

Simulation platform of an industrial propylene-propane splitter integrated to Advanced Process Control for Real Time Optimization experiments

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Abstract: The present paper shows the development of a dynamic rigorous model of a propylene-propane splitter connected to an industrial MPC controller via OPC-UA. The model includes the material and energy balances, thermodynamic equilibrium, and constitutive equations. Some of the PI controllers presented in the real plant have also been modeled. A dynamic model requires further information as the sizing of the equipments, heat transfer coefficients, thermodynamics data and a good initial value for the state and algebraic variables. The validation of the model was performed in open loop and in closed loop simulations. The simulation results were compared to the historical data of the process. As future work, the simulation platform created will be used to study new algorithms of RTO with Modifier Adaptation methodology.

Keywords: Real-time Optimization, superfractionator, Aspen DMC, MPC

1. INTRODUCTION

Dynamic models aim to simulate the behavior of a process over time and they are used in different stages of a plant life cycle. In the design stage, for example, a dynamic model is useful for studies of operability and controllability. In operation, dynamic simulations are used to train operators, validate safety procedures, and study different operations conditions for optimization and control.

There are different ways of describing a distillation column using a dynamic model. Generally, these models use conservation laws like mass, energy, and momentum, and time dependent constitutive equations that define the relation between intensive variables and extensive variables (as equations of state and equilibrium equations). These equations form a differential-algebraic equations (DAE) system.

In order to make further experiments of Real Time Optimization (RTO) algorithms, a mathematical model able to describe the effects of inputs (manipulated variables and disturbances) on the outputs over wider ranges of operation is required. Therefore, the present paper shows the development of a simulation based on a first-principle model (FPM) of an actual industrial-scale propylene-propane splitter, to be used as a benchmark for tuning the RTO layer before its implementation in the real process. The simulation is connected via OPC-UA with Aspen DMC controller to mimic the behavior of the industrial process studied. In future work, a RTO layer with Modifier Adaptation (Marchetti, Chachuat and Bonvin, 2009) will be added to the architecture in order to perform the tuning experiments.

The paper is structured as follows: Section 2 describes the propylene-propane splitter and the FPM created. Section 3 explains the data reconciliation performed. Section 4 summarizes some characteristic of the Aspen DMC controller. Finally, section 5 presents the model validation that compares the open loop and closed loop results with the process data after reconciliation and section 6 presents some conclusions.

2. PROPYLENE PROPANE SPLITTER

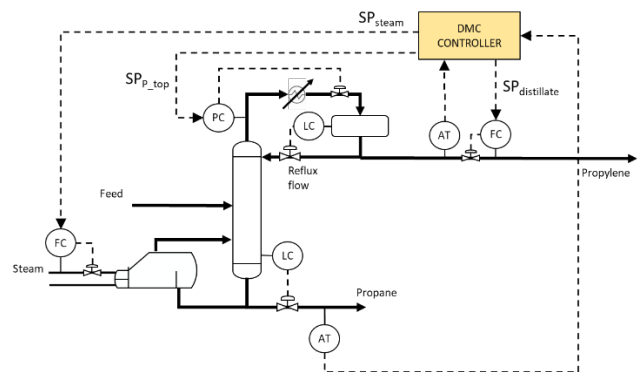


Figure 1. Control structure of the propylene propane splitter.

2.1 Modeling and simulation

The case study is a simulation of a real propane-propylene splitter of a Fluid Catalytic Cracking (FCC) of the Petronor refinery in Bilbao, northern Spain. The splitter studied aims to produce high purity propylene from a stream of propylene, propane and a small amount of impurities (C2-C4 hydrocarbons). The splitter consists of a total condenser, a partial kettle, and 135 equilibrium stages. The splitter has a DMC controller to maintain the propylene concentration in the

distillate and bottoms product within a range ($\geq 97.5\%$ molar on top and $\leq 10\%$ molar in bottoms); controlling the distillate, steam flow and top pressure (Figure 1). The process also has controllers to maintain the level in the accumulator vessel and base at a set point, manipulating the reflux and bottoms flowrate respectively.

2.2 Dynamic rigorous model

The rigorous model is a representation of the real process for use in the experiments with the DMC and RTO. A propylene propane splitter is a superfractionator, i.e., a distillation column that performs the separation of components with quite low relative volatility (<1.2) between the components, so the number of equilibrium stages required is very high.

The mathematical model considers the following simplification hypothesis:

- Constant pressure drop.
- The feed consists of four components: propylene, propane, isobutane and ethane.
- The condenser allows sub cooling.
- The column is thermally isolated.
- Only the top pressure and accumulator vessel level PI controllers are modeled. The level inside the reboiler is considered constant.

The nonlinear dynamic model described was developed with EcosimPro (EA Int., 2020). The model has 12090 equations and it was solved using the IDAS_SPARSE integration solver (Hindmarsh *et al.*, 2005).

Internal Trays

Equations (1) and (2) describe the total and individual component material balances for each stage. In Equation (1), the variable mol_n is the molar liquid holdup on stage n . l_{n+1} and l_n represent the liquid molar flow (kmol/h) that comes from the upper stage and goes to the downer stage respectively and, v_{n-1} and v_n are the vapor flow that comes from the stage below and goes to the upper stage.

$$\frac{dmol_n}{dt} = l_{n+1} + v_{n-1} - l_n - v_n \quad (1)$$

In Equation (2), the term $x_{j,n}$ corresponds to the liquid molar fraction of the component j in the tray n and $y_{j,n}$ is the vapor molar fraction.

$$\frac{dmol_n x_{j,n}}{dt} = l_{n+1} x_{j,n+1} + v_{n-1} y_{j,n-1} - l_n x_{j,n} - v_n y_{j,n} \quad (2)$$

The dynamics of the specific liquid enthalpy depends mainly on the change in the compositions, which is assumed faster than the dynamics of the total mass. Therefore, its effect on the energy balance can be negligible, avoiding a high index problem associated with the calculation of the temperature (equation (3)). In equation (3), h is the enthalpy of the liquid flow and H is the enthalpy of the vapor flow. Also, notice that equation (3) is used to calculate the vapor flow in each tray and not the temperature. The temperatures are calculated using the

thermodynamic equilibrium as will be explained next in Thermodynamics section.

$$h_n \frac{dmol_n}{dt} = h_{n+1} l_{n+1} + H_{n-1} v_{n-1} - h_n l_n - H_n v_n \quad (3)$$

Feed

In the feed tray, total, individual material balances are presented by Equations (4) and (5). f is the feed molar flow and z_j is the feed molar fraction for each component j . The subscript nf means the feed stage.

$$\frac{dmol_{nf}}{dt} = f + l_{nf+1} + v_{nf-1} - l_{nf} - v_{nf} \quad (4)$$

$$\frac{dmol_{nf} x_{j,nf}}{dt} = f z_j + l_{nf+1} x_{j,nf+1} + v_{nf-1} y_{j,nf-1} - l_{nf} x_{j,nf} - v_{nf} y_{j,nf} \quad (5)$$

The energy balance is presented by equation (6), similar to equation (3).

$$h_{nf} \frac{dmol_{nf}}{dt} = f h_f + h_{nf+1} l_{nf+1} + H_{nf-1} v_{nf-1} - h_{nf} l_{nf} - v_{nf} H_{nf} \quad (6)$$

Top tray

In the top tray, heat and mass balances similar to the internal trays could be considered (equations (7) to (9)). nt refers to the top tray and r is the molar reflux flowrate.

$$\frac{dmol_{nt}}{dt} = r + v_{nt-1} - l_{nt} - v_{nt} \quad (7)$$

$$\frac{dmol_{nt} x_{j,nt}}{dt} = r x_{j,r} + v_{nt-1} y_{j,nt-1} - l_{nt} x_{j,nt} - v_{nt} y_{j,nt} \quad (8)$$

$$h_{nt} \frac{dmol_{nt}}{dt} = h_r r + H_{nt-1} v_{nt-1} - h_{nt} l_{nt} - H_{nt} v_{nt} \quad (9)$$

Base and reboiler

The column base and reboiler are assumed to be tray number 1. Equation (10) corresponds to the total mass balance at the base, where mol_{base} is the molar liquid holdup and l_{base} is the liquid molar flow. Equation (11) is the total mass balance in the reboiler, where b is the bottom distillate molar flow and v_1 is the vapor flow leaving the reboiler. As the control level in the reboiler is assumed perfect, the equation (12) calculates the molar liquid holdup inside the reboiler and the level $h_{reboiler}$ is constant. Equation (13) corresponds to the individual component material balances inside the reboiler. Equation (14) is the energy balance in the reboiler. The heat dynamics is faster compared to the composition dynamics so equation (14) is used to calculate the vapor flow in each tray until the feed tray, as presented in equation (3). Equation (15) calculates the heat generated $Q_{reboiler}$ by the steam flow F_s with a heat of vaporization ΔH_{vap} in the pressure P_s , considering a steam quality τ_s . A τ_s of 0 indicates 100% liquid (condensate) and a τ_s of 1 indicates 100% steam.

$$\frac{dmol_{base}}{dt} = l_2 - l_{base} \quad (10)$$

$$b = l_{base} - v_1, l_{base} = K_{base} \sqrt{\frac{mol_{base} * MM_{base}}{A_{base} \rho_{base}}} \quad (11)$$

$$mol_{reboiler} = \frac{A_{reboiler} h_{reboiler} \rho_1}{MM_1} \quad (12)$$

$$mol_{reboiler} \frac{dx_{j,1}}{dt} = l_{base} x_{j,2} - v_1 y_{j,1} - b x_{j,1} \quad (13)$$

$$v_1 = \frac{h_2 l_2 - h_1 b + Q_{reboiler}}{H_1} \quad (14)$$

$$Q_{reboiler} = \tau_S F_S \cdot \Delta H_{vap}(P_S) \quad (15)$$

Condenser

The splitter has a flooded condenser to control the top pressure, manipulating the flooded area of the condenser using a control valve beneath. An increase in the condensate flow decreases the liquid level inside the condenser and the area available for condensation increases (Luyben, 2017).

Equations (16)-(23) describe the condenser with sub-cooling liquid. Equation (16) is the vapor molar material balance inside the condenser. $mol_{v,cond}$ is the vapor holdup inside the condenser, v_{nt} is the vapor leaving the top tray and l_{cond} is the amount of vapor that condensates to liquid. Equation (17) relates the molar liquid holdup inside the condenser ($mol_{l,cond}$) and the flow of liquid entering the liquid phase from condensation, l_{cond} , and the liquid flow that goes to the accumulator vessel, l_{accum} .

$$\frac{dmol_{v,cond}}{dt} = v_{nt} - l_{cond} \quad (16)$$

$$\frac{dmol_{l,cond}}{dt} = l_{cond} - l_{accum} \quad (17)$$

Equations (18) and (19), respectively, present the total latent heat lost by the vapor to condensate to saturated liquid and the total sensible heat lost to cool down the saturated liquid to a temperature below the bubble point. Both latent and sensible heat transfer processes are very fast, so the dynamics are not considered.

$$Q_{cond_sat} = l_{cond}(H_k - h_{cond_sat}) \quad (18)$$

$$Q_{cond_sub} = l_{cond} h_{cond_sat} - l_{accum} h_{cond_sub} \quad (19)$$

Equations (20) and (21) describe the change in temperature for the condensate flow and refrigerant flow, considering the equipment design data and the condensate level inside the condenser. The parameter α describes the percentage of the area available for condensation, equation (22).

$$Q_{cond_sat} = U_v(1 - \alpha)A_{cond}(T_{nt} - T_{in}^W) \quad (20)$$

$$Q_{cond_sub} = U_l \alpha A_{cond}(T_{accum} - T_{in}^W) \quad (21)$$

$$\alpha = \frac{V_{l_cond}}{V_{T_cond}} \quad (22)$$

Finally, equation (23) represents the total heat that the coolant extracts from the process flow. F_W is the coolant flow, C_p^W is the refrigerant capacity heat and T_{out}^W , T_{in}^W are respectively the coolant outlet and inlet temperature.

$$Q_{cond_sat} + Q_{cond_sub} = F_W C_p^W (T_{out}^W - T_{in}^W) \quad (23)$$

The composition inside the condenser is assumed to be the same of the vapor to be condensate.

Accumulator vessel

The accumulator is a horizontal vessel where the liquid from the condenser is collected. One part of the liquid is withdrawn as distillate and the rest is returned to the splitter as reflux liquid. The total and partial mass balance can be written as (24) and (25). The accumulator vessel has a huge volume so an energy balance is also necessary (26).

$$\frac{dmol_{accum}}{dt} = l_{accum} - r - d \quad (24)$$

$$\frac{dmol_{accum} x_{j,d}}{dt} = l_{accum} y_{j,nt} - r x_{j,r} - d x_{j,d} \quad (25)$$

$$\frac{d(mol_{accum} h_d)}{dt} = l_{accum} h_{cond_sub} - r h_d - d h_d \quad (26)$$

Note that, actually, $x_{j,r} = x_{j,d}$ as the reflux and distillate are the outlet from the accumulator vessel.

Thermodynamics

The high pressures (>10 bar) inside the splitter required the use of the Peng Robinson equation of state for the equilibrium constant, equations (27) and (28), and enthalpies calculations (Matsoukas, 2013). $\phi_{i,n}^{liq}$ is the liquid fugacity coefficient for component j in tray n , similarly $\phi_{j,n}^{vap}$ is the vapor fugacity coefficient and $K_{j,n}$ is the liquid-vapour equilibrium constant.

$$K_{j,n} = \frac{y_{eq,j,n}}{x_{j,n}} \quad (27)$$

$$K_{j,n} = \frac{\phi_{j,n}^{liq}}{\phi_{j,n}^{vap}} \quad (28)$$

The temperature values in each tray are calculated by using a convergence method. First, initial values for the temperature, K and x in each tray are guessed (for 3 of the 4 components presented in the mixture). Then y_{eq} for the three components are calculated by equation (27). The last component molar fraction is given by the sum of molar fractions (always equals to 1). After that, the last K -value and the fugacity coefficients are also calculated using (27) and Peng-Robinson. Finally, the fugacity coefficient equations are used as residue equations to verify the initial values given (temperature and K).

The Murphree tray efficiency, ε_n , is applied to calculate the actual performance of the splitter, Equation (29).

$$y_n = \varepsilon_n(y_{eq,n} - y_{n-1}) + y_{n-1} \quad (29)$$

Column hydraulic

A simple Francis weir equation that relates the liquid holdup in the tray with the liquid flow leaving the tray is used (Luyben, 1999), Equation (30). The flow depends on the fluid mechanics of the tray. l_{vol_i} is the liquid flow rate over weir, h_{ow} is the height of liquid over weir and L_w is the length of weir.

$$l_{vol_n} = 3.33L_w h_{ow}^{1.5} \quad (30)$$

Pressure profile

The rigorous model considers that the gas accumulates in the condenser as shown in Equation (16). The pressure drop is constant along the column and the maximum pressure drop between the base and top is approximately 1 bar. Equation (31) calculates the pressure profile in the column except for the top tray, which is given by equation (32) (Luyben, 1999). The term mol_{cond} is the holdup of the vapor phase inside condenser and z is the compressibility factor calculated from Peng Robinson.

$$P_n = P_{n+1} + \Delta p \quad (31)$$

$$P_{nt} = z \frac{mol_{v,cond} RT_{nt}}{V_{nt}} \quad (32)$$

PI controllers

The accumulator level and the pressure PI controllers have been modelled in the rigorous dynamic model. The first one manipulates reflux flow to maintain the level set point in the accumulator vessel and the second one manipulates the liquid flow from the condenser to the accumulator vessel to maintain the top pressure in the set point calculated from the DMC.

Parameters of the model

A dynamic simulation requires some information of the equipment involved in the process. The size and overall heat transfer coefficient for the vapor phase for the condenser, the size of the reboiler and the diameter, weir length and height of the column were founded in the respectively equipment specification sheet. Another parameters used in the model are the thermodynamic data. The data was obtained from the Simulis Thermodynamics software (Simulis Thermodynamics, 2021) and Wauquier (1995).

Initialization and convergence of the model

The splitter rigorous model presented forms a differential-algebraic equations (DAE) system with 12090 equations that require the initial values of 553 state variables and 549 algebraic variables (1102 variables in total). To find good initial values, the methodology proposed in Oliveira-Silva and Prada (2019) was applied. The methodology constructs simplified models based on the full rigorous model, applying assumptions that may not be suitable for the process studied, but decrease the number of initial values required. In each step, the simplified models approximate to the complete rigorous model and a subset of good initial values are found.

3. DATA RECONCILIATION

In order to find any errors, caused by measured devices malfunction, we used data for almost 4 months in 2019 (data per hour) to verify the mass and energy balance equations.

First, as only the propylene concentration is measured in all the inputs and outputs, we consider the presence of only propane and propylene in the mixture. Then all the volumetric flow measurements are converted to mass flow, and the molar fractions to mass fractions. So, the amount of total mass and propylene mass that flow in and flow out the column in this period of time could be calculated. We consider that integrating non-stationary flowrates over a period larger than the time constant of the control volumes, makes the accumulation negligible compared to inflow and outflow values. We also assume that the analyzers are more reliable than the flow meters, so the following optimization problem could be written as in equation (33), where $bias_F, bias_D, bias_B$ refers to the difference between the measured and the real value of the feed, distillate and bottoms flows respectively.

| | |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|
| $\min_{bias_F, bias_D, bias_B} \varepsilon_{total}^2 + \varepsilon_{C_3H_6}^2$ $\varepsilon_{total} = \sum_{t=0}^{t_f} [(F_t + bias_F) - (D_t + bias_D) - (B_t + bias_B)]$ $\varepsilon_{C_3H_6} = \sum_{t=0}^{t_f} [(F_t + bias_F)z_{i,t} - (D_t + bias_D)x_{D,i,t} - (B_t + bias_B)x_{B,i,t}]$ <p style="text-align: center;">s.t. steady state mass balances, process constraints</p> | (33) |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|

The problem was solved using the solver in Excel and the results founded were: $bias_F = 0.1624$, $bias_D = 0$ and $bias_B = 0.0920$. Two open loop simulations were performed: the first one using the input flow data and a second one with the input flow bias corrected data. The results of the percentage difference for the propylene molar fraction concentration in distillate are presented in Figure 2. The correction made in the process data with the bias decreased the difference between the simulation and process data. Similar results were obtained for other important simulation variables.

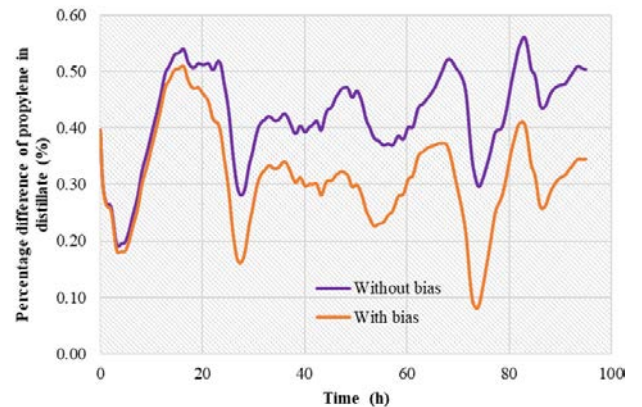


Figure 2 Percentage difference between simulations with and without reconciliation and process data.

4. ASPEN DMC CONTROLLER

The Aspen DMCplus Build and Aspen DMC3 builder are applications to develop and deploy a MPC (Aspen Technology Inc, 2021). At each sampling time, Aspen DMC executes a two-layer architecture: the first one, the optimizer, calculates the future targets to the second layer, the controller. Then, the controller calculates the future moves to achieve these targets and apply the first move to the process.

The DMC optimizer calculates the setpoints to the control variables (CVs) and manipulated variables (MVs), solving the Linear Programming (LP) problem (34) subject to the constraints ($\geq 97.5\%$ molar on top and $\leq 10\%$ molar in bottoms of propylene). The $LPCost_i$ values are the incremental cost of increasing the i -th MV by one unit, while all other MVs remain constant. By definition, a negative $LPCost$ tries to maximize the value of the MV and a positive $LPCost$ tries to minimize its value. $\Delta MV_{i,ss}$ corresponds to the change in the i -th MV in steady state. Note that the main objective of the LP is to fulfill the process constraints, as the controller is unconstrained.

$$\min_{MV} \sum_{i=1}^n \Delta MV_{i,ss} \times LPCost_i \quad (34)$$

5. MODEL VALIDATION

Model validation in open loop

In order to validate the model, some of the historical process bias-corrected data were compared to the model results. To do so, process data from four consecutive days (one data per hour during four days in June 2019) was used as input to the EcosimPro simulation, including the values of the manipulated variables: distillate flowrate, steam flowrate to reboiler and the top pressure. It means the following validation results does not consider the DMC controller (open loop simulation). Note that the results were normalized due to confidentiality reasons.

Figure 3 and Figure 4 show the behavior of the normalized molar fraction of propylene in the distillate and bottoms in time.

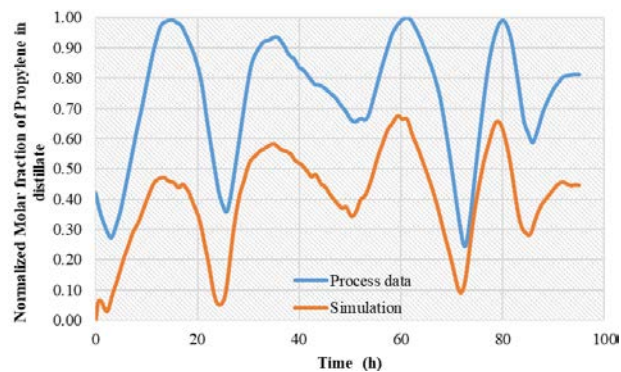


Figure 3 Normalized molar fraction of propylene in distillate, open loop.

The figures show that the rigorous model and the process have a very similar dynamic behavior. Figure 3 shows that process

and simulation have similar gains, but there is a bias between the values. In Figure 4, one can noticed that the dynamic model is able to match the real gain most of the time.

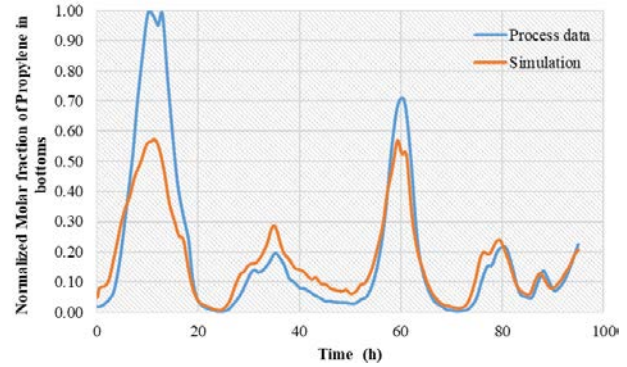


Figure 4 Normalized molar fraction of propylene in bottoms, open loop.

Model validation in closed loop

The closed loop simulation architecture is presented in the Figure 5. In order to connect the EcosimPro simulation with the Aspen DMC, first a deck was generated. A deck allows any experiment in EcosimPro to run as a standalone black box independent from the main program (EA Int., 2020). After that, the OPC-UA deck was connected to the Aspen DMC controller using the Aspen Cim-IO interface manager application. The same DMC application used in the process was changed to connect to the deck, updating the IO Tag in the Deployment section in DMC3 Builder, Figure 6. So the DMC used in the simulation and the plant are the same (same model and configuration). The DMC were monitored using the Aspen APC Web Interface. The code in Python connects to the EcosimPro deck by OPC-UA and call the deck commands to reset, run and integrate the simulation over time. During the simulation, the controller reads the data directly from the deck then calculates the MV control moves (distillate flow, steam flow and pressure) and send this information back to the deck.

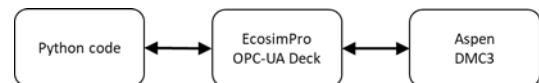


Figure 5 Closed loop simulation architecture.

| Tag Generator | | | |
|----------------|---------|---------------|--------------------|
| Variable Name | Type | Generate Tags | Measurement Prefix |
| new_dmcff3_... | General | | |
| 14FC0005.SP | Input | | |
| 14FC0002.SP | Input | | |
| 14FC0001.SP | Input | | |
| X14F001C | Input | | |
| 14AR005B. | Input | | |
| 3TR07001. | Input | | |
| 3PC0115B. | Input | | |
| 14AR001A. | Output | | |

| Variable Detail | | | |
|-----------------|-----------|------------------------|-------------|
| Parameter | IO Source | IO Tag | IO Datatype |
| Measurement | Splitter | ns=4s=mv out.signal[2] | Double |
| Setpoint | Splitter | ns=4s=mv in.signal[2] | Double |

Figure 6 Connection between deck and DMC.

The input data used was the same from the open loop simulation, except the MVs as already mentioned. The DMC controller started after 30 minutes of simulation.

Figure 7 and Figure 8 show the behavior of the concentrations of propylene in distillate and bottom. Note that as the DMC requires past input values to make predictions, the first 20 hours of simulation should be discarded. The simulation needs some time to update these values. After 48 hours of simulation, the results approach the process data.

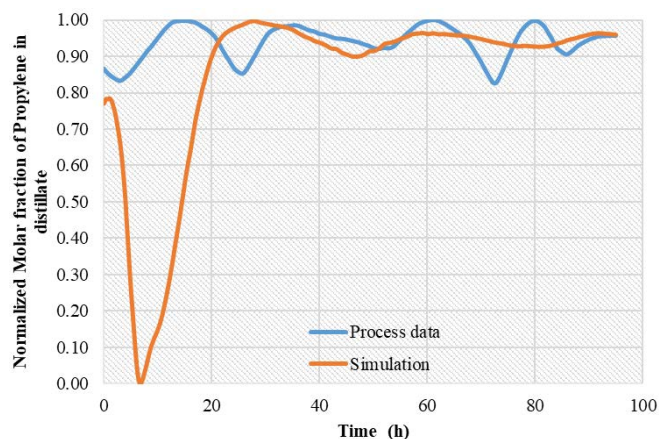


Figure 7 Normalized molar fraction propylene in distillate, simulation in closed loop with Aspen DMC controller.

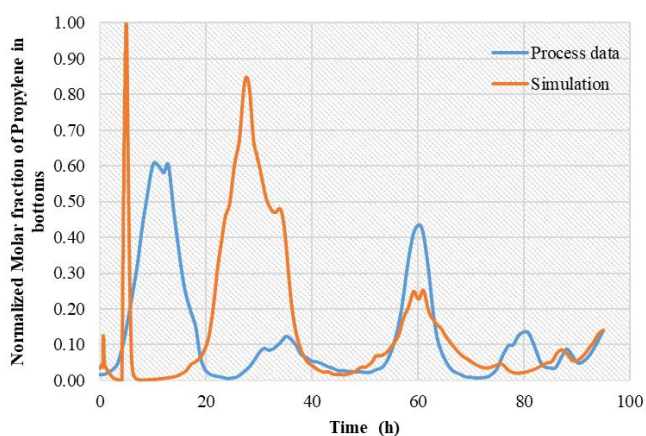


Figure 8 Normalized molar fraction propylene in bottoms, simulation in closed loop with Aspen DMC controller.

6. CONCLUSION AND FUTURE WORK

In conclusion, the open loop and closed loop validation show that the model can predict the dynamic behavior of the process. The main differences are in the propylene composition in bottoms. However, for control and optimization purposes, the dynamic response and gains are more important than the absolute values of process variables. So, the present model is considered good enough for the purpose of a virtual plant for RTO experiments.

As future work, the RTO+MA algorithm will be included in the Python code and the CVs setpoints calculated will update the DMC external targets. The inclusion of MA modifiers in the RTO layer permits to match the necessary conditions of optimality of the process and model. MA does not require an accurate model to find the real optimum of the process, since the modifiers, i.e., process gradients are calculated correctly (Marchetti *et al.*, 2020). Because of that, the model used in RTO+MA scheme will be the same linear model of the Aspen

DMC. The economic cost function will consider the profit by selling propylene and propane minus the cost to produce steam. The products prices will depend if the propylene specification is fulfilled ($\geq 97.5\%$ molar on top and $\leq 10\%$ molar in bottoms), i.e., the price of products out of specification will be drastically reduced.

ACKNOWLEDGMENTS

This work was supported by JCYL under programs CLU 2017-09 and UIC 233, as well as by project InCO4In, from Spanish AEI under project PGC2018-099312-B-C31, both with FEDER funds. The authors thank the European Social Fund and the “Consejería de Educación de la Junta de Castilla y León”.

REFERENCES

- Aspen Technology Inc (2021) *Aspen DMC3*. Available at: <https://www.aspentech.com/en/products/msc/aspen-dmc3> (Accessed: 22 November 2021).
- EA Int. (2020) *EcosimPro 6.2, User Manual*. Available at: <https://www.ecosimpro.com/>.
- Hindmarsh, A. C. *et al.* (2005) ‘SUNDIALS’, *ACM Transactions on Mathematical Software*, 31(3), pp. 363–396. doi: 10.1145/1089014.1089020.
- Luyben, W. L. (1999) ‘Process Modeling , Simulation and Control Chemical Engineers’, *Petroleum Refinery Engineering*.
- Luyben, W. L. (2017) ‘Dynamic simulation of flooded condensers’, *Chemical Engineering Research and Design*. Institution of Chemical Engineers, 118, pp. 12–20. doi: 10.1016/j.cherd.2016.12.001.
- Marchetti, A., Chachuat, B. and Bonvin, D. (2009) ‘Modifier-Adaptation Methodology for Real-Time Optimization’, *Industrial & Engineering Chemistry Research*, 48(13), pp. 6022–6033. doi: 10.1021/ie801352x.
- Marchetti, A. G. *et al.* (2020) ‘Modifier Adaptation as a Feedback Control Scheme’, *Industrial and Engineering Chemistry Research*, 59(6), pp. 2261–2274. doi: 10.1021/acs.iecr.9b04501.
- Matsoukas, T. (2013) ‘Fundamentals of Chemical Engineering Thermodynamics: With Applications to Chemical Processes’, p. 690. doi: 10.1111/j.1475-6803.2004.00096.x.
- Oliveira-Silva, E. and de Prada, C. (2019) ‘Methodology to achieve convergence in a rigorous dynamic model of a superfractionator’, in *X Congress of Eurosím*. Logroño, La Rioja, pp. 1–12.
- Simulis Thermodynamics* (2021) *Prosim*. Available at: <https://www.prosim.net/> (Accessed: 22 November 2021).
- Wauquier, J.-P. (1995) *Petroleum Refining, Volume 1 - Crude Oil, Petroleum Products, Process Flowsheets*. Technip, Institut Français du Pétrole. Technip. Paris.