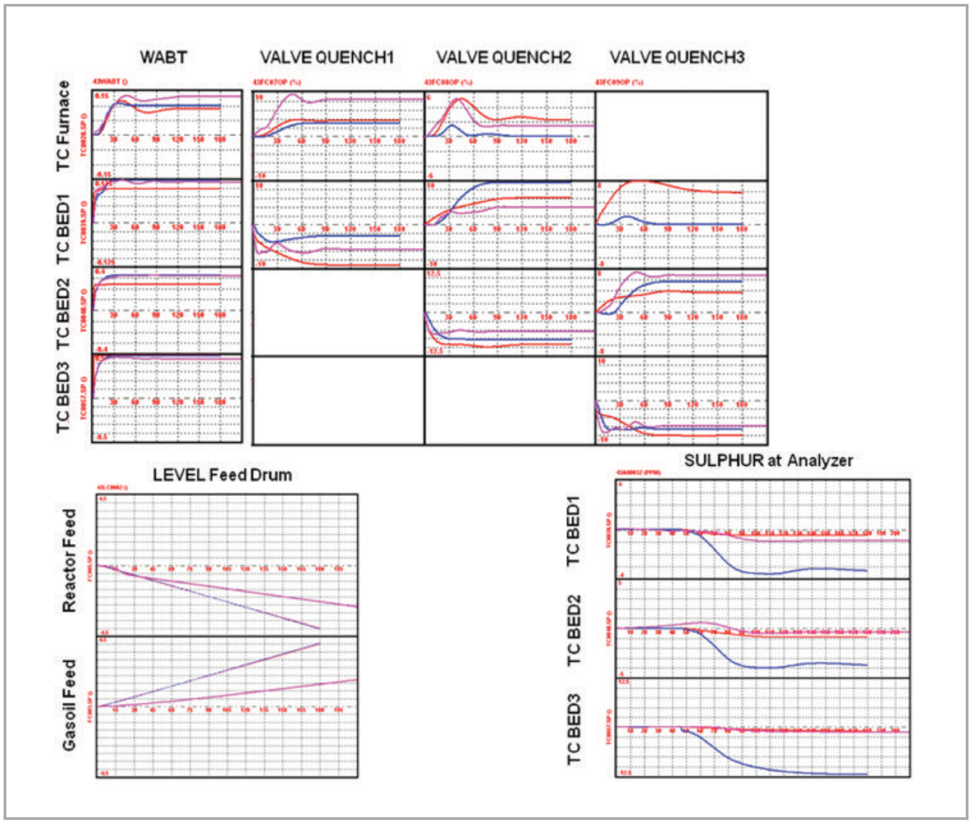


Figure 9. Aspen DMCplus model comparison

After an initial assessment of both Aspen DMCplus comparison models (one based on plant data and the other built with simulated data from the rigorous dynamic model), some adjustments in the HDS simulation were needed in order to achieve dynamic behavior closer to the real plant:

- **Valve characteristics.** Some valves, specially the quench valves, require a more accurate representation than the default isopercentage curve of the simulation platform. The real valve characteristic was obtained from historical process-plant data, flow vs. valve opening and configured in the custom valve characteristic of the simulation valve object.
- **Pure process dead times.** In the simulation platform it was not easy to simulate flow through a long pipe as pure plug-flow process dead-time. A typical solution is to use the "PIPE object" with several segments, but it still did not reproduce the actual "transport" phenomenon well.

More than 100 segments would be required to yield good results, but that would slow down solution speed of the model. An alternative solution was used with delay transfer function blocks (to represent the dead-time).

Figure 9 compares the DMCplus models obtained by simulation with the real plant. As a guideline:

- Original DMCplus with plant at 200 ppm (blue line)
- DMCplus from plant tests at 50 ppm (pink line)
- DMCplus from rigorous model (red line)

The DMCplus models generated with the first-principles model at 10 ppm (red) showed a good match in terms of gain and response time when compared with the existing DMCplus models at 50 ppm (pink) and also at 200 ppm (blue). These comparisons proved that the simulation model was sufficiently trustworthy for the control analysis objectives of the project.

Control, Operations Studies

Once the validation process was completed and suitable model adjustments made, the simulation showed a dynamic response very close to the real plant. The integrated simulation and APC controller was now ready for use in control and operations studies. It is possible to include new control objects in the simulation environment and new variables in the APC controller design to evaluate the incremental benefit that may be achieved by improving the existing control strategy.

Case 1: Including a sulfur-feed analyzer in the APC controller. Due to tighter sulfur levels required in the final product, the margin for correcting out-of-specification products by blending is now reduced. So it is critical for HDS plants to increase their capability to respond faster to plant disturbances.

Since changes in the sulfur feed content may greatly affect the final diesel, the effect of including a feed sulfur analyzer in the APC controller design has been tested.

The HDS dynamic simulation makes it possible to add this kind of analyzer as a new variable in the MPC controller and determine if an improvement in the control response would be achieved, both in terms of stabilization time and standard deviation (Figure 10).

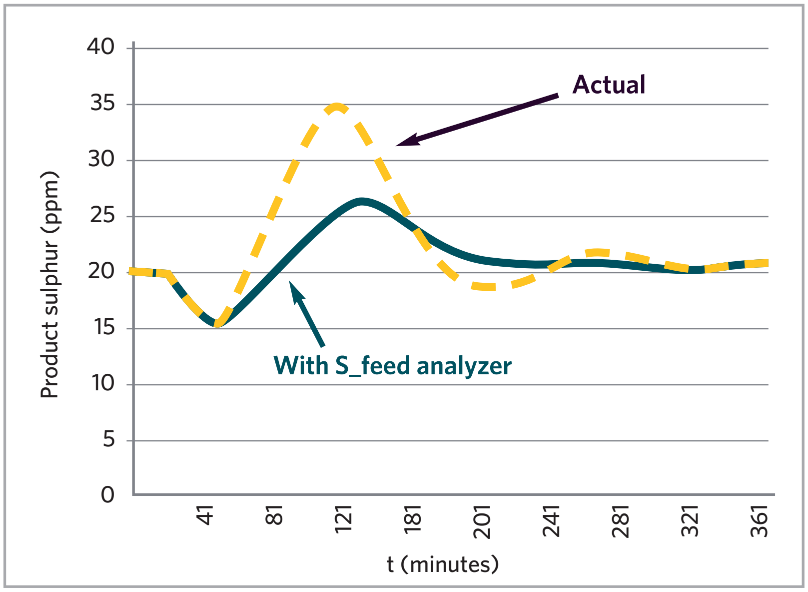


Figure 10. Control improvement by adding a feed sulfur analyzer

A new analyzer would allow operating the plant under less severe conditions, closer to the 10 ppm desired and with associated savings in energy, hydrogen consumption, and catalyst life cycle.

Case 2: Sulfur reactor outlet's inferential development. In a 10 ppm operation, the control needs to be very tight to avoid quality giveaways. A sulfur analyzer is located in the gas oil product line, but its response has a large dead-time and slow process response to perform accurate control.

During the APC revamp project for 10 ppm in the Puertollano HDS unit, a "fast model" (online inferential) was developed and tested to predict the product's sulfur, updated with the analyzer data periodically.

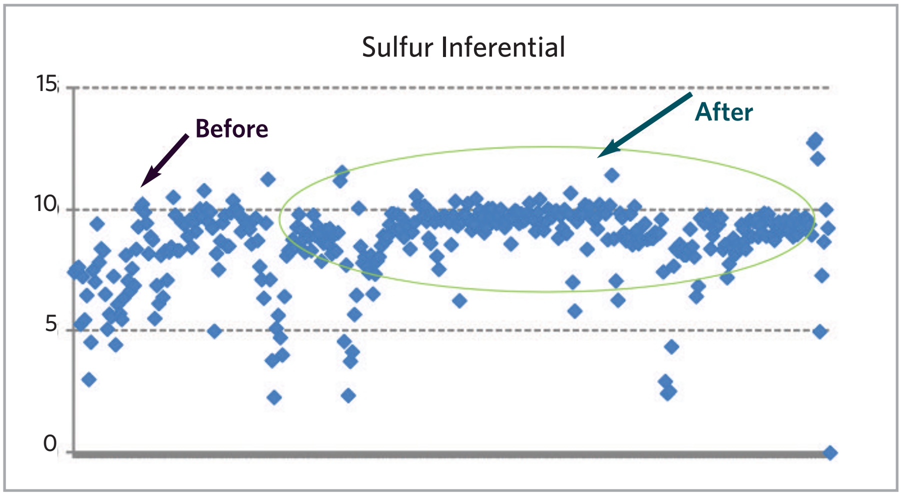


Figure 11. Gas oil product sulfur content before and after inferential implementation

An algebraic inferential, based on weighted average bed temperature, feed flow, and other parameters was calibrated with coefficients coming from step-test and from the simulation (Figure 11). After the inferential implementation, sulfur control is much better, reducing the WABT by 2°C.

Controlling the sulfur content tightly at 10 ppm makes it possible to save energy (fuel), reduce hydrogen consumption and increase catalyst life. Considering only energy consumption, (Figure 12) gives an indication of the percent increase in energy consumption when the operation moves away from the desired 10 ppm specification.

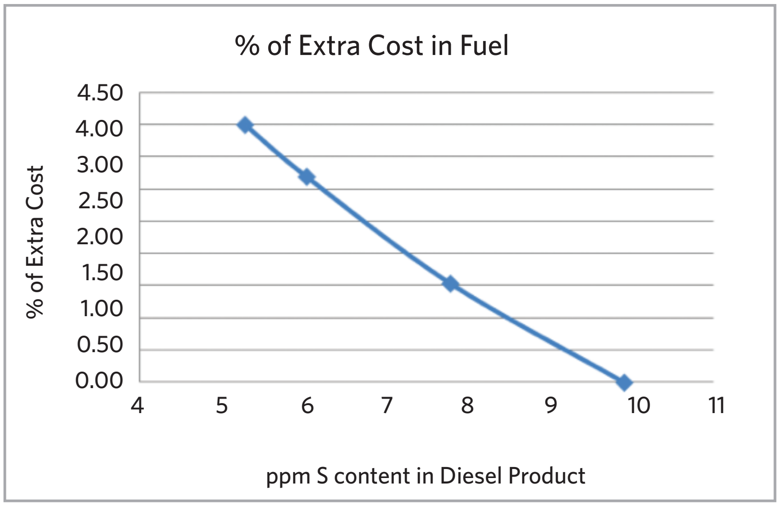


Figure 12. Percent increase in energy (fuel) consumption compared to a base case at 10 ppm sulfur specification

Conclusions

The integration in a single rigorous simulation of the whole HDS unit model provides a powerful tool that enables Repsol to:

- Use it as a tool to evaluate the impact of operational changes or feed quality changes to the unit (steady-state and dynamic "what-if" studies).
- Evaluate control strategy improvements in HDS plants without having to perform step-tests in the actual units, and therefore reduce operational, safety and product quality risks.
- Help develop online inferentials that may provide significant savings in energy consumption as well as in increasing catalyst life.
- Perform conceptual and basic engineering studies for unit revamps or evaluate new process schemes.
- Improve plant performance knowledge, especially useful to train plant operators.
- Use it as basis for HAZOP studies.

Moreover, this project has been very ambitious with high technical development goals, requiring an advanced level of simultaneous expertise in diverse areas to develop the simulation tools and a high effort to enhance the fluid flux of knowledge between all the groups involved.

Repsol's current objective is to apply this integrated model to other HDS units, and to extend and maximize model utilization in both steady-state and dynamics applications, thereby avoiding disruptions and minimizing the impact on real plant operations.

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