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TIME-SERIES MODEL: HYBRID FIRST-PRINCIPLE WITH OPERATIONAL DATA FOR OPTIMISATION OF AN INDUSTRIAL ENDOTHERMIC REACTOR SYSTEM

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ABSTRACT

It is crucial to identify and manage main pain point contributor(s) in the hydrocarbon value chain in maximising revenue and cash generation. Recently, PETRONAS has embarked on the initiative to maximise the production of propane value chain by addressing the run length limitation issue due to increasing coking rate in one endothermic reactor system. Hybrid of the first principle and plant operational data were used and modelled in a time-series manner. Several high impact influential variables were selected and incorporated into the model, i.e. hydrocarbon throughput, hydrogen-to-hydrocarbon ratio, reactor inlet temperature and days-on-stream. The hybrid modelling approach is used to find optimum start-of-run operating conditions, control coke formation rate in the presence of variations in operating conditions throughout the run length, and manoeuvre the intermediate operating strategies to achieve the desired run length. The current operation with the implementation of new operating strategies derived from the model shows coke formation reduction up to 70% compared to the historical trending, on-track to achieve the desired run length equivalent to the catalyst expected life, which has never been achieved since in operation. The model can be enhanced in future work to achieve the maximum possible yield throughout the run length and predict the anticipated production with the corresponding operating strategies.

INTRODUCTION

Many industrial petrochemical processes are complex because of unknown reaction chemistry, numerous parameters involved, and the potential to be highly dynamic over time. The same applies to the alkane dehydrogenation process, which involves multiple stage reactor and has many operating variables that can be adjusted. An acceptably accurate model will provide a better overview of potential ways to optimise the plant and increase productivity. The relationship between the key parameter and its influencer is modelled using operational data combined with the first principle.

This paper will focus on the impact of the operational variables on coke formation rate, reflected by the delta pressure (DP) across the reactor screens.

METHODOLOGY

Simulation Software

iCON (Symmetry) process simulation software is used to develop the steady-state simulation scope. Advanced Peng Robinson, a thermodynamic property package, is the extension.

Base Case Simulation

A base case simulation is developed to match existing operating conditions for a selected historical period. The selected period fulfilled the base case criteria: stable plant operation with average operating load and low material imbalance operational figures. The actual operating conditions are extracted from the Plant Information Management System (PIMS). The model was tuned to match within +/–2% of the operational data.

Screen Modelling Approach

Modelling in iCON (Symmetry) mainly intends to calculate the stream properties and represent the open area on the screen (labelled as effective diameter) with a standard measure derives from the measured variables, i.e. DP and mass flow rate of the stream entering the reactor.

This is important to establish a standard measure for the reactor screen effective diameter since there are possible changes in both volumetric and effective diameter, which can be explained in the equation below:

$$P_1 - P_2 = \rho\left(\frac{v_2{}^2 - v_1{}^2}{2g}\right) \tag{1}$$

The velocity is assumed to be a volumetric flow rate divided by effective diameter.

Hybrid Model Development

In this phase, the model development experimented with multivariable regression and a lookup table (represented as gradient table). The selection of key influencer was made closely together with Process Technology in-house experts in this phase to ensure its principles guide the model. This is important as modelling based solely on historical data can end up in an overfitting model, which can be misleading. This is also a way to reduce iteration in arriving at an optimum model. they are used to create the pump performance head curve profile at varying speeds.

Multivariable regression gave a poor fit to represent the coke formation rate daily. After an extensive run of279,927 permutations of influential variable sets and transformations, the best R squared value obtained was 0.3821.

Gradient table is then established by observing the slopes at varying snapshots throughout the operation of multiple cycles.

CASE STUDY

A case study was conducted to observe the expected DP profile for a single critical screen throughout the current cycle by varying selected influential variables. The effect of throughput, hydrogen-to-hydrocarbon ratio, reactor inlet pressure, and reactor inlet temperature were selected in observing the impact towards DP profile of reactor screen.

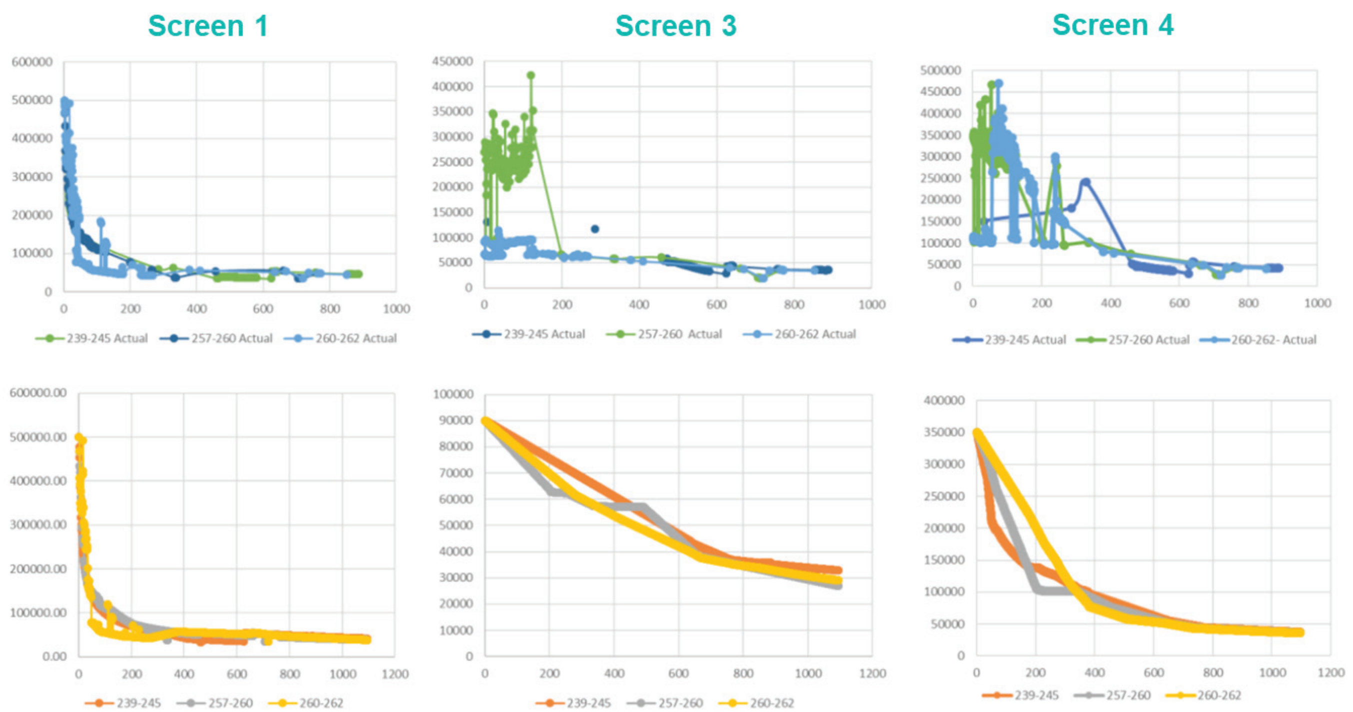

Figure 1 A sample of before and after transformation of a new set of variables profile at corresponding influential variable clusters. These profiles are translated into a gradient table which functions as the central database for the model

RESULTS

Case Study 1: Varying Reactor Throughput

Case 1 shows the impact of throughput to the reactor towards the prediction of DP profile throughout the expected operation. The rest of the variables are maintained the same in this case study.

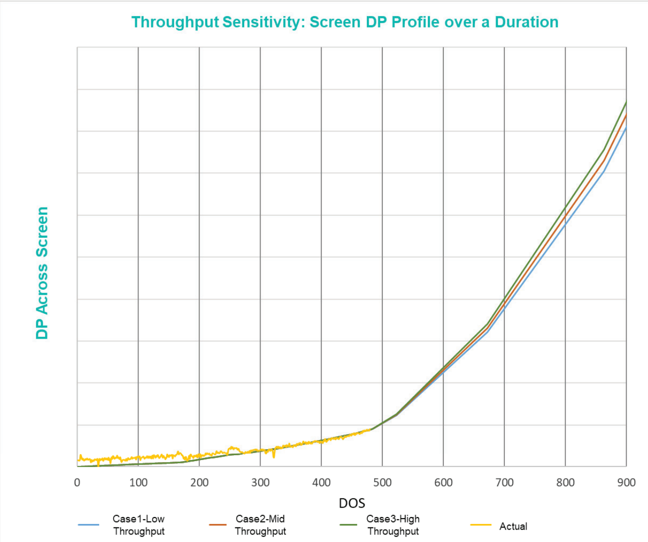

Figure 2 Expected DP profiles at varying throughput to the reactor

Case Study 2: Varying Reactor Inlet Temperature

Case 2 shows the impact of reactor inlet temperature (RIT) on the prediction of DP profile throughout the expected operation. The rest of the variables are maintained the same in this case study.

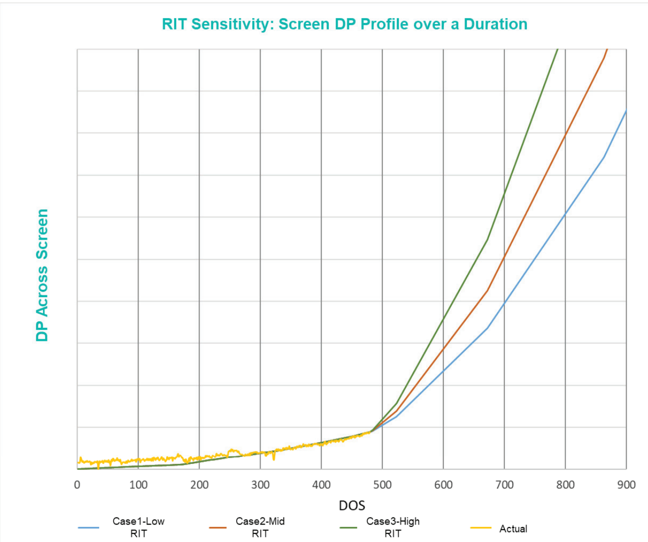

Figure 3 Expected DP profiles at varying RIT

Case Study 3: Varying Reactor Hydrogen-to-Hydrocarbon Ratio

Case 3 shows the impact of throughput to the reactor towards the prediction of DP profile throughout the expected operation. The rest of the variables are maintained the same in this case study.

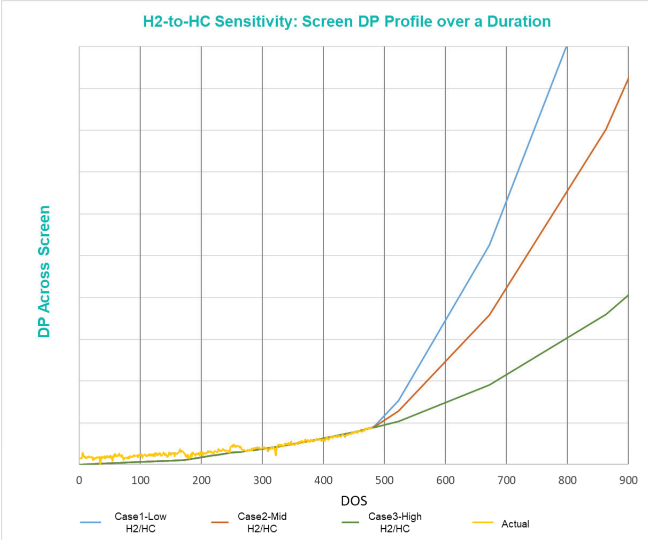

Figure 4 Expected DP profiles at varying H2/HC ratio

Case Study 4: Varying Reactor Inlet Pressure

Case 4 shows the impact of throughput to the reactor towards the prediction of DP profile throughout the expected operation. The rest of the variables are maintained the same in this case study.

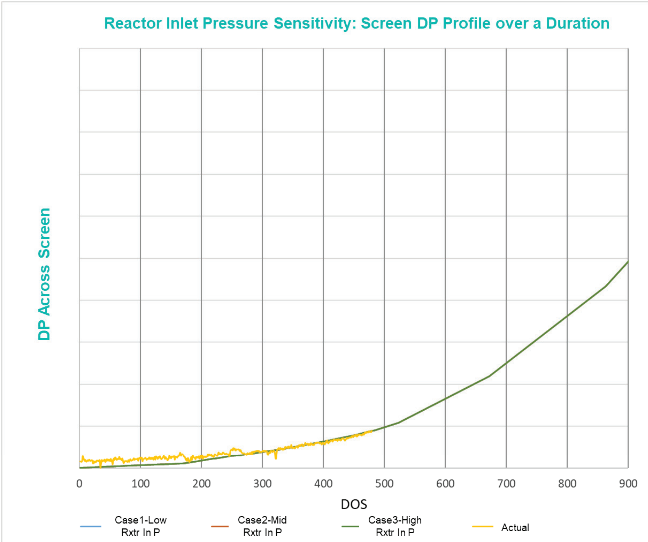

Figure 5 Expected DP profiles at varying reactor inlet pressure

CONCLUSION

The DP profile across the screen can be predicted by utilising the first principle model combined with analysis from historical data. This model enables the user to run the possible operating conditions and evaluate the estimated/predicted DP profile, which is the primary constraint in the reactor system due to inevitable coke formation.

FUTURE WORK

The improvement that can be introduced to the model can predict the desired product yield using common or overlapping influential variables.

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