# Process Optimization to Increase Productivity of Fixed-Bed Adiabatic Reactor

Das Babua* and Farah S. Anwar**

PETRONAS Group Technical Solutions
Level 16, PETRONAS Tower 3, 50088 Kuala Lumpur, Malaysia

*Corresponding e-mail: * das.babua@petronas.com ** farah_syamim@petronas.com

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**ABSTRACT** –This paper discusses the approach used to develop the productivity constraint prediction model and prescribes operating setpoints of fixed-bed adiabatic reactor operation. Most often, the productivity constraints which lead to lower reactor throughput and reduce on-stream time are high bed differential pressure, loss of catalyst selectivity and activity. Baseline assessment was conducted to validate and analyse operating data, experiences and compare with reactor design performance to identify main influencing variables, and system constraints. The behaviour of constraints are predicted by utilizing hybrid first-principle and mathematical regression-based constraint model. The hybrid model predicts the optimised setpoints such as feed water concentration limits, hydrogen-to-hydrocarbon ratio, which results in productivity enhancement up to seven months.

## 1. INTRODUCTION

Adiabatic hydrogenation catalytic reactors are used for hydrogenating unsaturated compounds to saturated compounds. Most often, the productivity constraints which lead to lower reactor throughput and reduce on-stream time are high bed differential pressure, loss of catalyst selectivity and activity.

As part of a systematic approach, baseline assessment is required to validate and analyse operating data, experiences and compare with reactor design performance to identify main influencing variables, and system constraints.

The inventory of operating data comprises continuous data historian, discrete laboratory data for feed contaminants and product quality, and reactor inspection data. To gain process insight and bridge gaps in instrumented data, first-principle simulation models are used.

The behaviour of constraints is predicted by utilizing hybrid first-principle and mathematical regression-based constraint model [1]. The predictive model requires to be trained and tested against actual plant operating data.

## 2. METHODOLOGY

Situational Assessment is conducted to assess the historical and current baseline reactor operating performance in terms of reactor run length, severity and capacity utilization. The objectives of reactor extended run length and capacity utilization are defined in alignment with the business case.

The plant data consists of data measured by transmitters located across the unit and also data coming from laboratory sampling to measure the compositions of crude aldehyde feed and crude alcohol product streams. Plant data measured by transmitters are normally continuous and updated frequently in the historian. However, data from laboratory sampling depends on the sampling schedule (frequency varying between once to twice a week, depending on the stream) to perform compositional analysis using gas chromatography (GC). The sampling data are updated and accessed from laboratory information management system (LIMS).

This discrete plant data impose substantial challenges in establishing consistent dataset to conduct model training and testing. Data generation through iCON first principle process models includes prediction of feed gas dew point, reactor heat balance for conversion prediction and prediction of physical properties. Modelling methodology flow diagram as depicted in Figure 1.

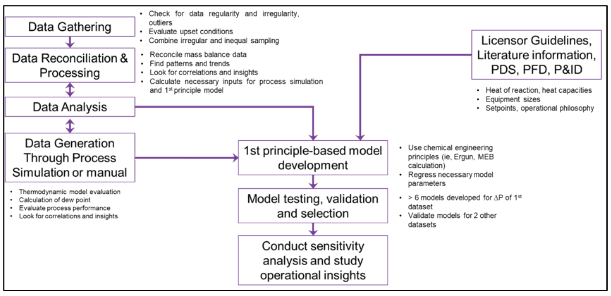

Figure 1 Modelling methodology flow diagram

Three (3) case studies are conducted for hydrogen-to-aldehyde molar ratio, higher water concentration in feed stream, and temperature approach to feed dew point in order to assess the impact on catalytic bed differential pressure and run length.

## 3. RESULTS AND DISCUSSION

All the three case studies show improvement opportunity to reduce differential pressure rise rate and extension of reactor run length.

For instance, an opportunity was identified to debottleneck the recycle gas compressor to sustain the hydrogen-to-aldehyde molar ratio at base value to increase the run length by one month. Refer to Figure 2. Operating above the minimum required hydrogen-to aldehyde ratio avoids the undesired secondary reactions such aldol formation, dimers and trimers [1] which can cause plugging of the catalyst bed. By avoiding the undesired reactions, the bed plugging rate is minimized leading to lower rate of dP rise of catalyst bed and longer run length.

In the second instance, an opportunity was identified to improve the water separation in the catalyst treatment section of upstream hydroformylation plant, which resulted in extension of run length by seven months. Refer to Figure 3. Water content reduction in feed by 2.7 times results in lower formation rate of butyric acid by undesired secondary reaction of ester hydrolysis in the hydrogenation reactor [2]. Butyric acid is a corrosive agent and corrodes the catalyst metal support forming salts, which damage the catalyst to fines formation. By lowering the formation rate of butyric acid, the catalyst degradation to fines is minimized leading to lower rate of dP rise of catalyst bed and longer run length [3].

## 4. CONCLUSIONS

Based on the model developed and case studies conducted, this approach provides a tool that enables the operations team to assess the reactor run length impact from any adjustment of the optimization handles, prior to making operating setpoint change in the actual plant.

This approach can be replicated for process optimization to increase productivity of fixed-bed adiabatic reactor in hydrogenation services.

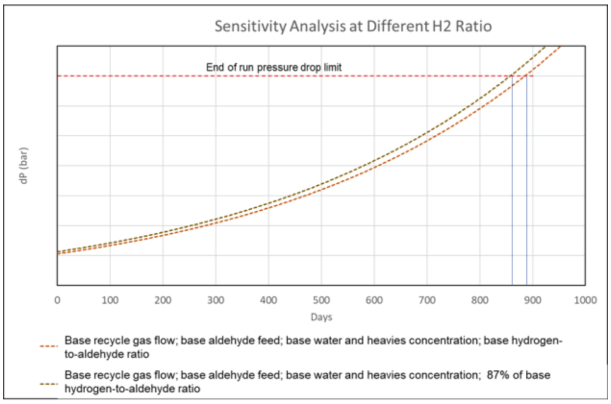


Figure 2 Sensitivity of differential pressure with respect to hydrogen-to-aldehyde ratio.

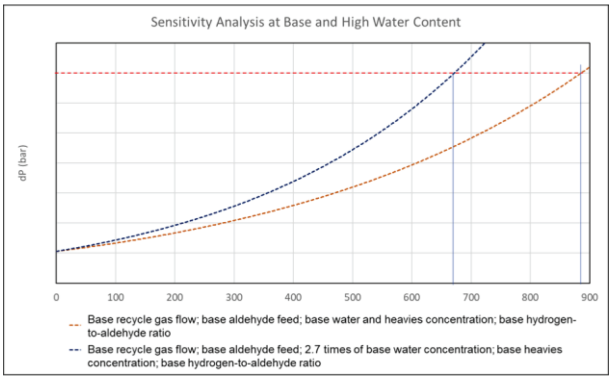


Figure 3 Sensitivity of differential pressure with respect to water concentration in feed stream.

## ACKNOWLEDGEMENT

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