ESTIMATION OF THE OPTIMUM PROPANE CONTENT FOR THE SPHERIPOL POLYPROPYLENE PROCESS

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ABSTRACT

A Real Time Optimization (RTO) algorithm was proposed[1] to optimize the reactors' propane content for the LyondellBasell's Spheripol Polypropylene process. This algorithm improved the existing approach of arbitrarily selecting "optimum" propane values, based on monthly/yearly average balances. The optimum propane content, is now calculated based on factors such as the costs of offgas and catalysts, the propane content in the feedstock and the catalyst mileage. A steady state process model was developed and tested over plant data to prove its predictive capabilities. In the present study, this model is extended to account for alternate destinations of the vented gas. Results from the off-line implementation of the algorithm are presented that demonstrate its applicability. Estimates on the amount of the expected savings for a medium size Polypropylene plant are also presented.

KEYWORDS: Optimum propane, RTO, Spheripol, polymerization

INTRODUCTION

In the Spheripol Polypropylene (PP) process, the liquid propylene feed (comprised of ~99,5% propylene, ~0,5% propane and small quantities of inerts), is transformed into polypropylene in circulated liquid loop reactors. The non-reacted monomer is recycled back into the process feed drum. Inside the loop reactors, liquid propylene, in the presence of Ziegler Natta catalyst, is converted to solid phase polypropylene particles. However, this is not the case for the non-reacting propane molecules that built up in the polymerization reactors reaching a content of 20-40% (depending on the individual producer speculations) before it is finally vented from the process. The purged mixture of propylene/propane is most of the times used as a fuel for the production of steam in gas-fired steam generators and therefore is billed much less than the propylene feed.

Although many researchers from both industry and academia have proposed sophisticated algorithms to model the kinetics and dynamic behavior of propene Ziegler-Natta Polymerization in liquid loop reactors [2, 3, 4], a solution to this problem has been only recently proposed[1], following the development of a Real Time Optimization (RTO) Algorithm[5]. It is based on the observation that the rate of reaction is proportional to the propylene and catalyst concentration in the polymerization reactors.

In the present study, the existing RTO algorithm[1] is updated to account for additional operating scenarios (i.e. a)selling the offgas to an LPG facility, b)burning offgas to the flare) thus extending its applicability in the PP Plant.

THE REAL TIME PROPANE OPTIMIZATION ALGORITHM (RTO)

In the present study, the classical version of the RTO algorithm shown at Fig.1 that follows, is employed[5]. It retrieves data from the plant's history database (PHD) every 20mins to 1hr (the sampling interval is adjustable). No gross error detection and data reconciliation is performed on the data by the specific algorithm. These operations are also routinely performed in process plants' by the DCS Application Engineering team. Nevertheless, the input data are checked for erroneous values (i.e. sporadic values with no physical meaning, out of range data, and data with excessive noise). Then, they are examined by the Steady State Identification (SSI) algorithm[6,7,8]. Once a steady state (SS) is detected, the system parameter (which is based on process data, such as production rate, the grade produced, loop densities, reactor energy balances et.c and kinetic constants), is first calculated, followed by the calculation of the objective function. Repeating the above steps for a range of offgas vent flowrates, produces a set of tabulated objective function values, among which the optimum one.

The optimum value may be applied as the new setpoint for the Plant's analyser/controller (online implementation) or the DCS (Distributive Control System) console operator may be advised to drive the plant to the optimum propane content by manually regulating the offgas venting rate (inline implementation). Finally, the RTO tool can be used for offline studies over existing DCS data.

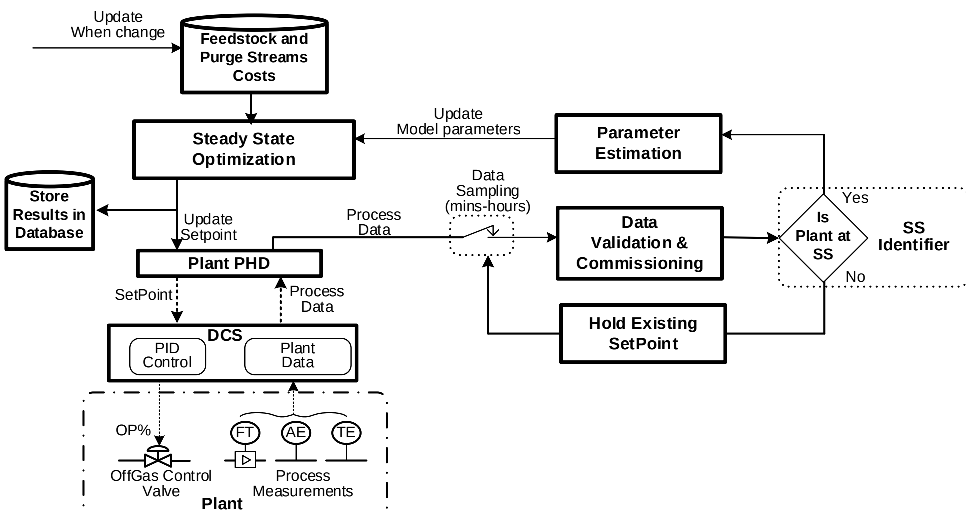

Figure 1. *Real Time Propane Optimization Scheme for the Spheripol Polypropylene Plant*

DEVELOPMENT OF THE OPTIMIZATION PROBLEM OBJECTIVE FUNCTION

It was mentioned earlier that the optimal propane content in the plant is a function of many factors. These are: a) the catalyst, propylene and offgas prices, b) the propane (propylene) concentration in the propylene feed, c) catalyst deactivation (spontaneous or due to poisons), d) the polymer grade that is produced (i.e. effect of hydrogen) and e) the production rate.

The effect of all these factors on the optimum propane content is shown in Figure 2 that follows. For example in Figure 2a, one may see that an increase in the catalyst price, will, (a)increase the production cost and (if all other factors remain unchanged) (b) necessitate for a decrease of the propane content (i.e. an increase of the offgas vent flow rate) to limit the amount of catalyst used and therefore it's cost contribution in the overall plant production cost.

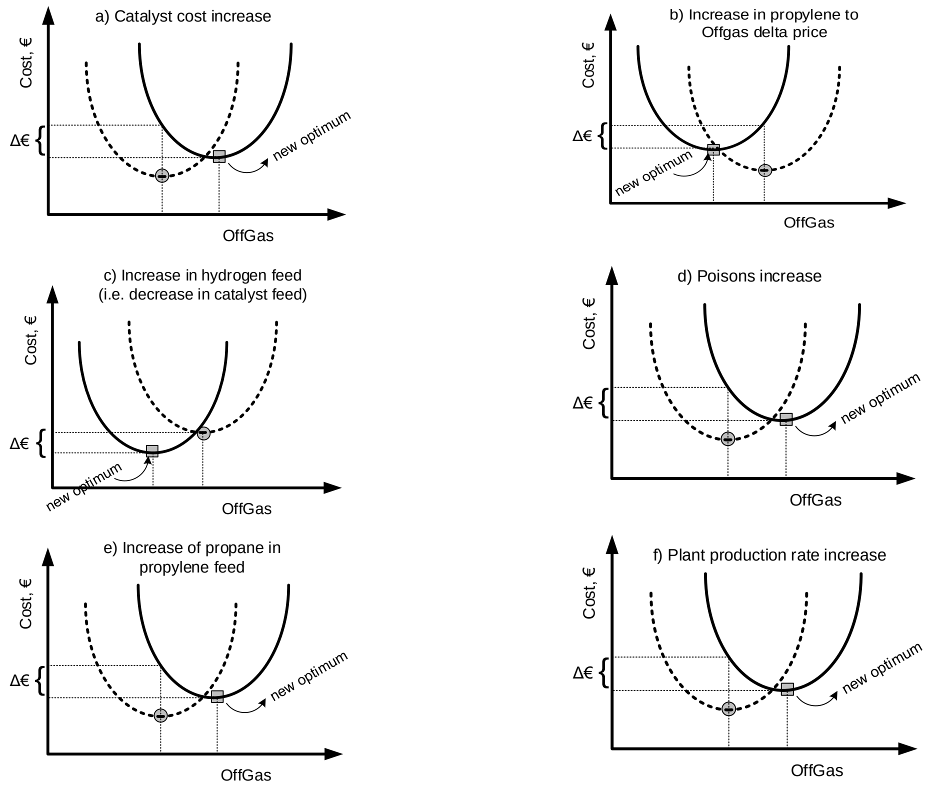

Figure 2. *Factors that affects the optimum propane content in the Spheripol Polypropylene Plant: a) Catalyst cost increase, b) Increase in propylene to offgas delta price, c) Increase in hydrogen feed (i.e. Grade change), d)Poison's increase (catalyst deactivation) e) Increase of propane in propylene feed, f)Production rate increase.*

In the present work, earlier analysis[1] is extended to account for additional operating scenarios for the PP plant. These include the following:

a) Feeding the purged gas stream to an LPG facility, to acquire a better selling price for this waste stream.
b) Account for the case where some propylene/propane needs to be sent to the plant's flare.

The Objective function of the optimization problem may now be written as follows:

Minimize: $P = F_{offgas}\,(C_{C3\text{-}} - C_{offgas}) + F_{LPG}\,(C_{C3\text{-}} - C_{LPG}) + F_{FL}\,(C_{C3\text{-}} - 0) + F_{cat}\,C_{cat}$ (1)

Sub to: The plant's mass balances (1a)

where, P is the summed catalyst and offgas cost (€/hr), C_{C3}, C_{offgas} C_{LPG}, C_{cat} are the unit costs for propylene (including propane), offgas, LPG and catalyst respectively (in €/kg) and F_{cat}, F_{offgas}, F_{LPG} , F_{FL} are the catalyst, vented offgas, vented gas to LPG and offgas to flare flow rates (kg/hr). At the same time, the solution should satisfy the process steady operation material balances[1].

Following the RTO algorithm of Figure 1, at each execution step, the above model should be periodically supplied with data from the Plant's History Database (PHD). These data should be first cross checked to: a) have meaningful values and be relieved of excessive noise and b) be retrieved while the plant operates under steady conditions. Then, the system parameters (such as reaction rates, loop densities, flowrates et.c.) may be recalculated. Last, the optimization problem should be supplied with the valid market prices for the propylene, offgas, LPG and catalysts.

MASS BALANCES DERIVATION FOR THE SIMPLIFIED POLYPROPYLENE PLANT FLOW CHART

A simplified description of the Spheripol PP plant[1, 2], is shown at Figure 3 that follows. Although simplified, Figure 5, depicts all the necessary information for the accurate derivation of the basic process material balances. The reaction is taking place in two loop reactors in series, operating in the liquid phase and under constant pressure and temperature. The reaction conversion is ~50% and the liquid phase polymer slurry exiting the loops, is now rich in propane which, in contrast to propylene, doesn't polymerize in the loops. The slurry is then treated in two recycled sections (a high pressure and a low pressure section) to extract the non-reacted monomer. The propane content in the Plant is kept under control by means of two vents (one in each degassing section). The use of a single vent stream from the plant's recycle section (instead of the actual two) at Figure 3 is still valid, given that downstream the reactors (after stream 9), the propylene/propane ratio is constant[1].

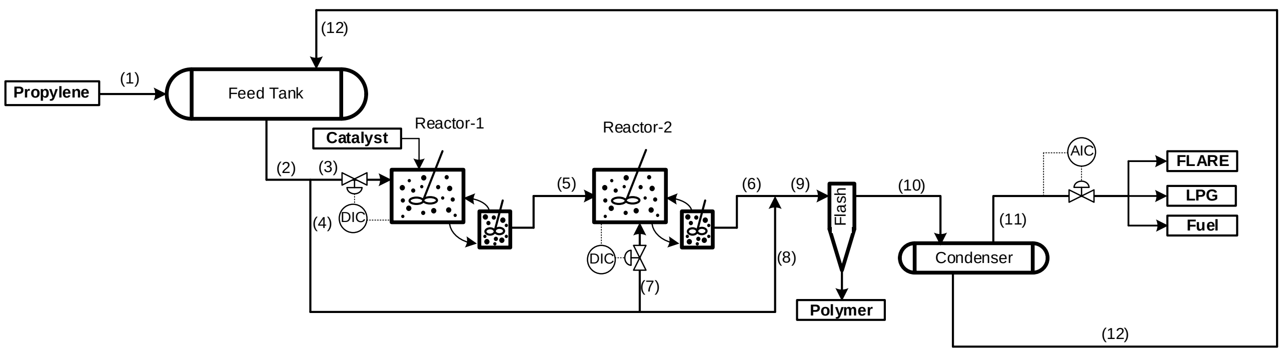

Figure 3. *Simplified Description of the Spheripol PP Plant (AIC: propane controller, DIC: density controller)*

Figure 3, differs from the simplified schematic of the earlier study[1], only with respect to its adaptation of the vented gas stream end-users. In this study, we are considering three possible destinations for the vented offgas (i.e. as a fuel for the production of steam, to be directed to an LPG facility and finally to be burned to the plant's flare).

Note that the above scheme, does not introduce any additional degrees of freedom in the original problem. Venting to flare is performed only for the case where the other two alternatives are not available. Selection between LPG and fuel offgas, depends on LPG installation availability and the price difference between LPG and FuelGas and is a decision that must be first taken by the LPG facility.

The plant's mass balance equations[1] and are only supplemented with the overall mass balance for the vented stream.

$$F^{(11)} = F^{(OG)} + F^{(LPG)} + F^{(FL)} \tag{2}$$

where, F denotes offgas flowrate and OG, LPG, FL denotes the vented gas destination (i.e. OG:for production of steam, LPG: to an LPG facility, FL: to the plant's flare).

SIMULATION RESULTS OVER PAST PLANT DATA

At the following, the above analysis is applied offline on Plants' data from year 2022 with the aim of calculating the deviation of the actual propane content in the Plant from the optimum one, for the two case studies.

During the specific time interval (i.e. 7-10 March 2022), the propane content in the incoming feed was much higher to the usual one (i.e. in the order of 2%, compared to the 0,5% of the normal polymer grade propylene content), thus highlighting even more the usefulness of the RTO tool. On top of this, the propylene price (1425€/tn), LPG price (910€/tn) and offgas price (689 €/tn) were closed to their 3-year high.

The following figures depicts the plant state and the RTO results for two modes of operation. First, the usual mode of venting gas to a steam production facility and second, that of venting gas to a LPG production facility at an agreed flowrate and then utilizing the rest of the vented gas for steam production.

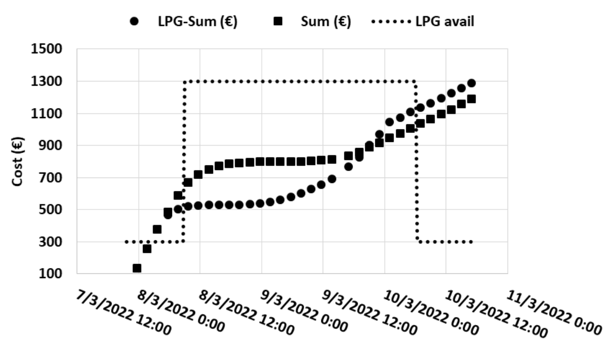

Figure 4. *Sum of catalyst and vented gas cost due to operating away from the optimum propane wt% for two operating scenarios, ●with/■ without, LPG availability (the latter denoted by ····)*

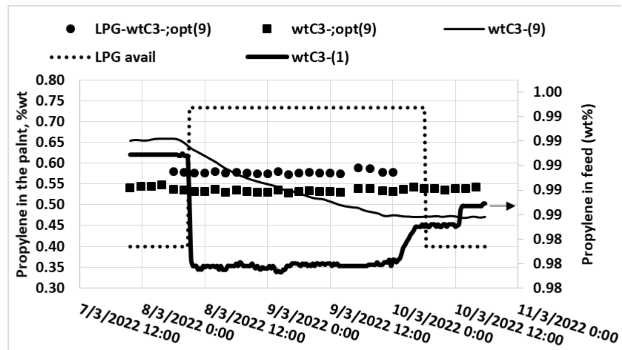

Figure 5. *Optimum propane concentration (wt%) for two operating scenarios ●with/■ without, LPG availability (the latter denoted by ····)*

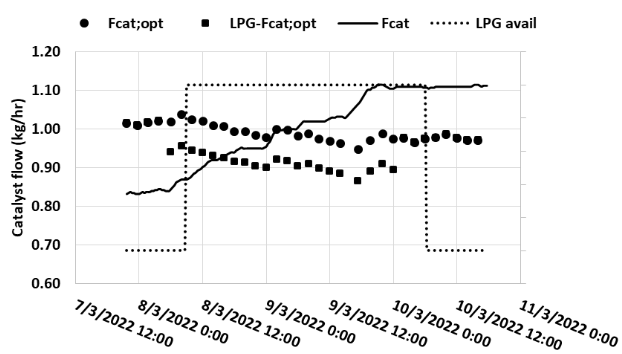

Figure 6. *Actual catalyst consumption (—) and optimal cat. consumption for two operating scenarios, ●with/■ without, LPG availability (the latter denoted by ····)*

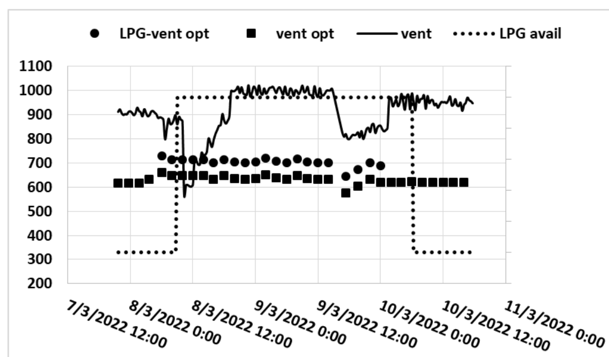

Figure 7. *Actual venting flow rate (—) and optimal venting flow rate for two operating scenarios, ●with/■ without, LPG availability (the latter denoted by ····)*

In the above figures, *LPG-Sum*(€) stands for the sum of vented gas and catalyst costs for the case where an LPG facility is available to treat 500kg/hr offgas and *Sum* (€) stands for the combined catalyst and offgas costs, when the offgas is used in a steam production facility. LPG-avail, simply denotes, the time interval where offgas can be sent to the LPG facility.

In a similar manner, $wt_{c3\text{-};opt(9)}$ refers to the optimal reactor propylene (wt%), $F_{cat\text{-}opt}$ is the optimal catalyst flow rate (kg/hr), and $vent_{\text{-}opt}$ stands for the optimal vented gas flow rate (kg/hr).

From Figs. 5, 6 above, it can be seen that the plant model, correctly predicts the dependence of propylene content in the loops to the catalyst flow. The decrease in propylene concentration is resulting in an almost proportional catalyst flow increase (i.e. decrease in catalyst mileage), to keep the plant production constant.

Figs 5, 6 captures the effect of a step change in the plant's propane feed (i.e. arrival of a new propylene cargo with increased propane content). The plant is moving towards a lower propylene content, and finally exceeds the optimum one (which is ~54% wt/600kg/hr offgas flow), settling at ~46%/900kg/hr offgas flow).

The cost impact, of these moves is shown in Fig. 4. It is calculated that within just 3 days, the plant suffered a ~1200€ loss, that could have been skipped if the RTO tool was in use. Note that, this result may only be seen as a rough estimation, since in the particular case, the operator is not applying the RTO tool predictions (i.e. it is an open loop operation).

The above figures also illustrate the RTO tool outcomes for the hypothetical case where an LPG facility could accept part of the vented gas. Due to its higher price (compared to the offgas), the plant would have to operate in a higher propylene content, i.e. we should expect an increase in vented gas flow. This is accurately predicted by the model and shown in Figs 5, 6.

Due to the higher vent flow predicted in the LPG availability case, the cost impact off the new feedstock is initially smaller to that of the offgas case. However, as the actual vent gas flowrate deviates from the optimum one, the cost impact, driven by the higher unit price of the vented gas, quickly recovers. At the end, where the LPG option is not available, the predicted costs for the two scenarios, move in parallel to each other.

CONCLUSIONS

In the present study, the problem of determining the optimum propane content in the polypropylene Spheripol process is presented.

The proposed solution, involves the development of a RTO algorithm, which is based on past and present plant data collected from the plant's PHD, as well as data for the prices of propylene, catalysts, offgas and LPG. The steady polymerization process model of the earlier study[1] , is extended to account for alternate destinations of the vented offgas (i.e. flaring and as a feedstock to an LPG facility).

From the offline simulation results over existing Plant data for the year 2022, it is seen that, depending on the unit prices of raw materials and the amount of propane in the plant's feed, the application of the RTO tool may have a significant cost impact in the PP plant economics.

The future availability of LPG, is expected to positively contribute to the PP plant economics in a twofold manner. It will first drive the plant towards an increased vent gas flowrate (having a higher unit price), thus improving the plant economics. As a side effect, it will also increase catalyst mileage, and therefore reduce the cost of catalyst utilization.

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