Optimisation of a diesel hydrotreating unit

A model based on operating data is used to meet sulphur product specifications at lower DHT reactor temperatures with longer catalyst life

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Meeting product specifications in diesel hydrotreating units is a challenging task requiring ongoing process adjustments as the feed sulphur content can vary significantly during the course of operations. Refinery operations will often run these units at higher reactor temperatures than required to ensure product sulphur specifications are always met but these higher temperatures can negatively impact product yield, energy costs, and catalyst life. This study uses a time series auto-regressive moving average model with explanatory variables (ARMAX) constructed using actual operating data to evaluate the performance of a diesel hydrotreating (DHT) unit at different sulphur operating targets. The optimum sulphur operating target ensures product specifications are consistently met while minimising the detrimental impact of higher reactor temperatures on product yield, energy costs, and catalyst life. The study focuses on the trade-off between sulphur operating target and catalyst life.

The methodology used in this study assumes operating data is available to evaluate the performance of the DHT unit within the sulphur operating target range of interest. The use of a process simulator in combination with Monte Carlo random sampling to evaluate the performance of a distillation unit outside of the current operating range was presented in a previous article.[1] The ARMAX model uses transfer functions to capture the relationships between key process variables and the produced diesel sulphur content. The model also contains a noise model to account for the variation in sulphur content not explained by the process variables and to properly represent the autocorrelation structure of model residuals.

The ARMAX model was used to determine the optimum sulphur operating target for the DHT unit by conducting a series of Monte Carlo simulations to model the unit performance under varying process conditions. The variability of the process due to changing conditions in the process variables was modelled using estimated probability distributions. The noise model is superimposed to account for unexplained process variability. Simple control logic was implemented as part of the Monte Carlo simulation that adjusted the reactor weighted average bed temperature (WABT) as necessary to maintain the produced sulphur content within pre-specified operating limits. To capture the effect of running at different WABTs on catalyst life, a term integrating WABT over time was also included. Integrated time on temperature has been previously used in predicting fouling/coking in fired heaters.[2] The ability of the process unit to meet diesel product sulphur specifications and the effect on catalyst life in light of reactor pressure drop (dP) and temperature constraints were then evaluated to determine the optimum sulphur operating target.

Figure 1 is a typical process flow diagram of a DHT unit. The raw diesel mixes with recycled hydrogen before entering the heater. The heated mixture

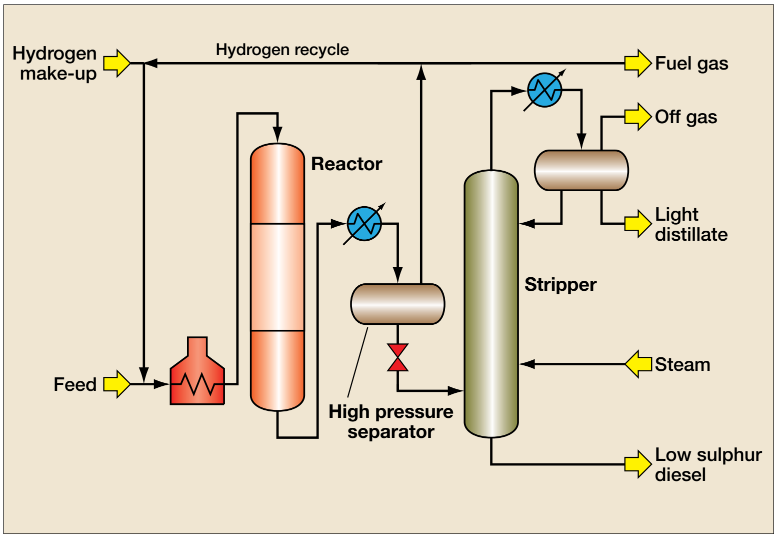

Figure 1 Diesel hydrotreating unit schematic

enters a reactor where hydrogen reacts with sulphur to produce hydrogen sulphide.[3,4] A steam stripper unit then removes the hydrogen sulphide from the diesel. The produced diesel needs to meet a maximum sulphur specification ranging between 10-11 ppm at the delivery point. The refinery configuration specific to this study combined the DHT reactor bottoms stream with the bottoms stream from a light cycle oil (LCO) hydrotreater hydrocracker reactor (HTHC) before entering the H_2S steam stripper. The bottoms stream from the steam stripper then goes into a downstream fractionator for final separation.

The following steps summarise the methodology used in this study:

1. Transfer functions for each of the process inputs developed using cross correlation charts between produced diesel sulphur content and the process input
2. Parameters of a noise model determined by examining autocorrelation and partial autocorrelation charts of residuals after accounting for the effect of process variables on sulphur content via the transfer functions
3. Probability distributions generated for input process variables
4. Monte Carlo simulations conducted for different sulphur operating target scenarios.

The simulation results are then used to evaluate the impact of the different sulphur operating targets on the ability of the process to meet the diesel sulphur specification and on catalyst life. A maximum reactor pressure drop (dP) of 90 psia and a maximum WABT of 760°F were assumed to estimate catalyst life.

A detailed description of the construction of the time series ARMAX model is provided below, followed by analysis results and conclusions.

ARMAX time series model construction

The first step in the construction of the ARMAX model is to identify the structure of the transfer function for each of the process inputs.[5] The cross correlation function chart (CCF) between the response and the input at different time lags of the input is needed. Quite often the generation of the CCF requires first differencing of both input and output time series. First differencing is calculated by taking the difference between the current value and previous value of a time series. Before building the CCF chart, the input is converted into an uncorrelated time series or white noise by removing any

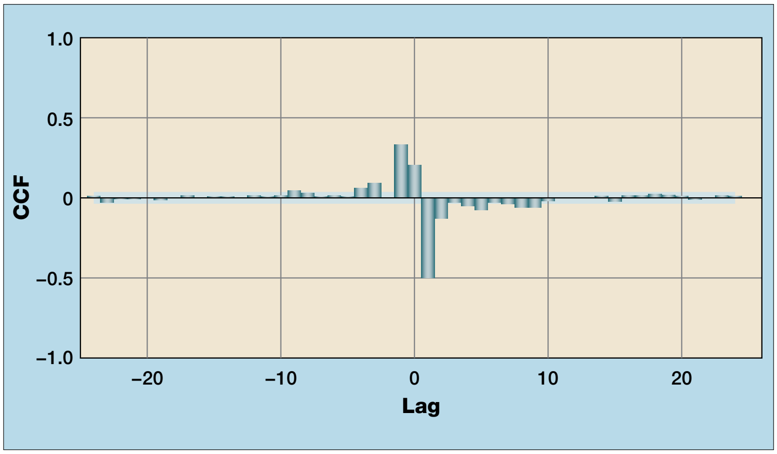

Figure 2 Sulphur vs WABT cross correlation chart

autocorrelation present in the input. This step is known as pre-whitening and the associated pre-whitening filter has an ARMA structure. The pre-whitening filter is also applied to the response prior to calculating the CCF. The SAS Analytics procedure Proc Arima[6] performs all of the necessary steps outlined above to generate the CCF for each input. The CCF is then used to identify the statistically significant time lags to consider in the transfer function. One-hour interval data were used in the construction of the ARMAX model.

Of all the variables considered in the study, reactor WABT was found to be the most influential variable impacting produced diesel sulphur content. Other variables considered and found to be statistically significant were DHT reactor weighted average temperature, DHT reactor recycle hydrogen purity, diesel production, and fractionator reboiler duty ratio. Process variables associated with the operations of the LCO HTHC reactor were not found to be statistically significant in predicting sulphur content during the period of operations considered.

Figure 2 gives the CCF chart for the WABT process variable. The CCF chart gives the correlation coefficient between the sulphur content response and WABT input at different time lags of the input. Positive lags represent previous values of input and negative future values of the input. Spikes or statistically significant lags in the CCF chart occur when the correlation coefficient value is outside of the 5% significance limits represented as the shaded area. High correlation between these variables at time lags of -1, 0, 1 and 2 periods can be seen in the CCF chart. When identifying the structure of the transfer function for an input, lags greater than or equal to zero are examined as we only consider causal models where the response is affected by previous or current values of the input. The negative spike at the time lag of 1 period indicates that an increase in WABT at time t-1 results in a decrease on sulphur content at time t. Spikes at

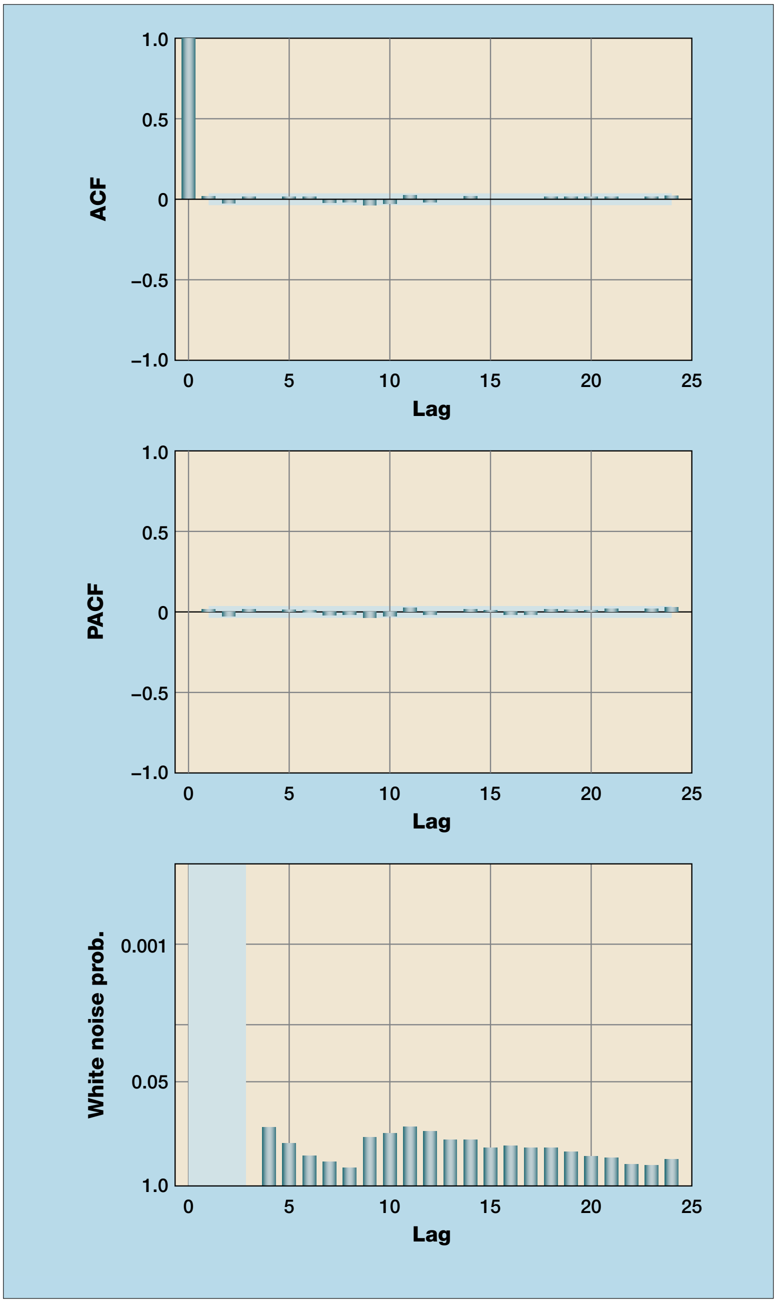

Figure 3 Final model residuals charts

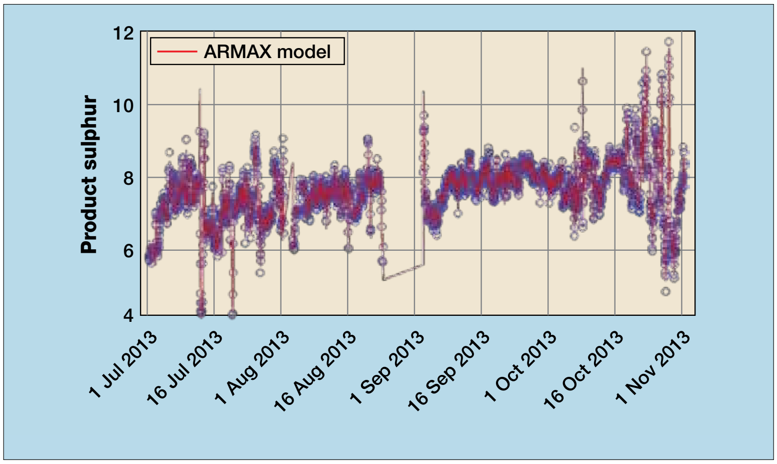

Figure 4 Predicted vs actual diesel sulphur content

% off-spec and estimated catalyst life results				
Sulphur target, ppm	1-hr data off-spec, %	24-hr data off-spec, %	Avg catalyst life months dP limited	Avg catalyst life months temp limited
5.0	0%	0%	15.6	31.4
5.5	0%	0%	17.3	33.1
6.0	0%	0%	19.1	34.8
6.5	0%	0%	20.8	36.6
7.0	0%	0%	22.3	38.3
7.5	0.0%	0.0%	24.1	40.1
8.0	0.1%	0.0%	25.9	41.9
8.5	1.3%	0.0%	27.7	43.6
9.0	7.4%	0.1%	29.5	45.4

Table 1

negative lags such as the one observed at lag -1 represent a feedback control mechanism. In this case, a high sulphur content signal value is followed by an increase in WABT and low sulphur content signal value by a decrease in WABT. This feedback control mechanism was considered in the simulations by using a one-period delay between a sulphur signal and the corresponding adjustment to WABT. Based on this analysis, time lags at 0, 1, and 2 were considered for the WABT transfer function.

The same general approach was followed for all other inputs to identify the structure of their transfer functions. None of the variables required use of a transfer function denominator term as this term was not found to be statistically significant for any of the variables. Once all transfer functions are defined, the next step focuses on the determination of the structure of the noise model. This step requires turning the model residuals into uncorrelated errors or white noise time series. Autocorrelation and partial autocorrelation charts are used to determine the statistically significant terms of the noise model. A noise model with second order autoregressive terms along with a lag 3 moving average term gave the best fit. The noise model accounts for unexplained variation including changes in feedstock quality not accounted for by the other explanatory variables in the model. The ACF, PACF, and white noise charts of the final model residuals are given in **Figure 3**. The final model residuals have been reduced to white noise as no significant spikes remained in ACF, PACF, and the white noise charts.

The final model is summarised below. The model includes a reboiler duty ratio term associated with the fractionator downstream of the DHT unit. The reactor dP model is also provided below. **Figure 4** below compares the observed produced diesel sulphur content values vs the model predicted values. Note that most of the variability in sulphur content was captured by the model.

$$Sulphur = 116.4+0.09*WABT_t-0.23*WABT_{t-1}-0.01812*WABT_{t-2} + 5.5E-5*DslProdt-0.064*H2_{t-1} -0.064*reb\_duty\_ratio_{t-1} + 5.74E-7*Integrated\_WABT_t+N_t$$

$$dP_t = -1.987+0.997* dP_{t-1} +0.0032*WABT_t$$

where:
$Sulphur_t$: diesel sulphur content at time t
dP_t: reactor pressure drop at time t
$WABT_t$: reactor weighted average bed temperature at time t
$Integrated\_WABT_t$: $Integrated\_WABT_{t-1}+WABT_t$
$H2_{t-1}$: recycle hydrogen purity % at time t-1
$reb\_duty\_ratio_{t-1}$: reboiler duty ratio at time t-1 in Mbtu/bbl of diesel produced

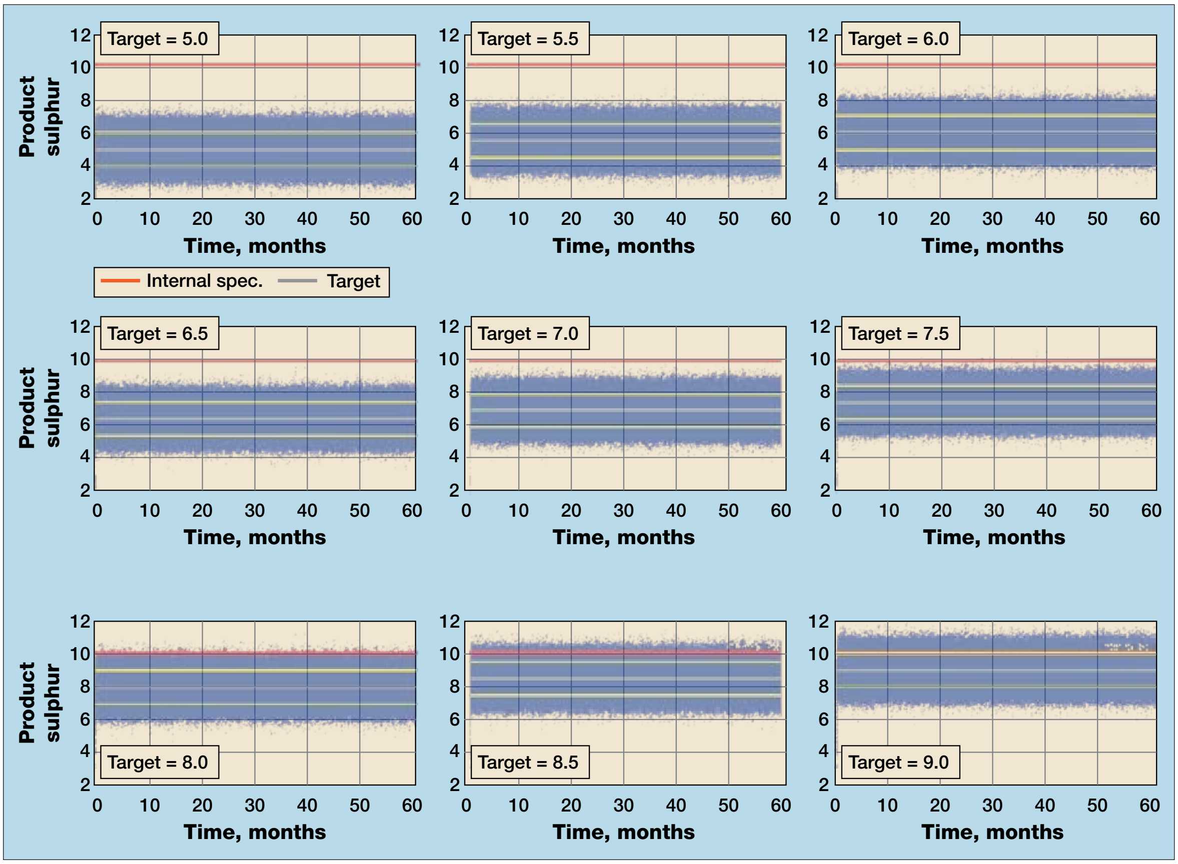

Figure 5 Diesel sulphur vs time

$DslProd_t$: diesel production at time t
N_t: process noise
$N_t=[(1+0.1132B^3)/(1-1.0959B+0.147B^2)]\ \varepsilon_t$
ε_t=white noise or uncorrelated random error

Analysis and results

The ARMAX model was used with Monte Carlo random sampling to examine the DHT unit performance at different sulphur operating targets under varying process conditions. Probability distributions were developed for diesel production rate, recycle hydrogen purity, and reboiler duty ratio using actual operating data. The unexplained variation in sulphur content was represented by the ARMAX noise model. Different scenarios were considered in which the sulphur operating target was specified. Sulphur operating targets ranging from 5-9 ppm at 0.5 ppm increments were considered. Upper and lower control limits of +/- 1 unit from the sulphur operating target were assumed. A simplified feedback control scheme was modelled using the predicted sulphur content values from the ARMAX model which was driven by Monte Carlo simulation. The distributions of diesel production rate, recycle hydrogen purity, and reboiler duty ratio were used to generate values for these inputs. The error disturbances associated with the noise model were also generated by random sampling. The simplified control scheme increased the WABT temperature in the subsequent time period if the predicted sulphur was higher than a pre-specified upper control limit or conversely decreased the WABT temperature if the sulphur was lower than the lower control limit. The analysis assumed a change of 1°F per 1 ppm offset from sulphur target would be required based on a simple regression model of WABT at time t vs the sulphur at time t-1.[7]

The term integrating WABT over time was used to model the required increase in reactor WABT over time due to catalyst deactivation. **Table 1** summa-

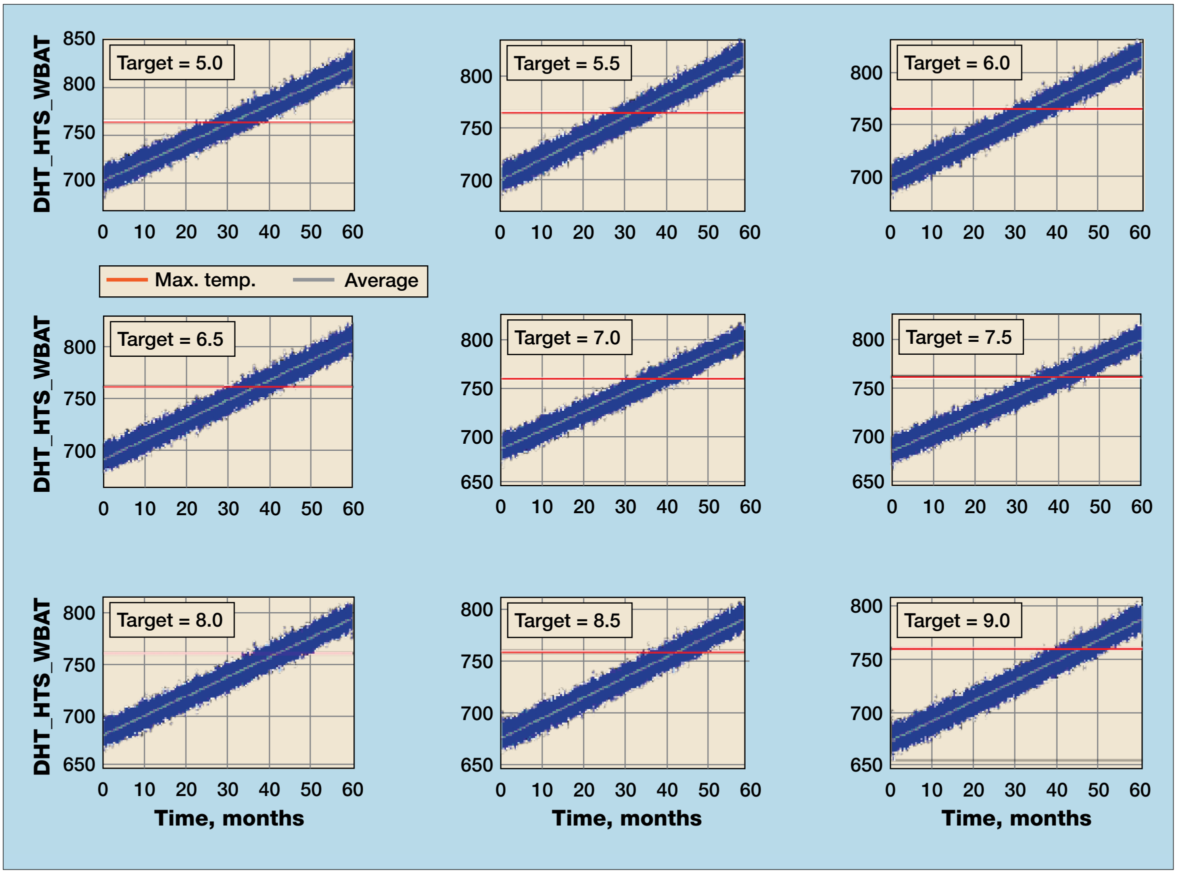

Figure 6 Reactor WABT vs time

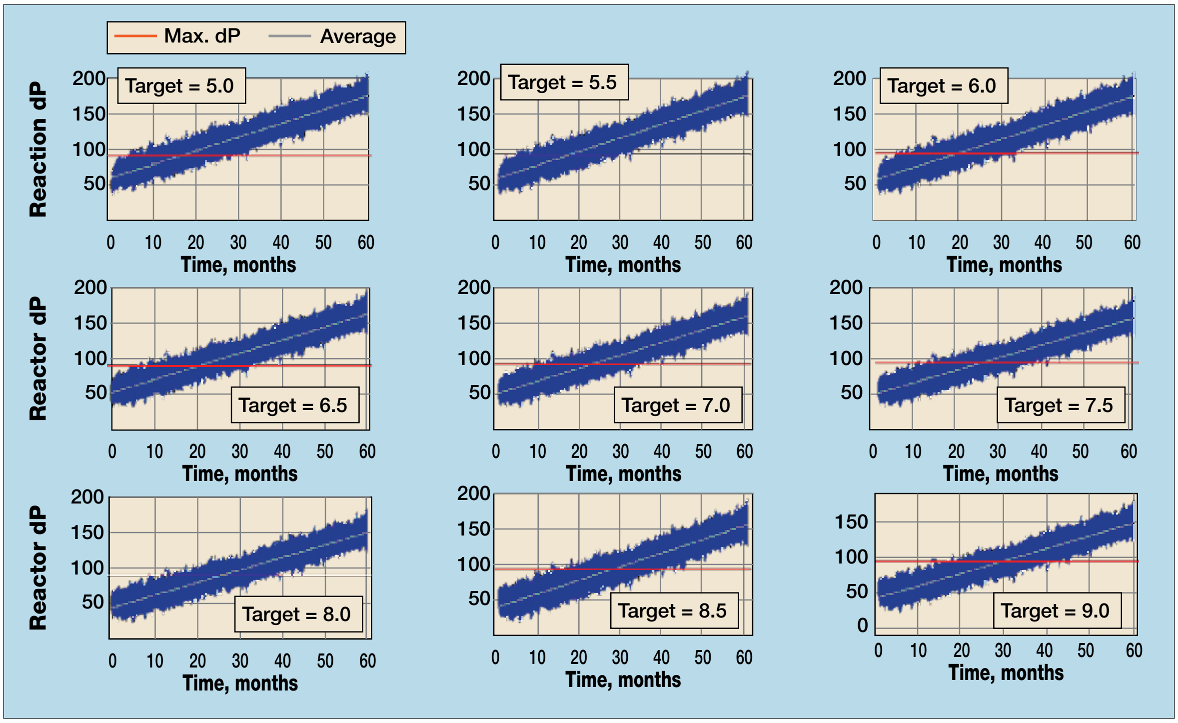

Figure 7 Reactor dP vs time

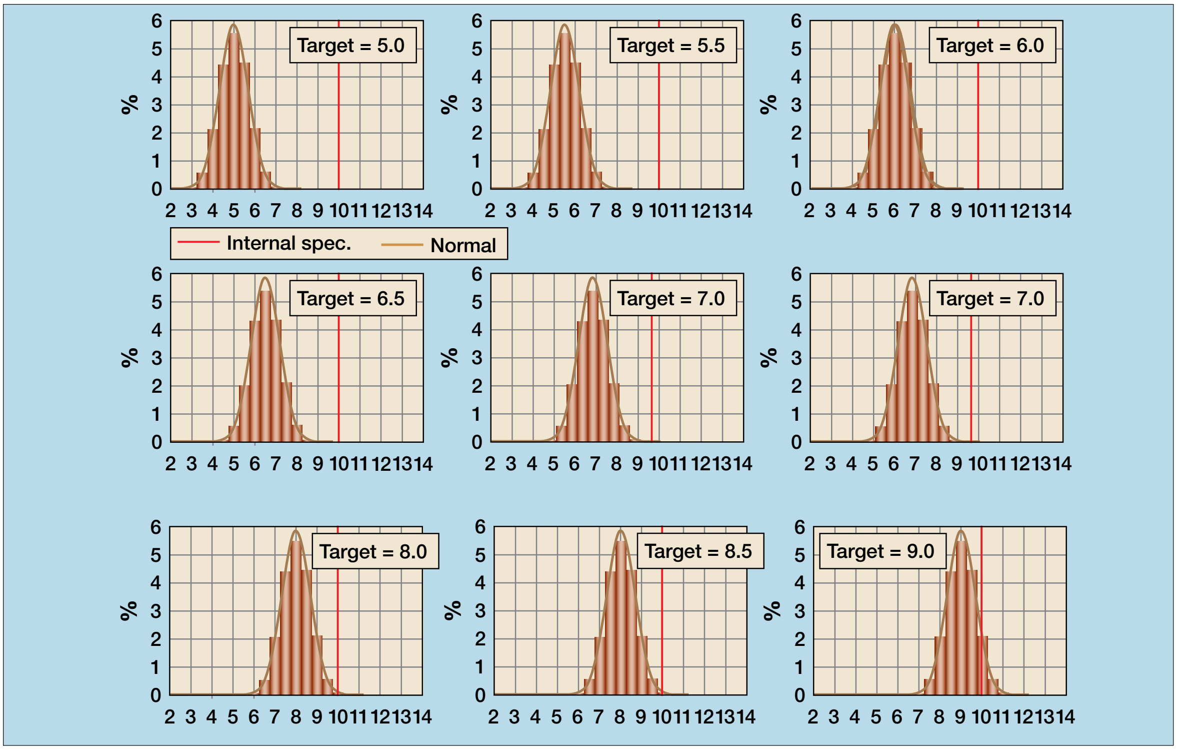

Figure 8 Sulphur distribution – one-hour data

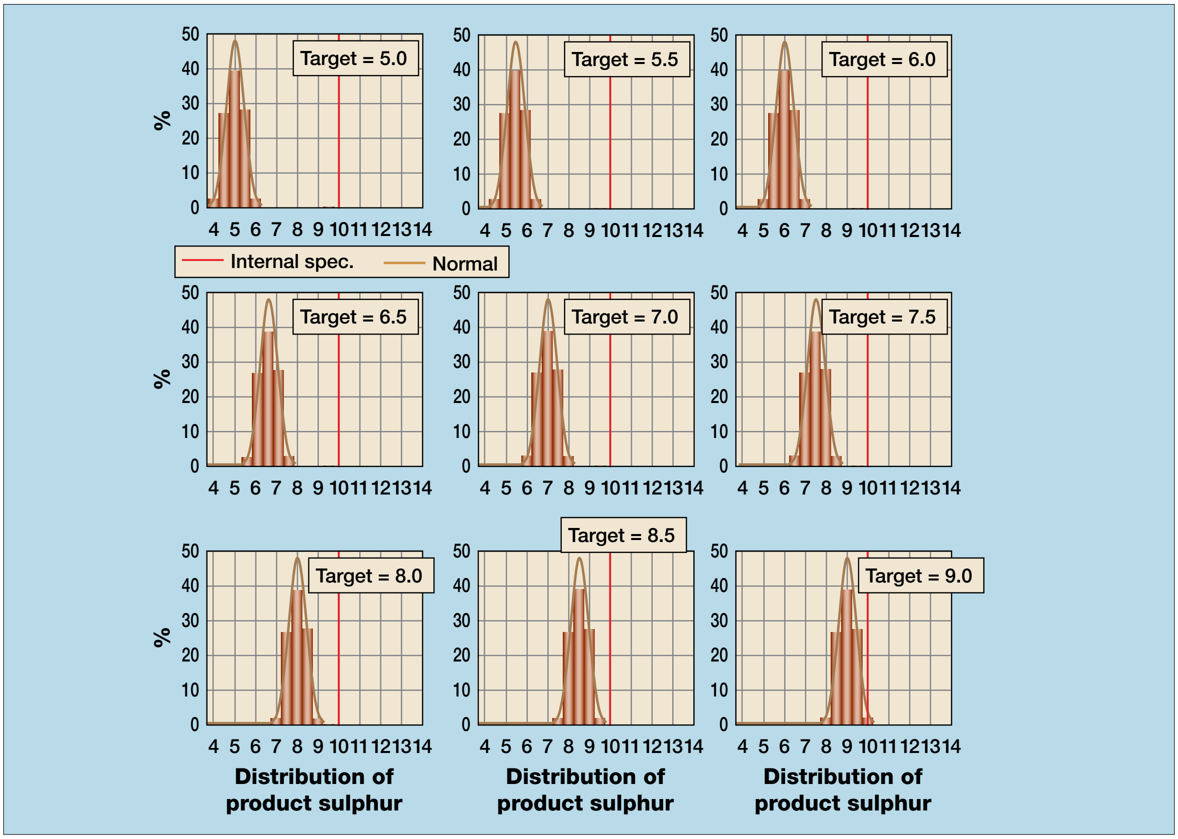

Figure 9 Sulphur distribution – 24-hour average

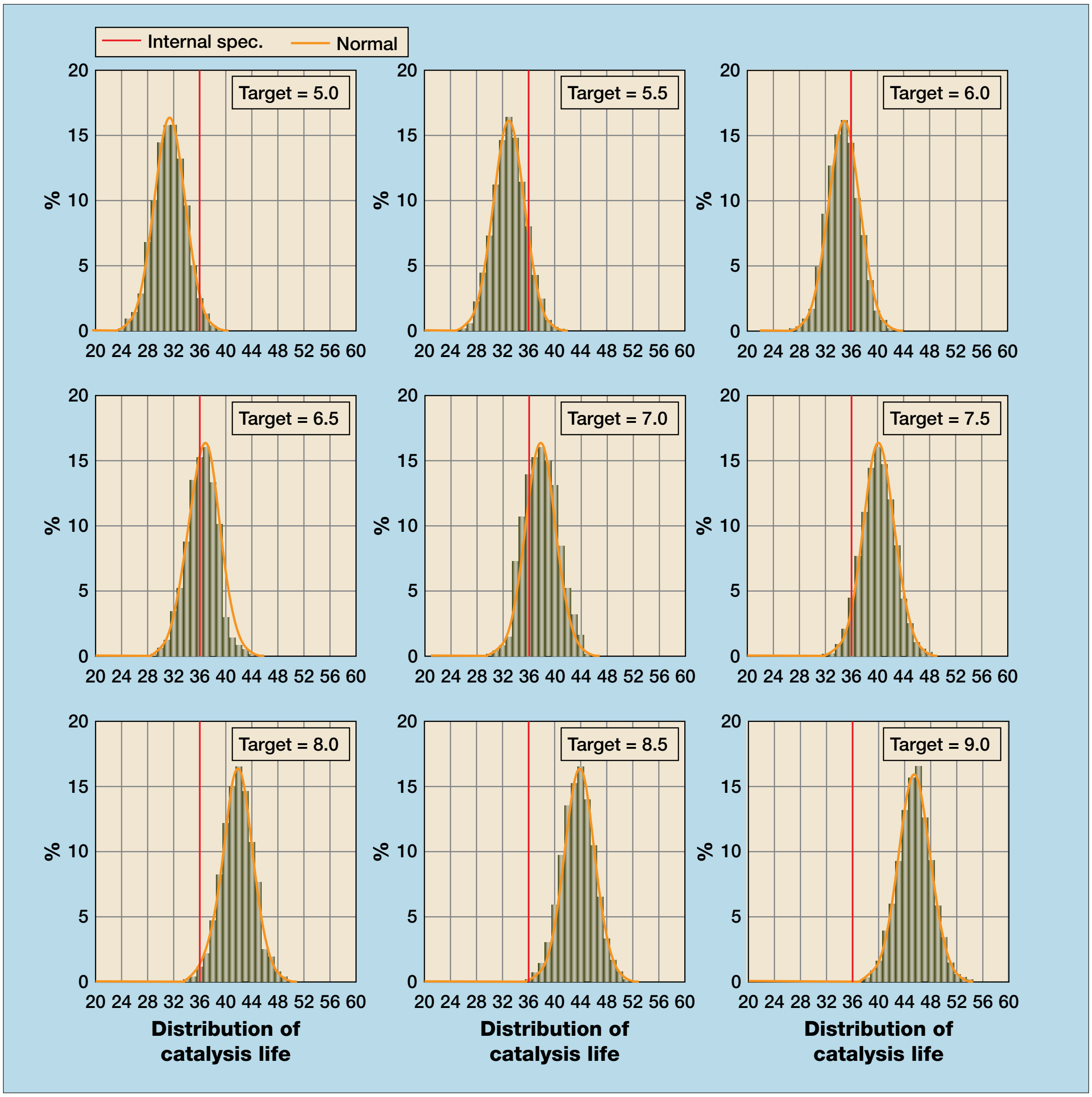

Figure 10 Catalyst life distribution – reactor temperature limited

rises the following simulation results for each sulphur operating target considered: % off-spec statistics using one-hour data, % off-spec statistics using 24-hour average data, estimated catalyst life when the reactor is pressure drop limited (dP), and estimated catalyst life when the reactor is temperature limited. The catalyst life estimates are based on the time when the average reactor dP reached 90 psi or the average WABT reached 760°F (400°C). The reactor dP was the limiting constraint in the simulations. The % off-spec statistics based on 24-hour average is a conservative estimate of the ability of the process to meet the final sulphur specification as the produced diesel goes into a tank with a capacity of 1.5-2 days of diesel production. Note that when 24-hour average data is used, the process is able to meet sulphur specification 100% of the time at a sulphur operating target as high as 8.5 ppm. The average sulphur operating target during the time frame of the study was 6.5 ppm so, according to these results, the estimated catalyst life would increase by about seven months when operating at the higher 8.5 ppm target.

Figure 5 shows the diesel

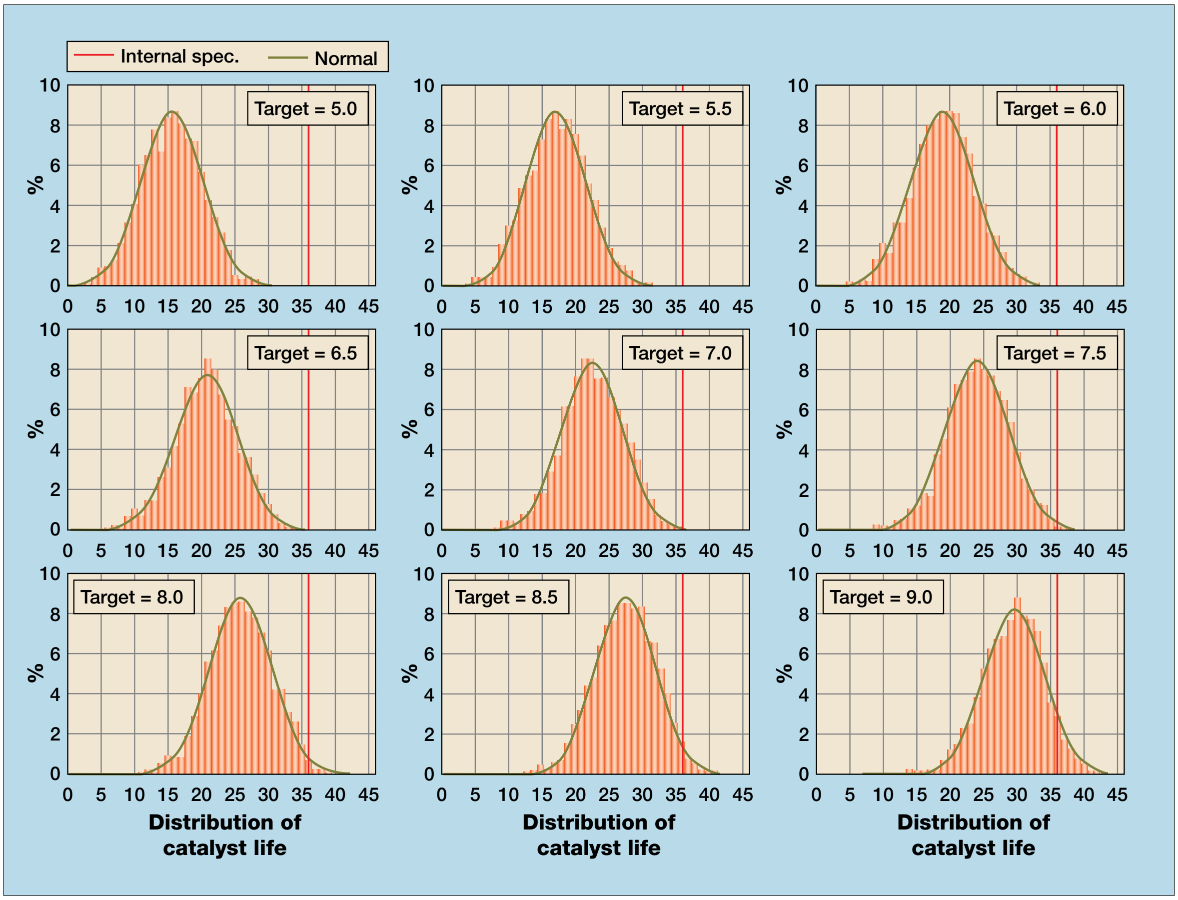

Figure 11 Catalyst life distribution – reactor dP limited

sulphur content vs time for the different sulphur operating targets using one-hour data. The assumed sulphur specification of 10 ppm is shown as the solid red line, the yellow lines represent the upper and lower control limits, and the solid grey line the sulphur operating target. Note that the 8 ppm sulphur operating target case has a few runs exceeding the sulphur specification of 10 ppm. **Figure 6** shows the predicted WABT and **Figure 7** the predicted reactor dP vs time. The grey line shows the average predicted value for reactor WABT and dP and the red line represents the assumed maximum reactor WABT of 760°F (400°C) and maximum reactor dP of 90 psi. A linear regression model using a one-period lag term for dP and the current value of WABT was used to predict the reactor dP.[7] Note that, as previously discussed, the predicted WABT and predicted dP intersect their respective maximum constraints sooner at the lower sulphur operating targets resulting in shorter catalyst life.

Figure 8 shows histograms of the produced diesel sulphur content for the different sulphur operating targets using one-hour interval data. The sulphur specification of 10 ppm is shown as the red line. **Figure 9** shows the estimated sulphur content distribution using the 24-hour average data which, as stated previously, is a conservative estimate of the produced diesel sulphur distribution as the produced diesel goes into a tank with 1.5-2 days of diesel production capacity.

Figures 10 and **11** show histograms of catalyst life for scenarios where the reactor is temperature and dP limited, respectively. A reference line of 36 months is shown which is representative of the expected catalyst life when the reactor is temperature limited. Note that the histograms shift to the right at the higher sulphur operating targets.

Conclusions

This article illustrates the optimisation of a diesel hydrotreating unit using a time series ARMAX model. This model was used in combination with Monte Carlo random sampling to determine the optimum sulphur operating target to ensure sulphur specifications are always met while maximising catalyst life. The results of the simulation were used to predict WABT and reactor dP as a function of time and the associated catalyst life for the different sulphur operating targets. Simplified control logic was implemented to simulate the unit's APC operation.

The results of this study were used to determine the optimum sulphur operating target for implementation into the APC system. The model will also be used to determine remaining catalyst life given operating data from the beginning of the run including produced diesel sulphur content, diesel production rate, recycle H_2 purity, reactor WABT, and reactor dP as well as the expected sulphur operating target for the remainder of the run. The methodology presented in this study can be used to optimise other refinery process units where sufficient operating data is available to construct a reliable time series ARMAX model to predict process unit performance.

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