Analytical RTO for a critical distillation process based on offline rigorous simulation

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Abstract: The economic performance of distillation processes has been always addressed by techniques supporting and completing Model Predictive Control (MPC), which are known as Real Time Optimization (RTO). RTO, via simulation model, has been deeply studied and applied to distillation processes, nevertheless, the cost associated with the development of such online simulation models is often an obstacle for industries to change their operations. Hence, this work presents an unconventional RTO approach, named “analytical RTO”, which calculates the setpoint of manipulated variables according to operating strategy exploiting an analytical generalized formulation. The proposed RTO is built for a specific unit, that is a Propane-Propylene super-fractionator producing polymer grade Propylene (99.5%), and it is based on an offline simulation model developed in UniSim Design. Sensitivities analysis of the revenue with the manipulated variables is obtained with the simulation model and used to derive a simple, yet quite effective analytical RTO formulation, taking into account the fluiddynamic limit of the unit studied. Comparing such an approach with the simulations, the results show a satisfactory match of the analytical estimations with the optimal points calculated by the rigorous model.

Keywords: Real-time optimization, distillation, optimization.

1. INTRODUCTION

Operation excellence represents the primary target of the process industries pursued by the application of advanced digital technologies (Warner and Wäger, 2019). In distillation processes, Advanced Process Control (APC) has been part of that effort for the last two decades through the Model Predictive Control (MPC) technology (Shin et al., 2020). Other advanced technologies supporting and completing APC are today available as Real Time Optimization (RTO) (Darby et al., 2011). RTO tools enforce the achievement of economic benefits in different scenarios when managing directly the systems operability (Vaccari et al., 2019) or assigning optimal economic targets to MPC (Vaccari et al., 2021). Clearly, the proper design of an RTO structure that leads to a substantial improvement in process performance is a critical and complex subject that needs the right tools and considerations (Câmara et al., 2016).

In this fashion, one of the most studied chemical processes, in terms of optimizing the operating performance, is distillation. Different models have been developed in both academic (Zhang et al., 2019) and industrial (Mendoza et al., 2013) environments to increase operating profit via RTO. Other distillation processes have been optimized via RTO in a closed-loop dynamic fashion (Pataro et al., 2020) or focused on robustness aspects (Haßkerl et al., 2018). Variations of RTO when subject to plant-model mismatch have been tested on a depropanizer column (Rodríguez-Blanco et al., 2017), and also one-layer MPC-RTO solutions have been analyzed (Hinojosa et al., 2017).

The Propane-Propylene super-fractionator producing polymer grade Propylene (99.5%) is the distillation unit where those advanced technologies have been profitably applied because of operation peculiarities. The MPC design concerning specifically the required Propylene purity of super-fractionator is reported in (Pannocchia and Brambilla, 2005). Among the mentioned examples for distillation RTO, the common denominator is model simulation, whose complexity varies upon the peculiarity of the process studied. Process simulation optimization is a powerful tool that gives the possibility to analyze complex industrial systems and identify potential improvements (Melouk et al., 2013) or perform data reconciliation (Vaccari et al., 2020) in a short time frame (minutes). On the other hand, online process simulation represents a cost in terms of equipment, model development, often licensing, and training of personnel. Thus, this paper describes an unconventional approach adopted for RTO which calculates the set point of the manipulated variables of the super-fractionator in Pannocchia and Brambilla (2005). This approach relies on an offline simulation model and on an objective function that changes according to operating strategy and to the online measurement of the feed composition, generally measured in this application.

The remainder of the paper is organized as follows. Section 2 presents the unit description, generalities, and main problematic. A detailed definition of the RTO strategy based on the different operating scenarios is illustrated in Section 3. Confrontation of the proposed method with optimal data calculated by the simulation model is shown in Section 4, while Section 5 concludes the paper underlining the main achievements.

2. UNIT DESCRIPTION

The chemical unit operation considered in this paper is the Propane-Propylene super-fractionator producing polymer grade Propylene (99.5%). The unit represents a real plant unit that can be found in most of the petrochemical plants producing monomers. The distillation unit is often composed of at least
Table 1. Separation characteristics and typical values of main operation parameters.

| Quantity                              | Unit   | Value |
|---------------------------------------|--------|-------|
| Overhead pressure (gauge)             | kg/cm² | 18    |
| Rel. volatility C₃/C₃                 |        | 1.07  |
| Total tray number                     |        | 200   |
| Propylene distillate spec.            | %w     | 99.5  |
| Throughput                            | t/d    | 270-390 |
| Propylene feed comp.                  | %w     | 70-80  |
| C2 feed concentration                 | %w     | max 0.1 |
| C4 feed concentration                 | %w     | 2-3   |
| Reflux ratio                          |        | 18    |

Then, the distillate and steam to reboiler flow controllers are the variables adopted for the separation targets. The throughput flow controller is set based both on planning requirements, and for optimization. The only drawback of the regulatory control takes place sometimes at the bottom level due to the low bottom product flow compared to the liquid flow from the bottom tray (boil-up ratio > 40), and the low hold-up that often can afflict this kind of unit. The bottom baffled arrangement reduces the sump hold-up for the level control but assures the reboiler stability. However, the reduced bottom volume available for the level together with the high liquid flow coming from the bottom tray, boil-up ratio about 60, can cause strong oscillations of the bottom product flow when vaporization variations occur due to bottom composition. As a consequence, using a controller of the bottom product Propylene, a measurement with the analyzer sample taken on the bottom product line can be problematic since there could be no sample to be analyzed.

2.2 Column dynamics

Two major problems are associated with the control of distillate Propylene concentration, xₚ. The first one is linked to the very large time constant (more than 15 hours) that produces a very slow response; the second process criticality is represented by the nonlinearity of the response gain from MV1 and MV2 to xₚ. In particular, the first one would make it difficult for plant testing and subsequent model identification. This problem has been overcome by adopting reduced-order integrating models (pseudo-ramp) with delay (Pannocchia and Brambilla, 2005). In this regard, rigorous simulation models were used to generate data for model identification. In the present work, a simulation model has been developed using the software UniSim Design, and its details are omitted for the sake of brevity.

2.3 Hydraulic limit

Many test runs have been performed on the plant to detect the maximum column capacity and they have confirmed that flooding occurs below the feed location triggered by a downcomer backup mechanism. The pressure difference between the bottom and the feed trays is the measured variable that gives the best indication of incoming flooding. Taking into account that the approach to flooding conditions is associated with a reduction of tray efficiency (Brambilla, 2014, chap. 5.2), the following operating limits have then been set from plant tests: the maximum throughput is 393 t/d while the maximum steam flow to reboiler Vₚₘₐₓ = 22.7 t/h, that using latent heat of vaporization 2.260 MJ/kg, corresponds to 14.23 MWt.

3. REAL-TIME OPTIMIZATION OPPORTUNITY

The opportunity for an RTO implementation has been considered due to the economic and process parameters variability. Feed, products, and energy prices are subjected to the oil price and Propylene season market, hence quite variable. Moreover, the throughput planning strategy has to deal with feed and product storage capacity and feed purchase availability and dynamics. Following these considerations, the unit revenues can be written in terms of MVs by the following equation:

\[
REV\text{ENUE} = DD_{p_{d-b}} - FF_{p_{f-b}} - VP_e \quad \text{(1)}
\]

where \( \Delta p_{d-b} \) indicates the cost difference between distillate and bottom products, \( \Delta p_{f-b} \) stands for the cost difference...
One additional parameter that can be considered as a measured disturbance is the Propylene concentration in the feed \( x_F \), as it affects indirectly the unit revenue through distillate product yield, much more as revenue value rather than as optimum operating parameters. An example of revenue trends with steam to reboiler is shown in Figure 2 for some typical costs reported in Table 2 and \( x_F \approx 79\% \). The right panel of Figure 2 compares revenue with different \( x_F \). Revenue trends have been obtained by rigorous simulation with the model validated with plant data. As it can be seen in Figure 2, by augmenting the throughput, the revenue augments almost linearly, while its relation with the steam to reboiler is similar to a reverse parabolic one. As a matter of fact, for a fixed throughput, the maximum revenue does not necessarily correspond to maximum steam, that is, working at the high hydraulic limit (red vertical line in Figure 2), or very near to it, could mean wasting raw materials. The right panel of Figure 2 shows instead a practically linear behavior of the revenue with the Propylene concentration in the feed, \( x_F \).

**Remark 2.** The analytical RTO model is intended above the MPC level in the process control hierarchy. Therefore, when the RTO model calculates the setpoint for the manipulated variable, the steady-state optimization problem of the MPC is not performed (functional design). Clearly, this is true if the RTO operability range is compatible with the MPC one. On the contrary, the MPC dynamic optimization is always performed, and it is deputed at controlling the distillate purity by rejecting unmeasured disturbances while fulfilling process constraints.

### 3.1 Optimization scenarios

The proposed analytical RTO has to face two operation scenarios: 1) revenue maximization with assigned throughput, and 2) revenue maximization with the only limit of maximum column hydraulic load assuming throughput availability.

**Scenario 1**  Assigned the throughput \( F \), the steam rate to reboiler \( V \) giving the maximum revenue satisfies the following equations:

\[
\frac{\partial \text{REVENUE}}{\partial V} = \frac{\partial (D \Delta p_{d-b} - F \Delta p_{f-b} - V p_e)}{\partial V} = 0 \quad (2)
\]

being \( F \) assigned, and therefore constant:

\[
\left| \frac{\partial (D \Delta p_{d-b} - V p_e)}{\partial V} \right|_F = 0 \quad (3)
\]

then let us define the revenue trend:

\[
\left| \frac{\partial D}{\partial V} \right|_F = \frac{p_e}{\Delta p_{d-b}} = R\text{V} \quad (4)
\]

The revenue trend is easily explained by the trend of distillate \( D \) (Propylene at 99.5\%) with the steam to reboiler \( V \) for a given throughput; both are shown in Figure 3. Increasing the steam to reboiler, the distillate \( D \) increases towards the asymptotic value \( D^* \approx 6 \text{kg/cm}^2 \text{y/(t h)} \) (Propylene recovery=100\%). When \( D \) is approaching its asymptotic value, the negative term of the steam to reboiler \( V \) in Eq. (3) begins to reduce the effect of the slow increment of distillate until it overwhelms. That point corresponds to the maximum revenue and is located where Eq.(4) is satisfied. The bottom panel of Figure 3 shows maximum revenue points for two values of cost parameter \( RV \); for increasing values of \( RV \), the maximum revenue point (the tangent points) moves from the fluidodynamic upper limit to the safer conditions.

**Scenario 2**  The maximum hydraulic column load, known from operation, is converted in terms of steam to reboiler \( V_{\text{max}} \). That value has been chosen not too close to flooding conditions to avoid heavy tray efficiency drop (Brambilla, 2014, chap. 5.2). The red dashed line in Figure 2 shows \( V_{\text{max}} \) at 22.7 t/h.

At the highest hydraulic limit \( (V_{\text{max}}) \), the throughput \( F \) giving the maximum revenue occurs when:

\[
\frac{\partial \text{REVENUE}}{\partial F} = \frac{\partial (D \Delta p_{d-b} - F \Delta p_{f-b} - V p_e)}{\partial F} = 0 \quad (5)
\]

as \( V = V_{\text{max}} \) is constant,

\[
\left| \frac{\partial (D \Delta p_{d-b} - F \Delta p_{f-b})}{\partial F} \right|_V = 0 \quad (6)
\]

and then:

\[
\left| \frac{\partial D}{\partial F} \right|_{\Delta p_{d-b}} = \frac{\Delta p_{f-b}}{\Delta p_{d-b}} = R\text{F} \quad (7)
\]

As for Scenario 1, the revenue trend is easily explained by the distillate \( D \) trend (Propylene at 99.5\%) with throughput \( F \) for the given steam flow to reboiler \( V_{\text{max}} \); both trends are shown in Figure 4. Increasing the throughput \( F \), the distillate \( D \) increases to a maximum and then decreases. When \( D \) is approaching its maximum value, the negative term of the feed rate in Eq. (6) begins to reduce the effect of the slow increment of distillate until it overwhelms. That point corresponds to the maximum revenue and should satisfy Eq. (7). The bottom panel of Figure 4 shows maximum revenue points for two values of the cost parameter \( R\text{F} \).

### 4. GENERALIZED OPTIMIZATION APPROACH

On-spec distillate trends are the base for the detection of maximum revenue operating points, hence, using the rigorous simulation model, different sensitivity analyses have been performed. Figure 5 shows these analyses with operating parameters. For Scenario 1, the left panel of Figure 5 shows distillate trends with steam to reboiler \( V \) for different throughput \( F \), while, for Scenario 2, in the right panel of Figure 5 the throughput \( F \) is varied and the steam to reboiler \( V \) is used as a parameter; in both cases, also different possible values of the Propylene feed concentration \( x_F \) have been tested. From this analysis, on-spec distillate trends seem to share similar values when \( x_F \) is maintained fixed until a limit value that is dependent on the specific \( V \) or \( F \) selected. On the other hand, the effect of varying \( x_F \) results in a translation of the curve: the lower is \( x_F \) the lower is the resulting \( D \).

To find a generalized approach for the estimation of maximum revenue condition, new coordinates are adopted so that only one curve could represent, adequately, all operating conditions. The

| Stream                  | Cost e/t |
|------------------------|----------|
| Distillate product - Bottom product | ∆pd−b 196 |
| Feed - Bottom product  | ∆pf−b 81 |
| Steam                  | p_e 18.8 |
Fig. 2. Revenue trends with steam to reboiler \( V \) for different throughputs for which cost parameters are in Table 2. On the left panel \( x_F = 79\% \) is fixed while on the right one two different value of \( x_F \) are tested; the red dash-dotted vertical line represents flooding conditions limit.

Fig. 3. On-spec distillate flow and revenue trend with \( V \) (top) and a close-up with tangent lines representing two cost parameters \( RV \) indicating the maximum revenue (bottom). Throughput \( F = 360 \text{ t/d} \) and \( x_F = 79\% \); the red dash-dotted vertical line represents flooding conditions limit.

Fig. 4. On-spec distillate and revenue trend for \( V = 22.7 \text{ t/h} \) and cost parameter \( RF = 0.7 \) (top) and a close-up with tangent lines representing two cost parameters indicating the maximum revenue throughputs (bottom).

Distillate \( D \) is normalized with the asymptotic value \( D^* = \frac{F x_F}{99.5} \) and is reported as function of the ratio \( V/F \) as in Figure 6. Although the curve that best fits the data displayed in Figure 6 is a “hyperbola-like”, a simpler function can be used in the operating range of interest. The \( D/D^* \) data between the asymptotes can also be analytically expressed by a 2nd (or 3rd order) polynomial function, i.e. \( D/D^* = f(z) \) with \( z = \frac{V}{F} \).

Figure 7 shows a close-up of the curve \( D/D^* \) in this interval. In particular, the trending line in Figure 7 represents the 2nd order polynomial function chosen in this paper to interpolate the data obtained for two different values of \( x_F \). The polynomial function is the following:

\[
f(z) = -2.0169z^2 + 6.0702z - 3.5722 \quad (8)
\]

and it interpolates the data with sufficient accuracy \( (R^2 = 0.9912) \). Note that the data interpolated with the function in Eq. (8) span almost the complete range of the typical values for the Propylene feed concentration listed in Table 1. From the generalized on-spec distillate polynomial in Eq (8), the maximum revenue conditions set by Eq. (4) and Eq. (7) are derived, respectively for the two scenarios considered.

**Scenario 1** To calculate the maximum of the distillate normalized curve for Scenario 1, the first derivative of \( f(z) \) is calculated as follows:

\[
f'(z) = \left. \frac{\partial f}{\partial z} \right|_F = \frac{1}{D^*} \left. \frac{\partial D}{\partial z} \right|_F = \frac{1}{D^*} \left. \frac{\partial D}{\partial V} \frac{\partial V}{\partial z} \right|_F = F \left. \frac{\partial D}{\partial V} \right|_F \quad (9)
\]
Fig. 5. On-spec distillate trends with steam to reboiler (on the left) and throughput $F$ (on the right). Where not specified, $x_F = 79\%$; the red dash-dotted vertical line represents flooding conditions limit.

Fig. 6. Normalized on-spec distillate trend with ratio steam to reboiler - throughput ($\frac{V}{F}$). Throughput data in the range $290 - 400$ t/d and $x_F = 79\%$.

Fig. 7. Close-up of Figure 6 between the asymptotes with two different values of $x_F$. The trending line is the green dash-dotted one.

with $a = \frac{99.5}{F}$. Then, according to Eq. (4), the value of the steam to reboiler that gives the maximum revenue is $V^* = z^* F$ where $z^*$ is the consistent root of the following second order equation:

$$f'(z^*) - a \frac{\partial D}{\partial V_F} = f'(z^*) - aRV = 0 \quad (10)$$

Then, according to Eq. (7), the throughput that gives the maximum revenue is $F^* = \frac{V_{\text{max}}}{z^*}$ where $z^*$ is the positive root of the following Equation:

$$f'(z) \left|_{\frac{\partial D}{\partial V}} \right| = a \left| \frac{\partial D}{\partial F} \right| \frac{\partial D}{\partial V}$$

$$-a \left( \frac{D}{F} \frac{\partial D}{\partial F} \right) \left( -\frac{V}{F^2} \right)^{-1} = F \left( \frac{D}{F} \frac{\partial D}{\partial F} \right) - a \left| \frac{\partial D}{\partial F} \right| \frac{\partial D}{\partial V} \quad (11)$$

In Eq. (10), the parameter $RV$ is the one most affecting the root value $z^*$, that is, when the throughput is fixed the major impact is given by the energy price and the price gap between top and bottom products. The accuracy of the analytical RTO estimations from Eq. (10) is shown in Figure 8 where they are compared with those obtained by the rigorous simulation model for $RV = 0.0328$ and $x_F = 79\%$. As can be seen, all the points calculated from the rigorous simulation model are matched by the analytical RTO model developed.

**Scenario 2** As for Scenario 1, we calculate the maximum of the distillate normalized curve for Scenario 2 using the following equation:

$$f'(z) = \left[ \frac{\partial D}{\partial F} \right]_{V} = a \left[ \frac{\partial D}{\partial F} \right]_{V} \frac{\partial z}{\partial F}$$

$$-a \left( \frac{D}{F} \frac{\partial D}{\partial F} \right) \left( -\frac{V}{F^2} \right)^{-1} = F \left( \frac{D}{F} \frac{\partial D}{\partial F} \right) - a \left| \frac{\partial D}{\partial F} \right| \frac{\partial D}{\partial V} = \frac{1}{z} \left( a \left| \frac{\partial D}{\partial F} \right| \frac{\partial D}{\partial V} - f(z) \right) \quad (11)$$

In Eq. (11), the parameter $RV$ is the one most affecting the root value $z^*$, that is, when the throughput is fixed the major impact is given by the energy price and the price gap between top and bottom products. The accuracy of the analytical RTO estimations from Eq. (10) is shown in Figure 8 where they are compared with those obtained by the rigorous simulation model for $RV = 0.0328$ and $x_F = 79\%$. As can be seen, all the points calculated from the rigorous simulation model are matched by the analytical RTO model developed.
In Eq. (12), the largest effect on the root value $z^*$ is given by the parameter $RF$, that is, the ratio between price difference among the feed and the product streams is determinant with respect to the cost of energy (see Eq. (7)). The accuracy of the estimations calculated via Eq. (12) is shown in Figure 9 where estimations are compared with those obtained by rigorous simulation for $V_{\text{max}} = 22.7\ t/h$ and $x_F = 79\%$. The effect of propylene feed concentration $x_F$ on optimum throughput at $V_{\text{max}} = 22.7\ t/h$ has confirmed a weak effect compared to the cost parameter $RF$. In fact, another simulation run with $RF = 0.537$ has returned an increase of 0.53% in the obtained maximum revenue throughput with a linear trend between $x_F = 73\%$ and $x_F = 79\%$, but, for the sake of brevity, it is not shown.

5. CONCLUSION

RTO has become a crucial instrument to optimize the economic aspects of chemical processes. Usually, such techniques need an online simulation model of the process which is often costly to implement. Hence, in this paper, the problem of optimizing the operation of a critical distillation unit, a Propane-Propylene super-fractionator, has been addressed. Two operative optimization scenarios implemented in the distillation process have been discussed and each of them has been reformulated to obtain the optimal setpoints analytically, as a function of the feed composition and price change disturbances. Such a procedure has been generalized and the obtained estimations have been compared with results calculated by a rigorous simulation model of the process developed offline in UniSim Design, matching them satisfactorily. We underline how the measurement of the Propylene feed concentration is a key parameter in the development of such procedure, hence, extending the same approach to general distillation processes where this measurement can be impractical is the real challenge to be explored in future works. In addition, it is assumed that the developed analytical RTO is operated in accordance with operation constraints that need to be handled in industrial practice. On the other hand, the MPC level is supposed to address unmeasured disturbances or plant-model mismatch accordingly, while eventually getting as close as possible to the RTO setpoint. Finally, compared with the common approach adopted in RTO where the rigorous model is used online, i.e., with regard to uncertainties on feed composition, the proposed one shows a simplicity of implementation also within the MPC itself that has to be remarked.

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