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Design, Economic Evaluation and Control of Olefin Metathesis Processes

SUMMARY

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Contents

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Introduction

Motivation

The current ethylene and propylene market is continuously growing year over year. More technologies are necessary to keep up with the high demand, in addition to the already existing technologies (naphtha cracker and fluid catalytic cracking) where light olefins are obtained as a co-product. An attractive alternative for on-purpose light olefins production is olefin metathesis process. The 2-butene metathesis is a novel process to convert low-value by-products of fluid catalytic cracking (FCC) into more attractive products such as propylene and ethylene. Therefore, the first part of the thesis is to present the design, economical optimization and conventional control of the 2-butene olefin metathesis unit.

The unpredictable market challenges for consistent attainment of high product quality, more efficient use of energy, reduction of greenhouse gases emissions (GHG) and an increasing awareness of circular economy have all combined to impose more demands on control systems than can be met by conventional techniques alone. The implementation of advanced process control techniques in chemical and petrochemical industries, such as linear model predictive control (LMPC) offers an attractive and effective way to tackle the problems in multivariable control systems by including the process model in the computation of control actions. However, limited published literature is available about LMPC applied on a plant-wide control process. Often, linear model predictive control is implemented exclusively on single equipment (e.g., reactor, distillation column) and not on an entire unit.

Therefore, the aim of the second part of this thesis is to address the challenges and benefits of implementing a linear model predictive control (LMPC) on a plantwide control of olefin metathesis unit. The performance of conventional and model predictive control applied on the olefin metathesis unit is evaluated to reflect the benefits and as well as the challenges identified during this work.

Thesis overview

The thesis consists of six chapters.

Chapter 1 presents the motivation of the current thesis related to the conceptual design, economical optimization, conventional and model predictive control of olefin metathesis unit.

Chapter 2 briefly describes the research literature and existing industrial applications for propylene production, either as a co-product - currently dominating the market, or as a stand-alone product - via several on-purpose technologies.

Chapter 3 presents theoretical aspects related to dynamic model development based on first principles and system identification, and process control through conventional and advanced strategies, such as model predictive control. A case study on a binary distillation column is used to compare the performance of conventional control and linear model predictive control.

Chapter 4 presents the conceptual design of on-purpose propylene production via 2-butene metathesis process. Several process alternatives are investigated by hierarchical approach. A simple Reactor-Separation process turns out to be the most economical alternative. Economical optimization of the "best" flowsheet is carried on. The objective function of the economical optimization is the total annual cost.

Chapter 5 presents the process control of 2-butene metathesis unit using two control strategies; conventional and model predictive control. The benefits and challenges of both control strategies are demonstrated based on the controllers' performance in achieving the required product specifications.

Chapter 6 presents the main achievements of the thesis together with the challenges, limitations or even issues encountered during the work development, ending with recommendations to assist the end user in avoiding repeating the same errors as the author.

All chapters could be read independently; each chapter begins with an introduction or brief overview, followed by methodology and original contributions, ending with conclusions. The references are listed at the end of each chapter.

Producing ethylene and propylene from low-cost feedstock (2-butene) by metathesis process using tungsten mesoporous catalyst is feasible. The economics suggest using the once-through reactor-separation flowsheet (without recycling). The plant dynamics can be controlled by means of conventional control system and for superior control performance, by model predictive control. Future work should focus on improving unit's by-products generation (circularity) due to economics (recycling reactants) and enabling more effective operator interaction with MPC through user-friendly interfaces.

Propylene production technologies

In this summary chapter, the focus is on the emergence of on-purpose routes for propylene production, in response to the increasing demand for plastics and to a shift to shale gas as a feedstock for ethylene production over the last few decades. Among these routes, propane dehydrogenation has proven to be an efficient and selective method for propylene generation, attracting significant investments to address the propylene supply gap.

Additionally, the metathesis technology, originally introduced in the 1960s, is currently experiencing renewed interest, particularly in the context of the propane to olefins process. The integration of metathesis technology with existing assets holds the potential to optimize economic margins for refineries. This ensures production flexibility and resource efficiency, both crucial for adapting to the dynamics of the chemical and petrochemical market. On-going research activities in this field are highlighted and outlines future perspectives.

Process Dynamics and Control

Dynamic behavior of chemical plants is characterized by complexity with numerous challenges from operability and safety standpoint of view. Process dynamics and control represents a fundamental pillar in design phase for assessing the operability of a process, product specifications and developing safe and reliable process designs.

In this summary chapter, a methodology for dynamic model developing based on first principles models is presented. An apparent more simplistic approach for building process models by system identification derived from process data (input-output data) is also explained together with its challenges. Integration between several software packages (Aspen Dynamics-Simulink co-simulation) is described and exemplified on a unit's operation models in the next chapters. Basic process control (conventional) and more advanced control strategies, such as model predictive control (MPC) are applied on a binary distillation column to compare their performances.

Conventional control and MPC applied to a benzene-toluene column

The study focuses on a benzene-toluene distillation column, assessing dynamic behavior and control system responses with two control approaches: conventional control (combining feedforward and feedback) and model predictive control (MPC). The conventional control system and process dynamics are established in Aspen Dynamics, while the model predictive control is implemented in Simulink/MATLAB. The MPC approach is categorized into two cases based on model development: (1) linearization from Aspen Dynamics and (2) system identification using simulation data.

The distillation column is inherently nonlinear. To obtain a model suitable for control purposes, the nonlinear column model undergoes linearization near its steady state operating conditions, using Aspen Dynamics. This yields state-space matrices A, B, C, and D. This state-space model is then used to design the MPC controller.

In a second approach, the (nonlinear) dynamic simulations model is used to conduct multiple step tests, and the data obtained is processed using the System Identification tool in MATLAB. Similar to the first case, this results in a state-space model representation.

The choice of representing both models in the state-space form is primarily driven by the requirement of the MPC Designer tool, which mandates a state-space model representation for constructing the MPC algorithm.

The report outlines the steps involved in developing both steady-state and dynamic simulations. It also explains the integration between the Aspen Dynamics environment and Simulink/MATLAB for configuring the model predictive algorithm. The document includes recommendations and practical tips for working with the various software applications involved.

Emphasis is placed on the necessary steps to enable data exchange between AspenTech software and MATLAB. It is important to note that both the MPC Designer and System Identification tools are integral parts of the MATLAB software suite, while Simulink serves as the platform for interaction with the Aspen Dynamics simulation environment. The report includes dynamic performance and control results for both conventional control and model predictive control (MPC). The conclusions section provides a comparative analysis of the performance of each control strategy.

Combined feedforward/ feedback control

Feedforward control is a control strategy often implemented together with feedback control to reject disturbances especially if the identified disturbance is influencing significantly the process outputs. The easily measurable feed rate is ideal for integrating feedforward control, substantially boosting the control system's performance.

The ideal feedforward controller is the negative ratio of the disturbance transfer function divided by the process transfer function.

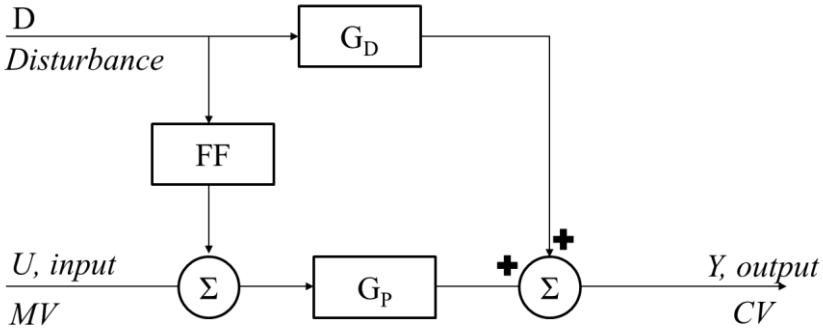


Figure 1. Block flow diagram of FF

$$Y(s) = D(s) \cdot G_D(s) + U(s) \cdot G_P(s) = 0$$

$$U(s) = -\frac{G_D(s)}{G_P(s)} \cdot D(s) \tag{0.1}$$

$$G_{FF} = -\frac{G_D(s)}{G_P(s)}$$

In this example, the feed flow is a measured disturbance and is added as feedforward action on both the distillate composition controller and bottoms composition controller. The objective is to ensure a better and much faster dynamic response to different measurable disturbances. A good approximation in most of the applications of feedforward control is to set the gain equal to the ratio of the disturbance and process gains, particularly when both of the controller outputs act on the process with similar dynamics, $\tau_p \approx \tau_d$. Thus, the following equation may be applied,

$$K_{FF} = -\frac{K_D}{K_P} \tag{0.2}$$

Since the composition controllers are PI controller, the feedforward controller is added to it with the following addition of the measured disturbance, d.

$$u(t) = u_{bias} + K_C e(t) + \frac{K_C}{\tau_I} \int_0^t e(t)dt + K_{FF} d \tag{0.3}$$

In Figure 2, the combined feedforward and feedback control on the benzene-toluene distillation column is illustrated.

The feedforward action is configured in Aspen Dynamics by a comparator block that calculates the deviation of feed flow, a lead-lag block configured with the feedforward characteristics. The signal coming from the lead-lag block together with the composition controller action are together introduced in a sum block with the output signal controlling the reflux rate for one feedforward controller, FF1 and the reboiler duty for the second controller, FF2. Step tests on the feed flowrate were performed to determine the response on the products composition, and consequently the controller parameters for both feedforward controllers (e.g., benzene CC1, and toluene CC2) from their corresponding transfer functions and by applying Eq. (0.2).

Table 1. Feedforward controller parameters

	Feedforward on benzene composition controller	Feedforward on toluene composition controller
Feedforward control gain, K_{FF}	-19.8	0.0148
Disturbance gain, K_d	0.0009, ([-]/kmol/hr)	-0.0121, ([-]/kmol/hr)
Disturnbance time constant, τ_d	0.53 h	0.95 h
Feedforward transfer function	$G_{FF1} = -\frac{\overbrace{0.0009}^{G_d}}{0.53s+1} \cdot \frac{\overbrace{0.56s+1}^{G_P}}{4.54\times10^{-5}}$	$G_{FF2} = -\frac{\overbrace{-0.0121}^{G_d}}{0.95s+1} \cdot \frac{\overbrace{0.56s+1}^{G_P}}{0.82}$

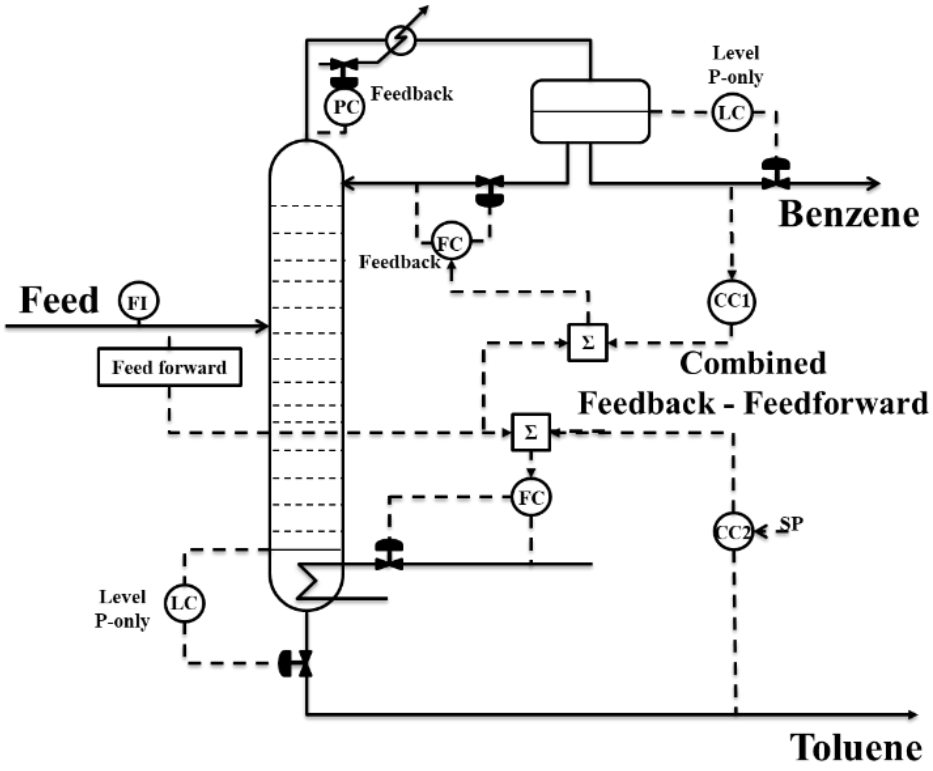


Figure 2. Combined Feedforward/Feedback on benzene-toluene distillation column

Model predictive control applied on benzene-toluene distillation column

The applicability of a model predictive controller for a benzene-toluene distillation column is demonstrated, including some valuable recommendations and hints that may save the reader tremendous time and effort in finding the resolution or way forward for designing and setting up a model predictive controller in Aspen Dynamics simulation.

Several prerequisites are necessary to facilitate the link and data transmission between Aspen Dynamics simulation and Simulink/ MATLAB. Obviously, the software packages of AspenTech (e.g., Aspen Plus and Aspen Dynamics) should be available. In order to enable data transfer between Aspen Dynamics and MATLAB, compatible version should be employed (either 32bits, or 64 bits); hence, in this case Aspen Plus v10 and MATLAB R2015b is used for the current research. Simulink is an application within MATLAB, so it should be available together with the other applications or tools as MPCdesigner and System Identification Toolbox. The latter applications are also required for the design and set-up of MPC on the benzene-toluene distillation column.

The Control Design Interface (CDI) from Aspen Dynamics enables a linear state space model to be extracted from the non-linear simulation of Aspen Dynamics, which can be used further in the Control System Toolbox in designing a process control system, hence a model predictive controller (Mathworks), (AspenTech, 2016). A similar example with the design and co-simulation of a distillation tower for separating benzene, toluene and p-xylene is provided and available on the Mathworks website.

Results

The results for each control structure are presented below to illustrate the performance and control response for a feed disturbance consisting in a step change of +/- 10% of feed flow.

- Conventional control represented by the three (3) scenarios:
  - CS1: Proportional-Integral (PI)
  - CS2: PI and Feedforward (FF) on benzene purity
  - CS3: PI and Feedforward (FF) on benzene and toluene purity
- Model predictive control represented by two (2) scenarios:
  - CS4: Model developed by System Identification with measured disturbance
  - CS5: Model developed by linearization with Aspen Dynamics (CDI)

CS1: Performance evaluation of PI control

The dotted line presents the control response for a step decrease of 10% of feed flow, while the solid lines represent an increase of 10% of feed flow. The PI-control structure consists in basic inventory control loops (e.g., two (2) level controllers for reflux drum and sump and one (1) overhead pressure controller) and two (2) composition controllers on the product purities.

In Figure 3 the dynamic results of CS1 are presented for the input and output variables considering a feed disturbance of ±10% of feed flow. Prior triggering the feed disturbance a

hold time of 1 hour is maintained with the nominal values for the distillation column. The product purities reach in approximately 3 hours a new steady-state and the reboiler duty and reflux rate reject nicely the feed perturbation with less than ±9% deviation from their nominal value. The fluctuations of product purities are less than 0.5 %, the highest corresponding to the toluene purity.

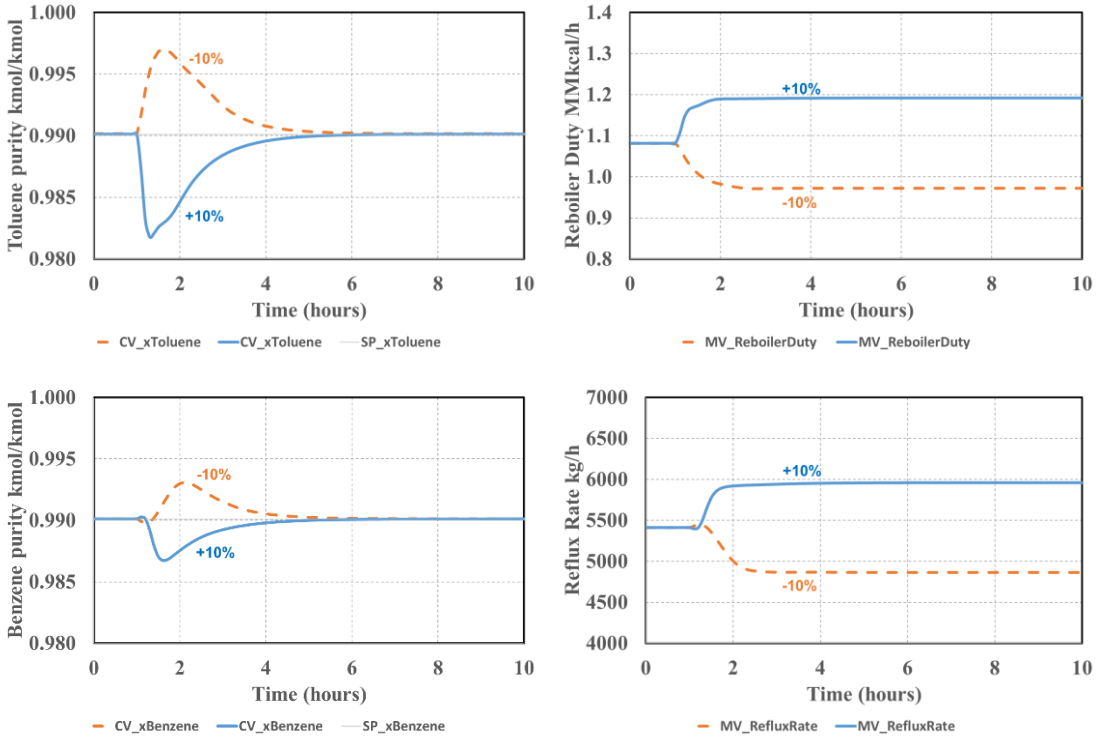


Figure 3. Dynamic response of benzene-toluene distillation column for ±10% of feed flow disturbance (PI control)

CS2: Performance evaluation of PI control with feedforward on benzene purity

In addition to the previous control structure, a feedforward strategy for benzene composition is included to improve the control performance. The result consists in a slightly lower deviation than conventional PI, in the range of 0.2% for benzene purity. The control response is slightly slower compared with the CS1, hence in approximately 4 hours the new steady-state is reached. The results are presented in Figure 4 for the controlled and manipulated variables.

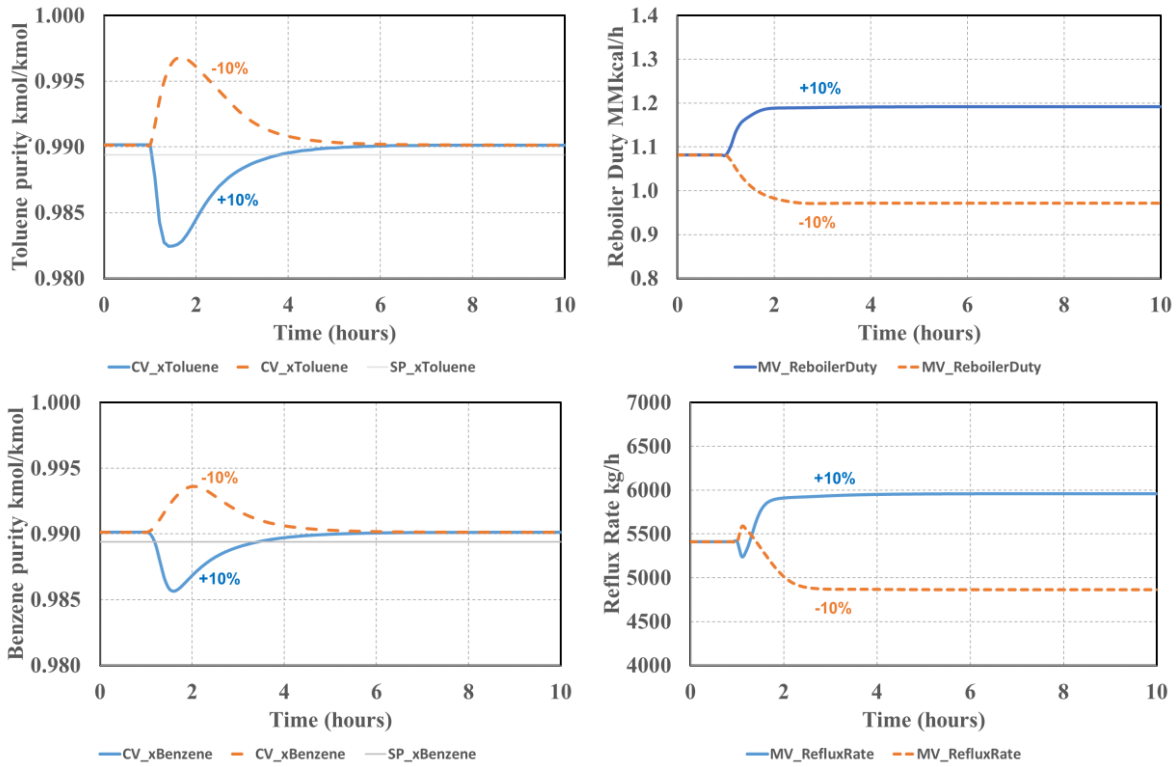
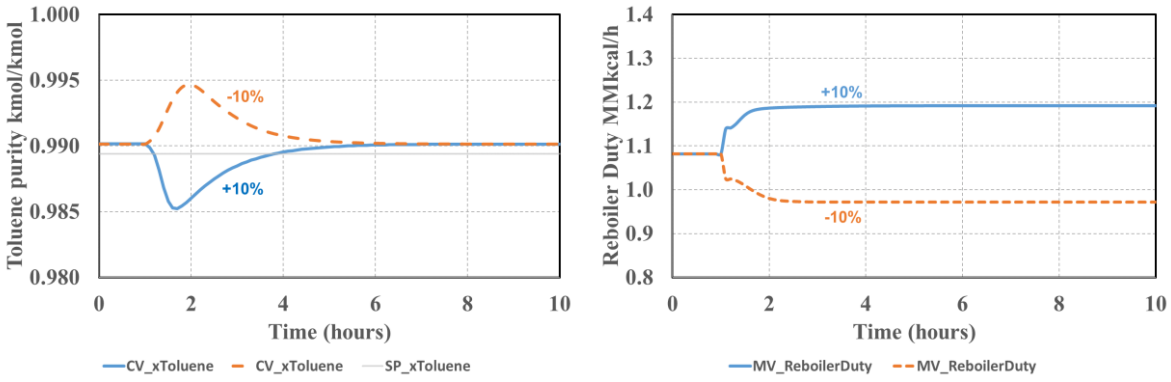


Figure 4. Dynamic response of benzene-toluene distillation column for ±10% of feed flow disturbance (PI control and FF on benzene purity)

CS3: Performance evaluation of PI control with feedforward for benzene and toluene purity

The control response is similar for the product compositions, whereas toluene purity is adjusted in less than 3 hours since the feed step changes. Moreover, the deviations for toluene purity are considerable low, with less than 0.1% deviation from the nominal value. The manipulated variables (reboiler duty and reflux rate) are nicely adjusted to reject the feed perturbation and reach steady-state in less than 1 hour. (Figure 5)



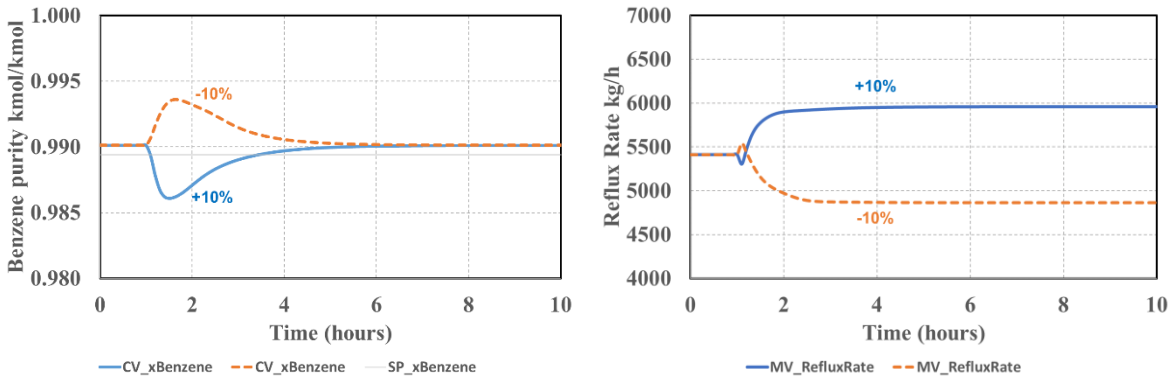


Figure 5. Dynamic response of benzene-toluene distillation column for ±10% of feed flow disturbance (PI control and FF on benzene and toluene purity)

CS4: Performance evaluation of MPC by System Identification with measured disturbance (MD)

In the model development, the feed flow is included in the distillation column process model as a measured disturbance (MD). The identified model incorporated in the model predictive controller shows a deviation in product purities in the range of 0.4% with a modest control performance, being required approximately 5 hours to adjust the controlled variables to their setpoints. The manipulated variables (MVs) reach the new steady-state in approximately 3 hours.

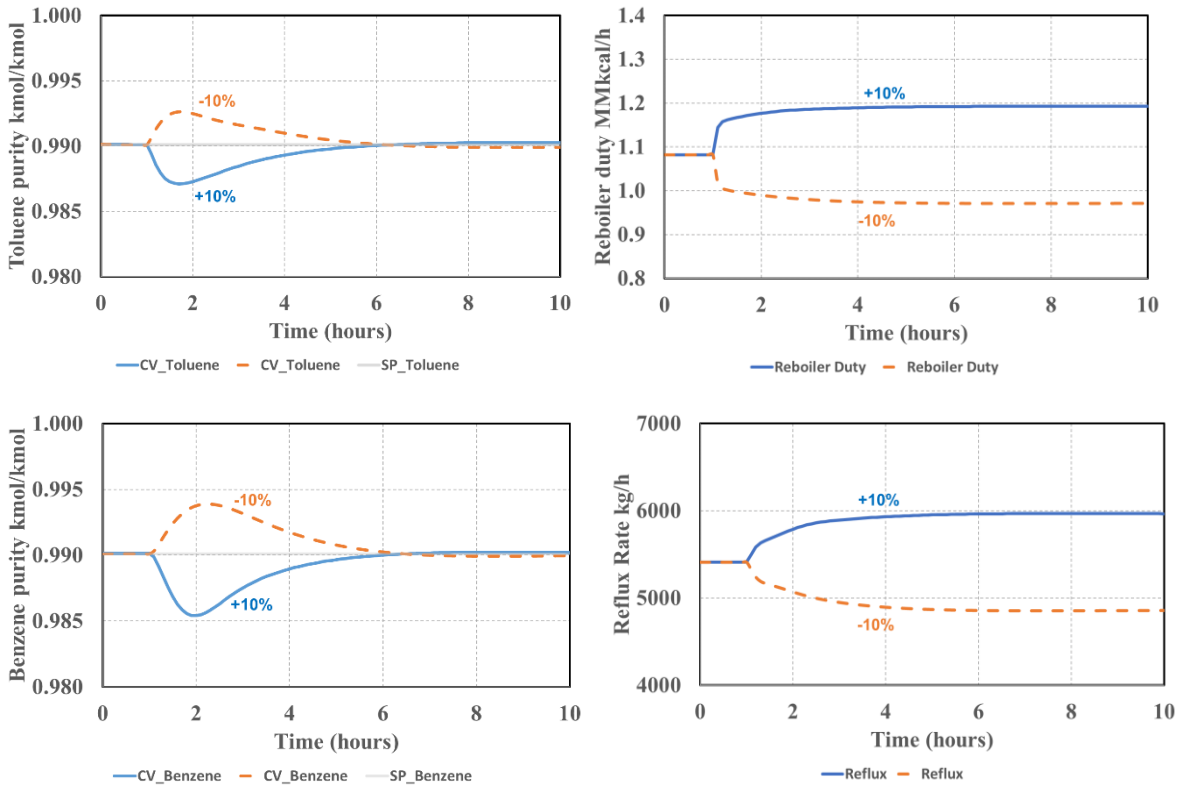


Figure 6. Dynamic response of benzene-toluene distillation column for ±10% of feed flow disturbance (MPC by System Identification)

CS5: Performance evaluation of MPC with Aspen Dynamics linearization

The model predictive control achieves a very good performance being able to adjust the product purities with very little deviations under < 0.1% and the control response is very fast since the feed perturbation occurs.

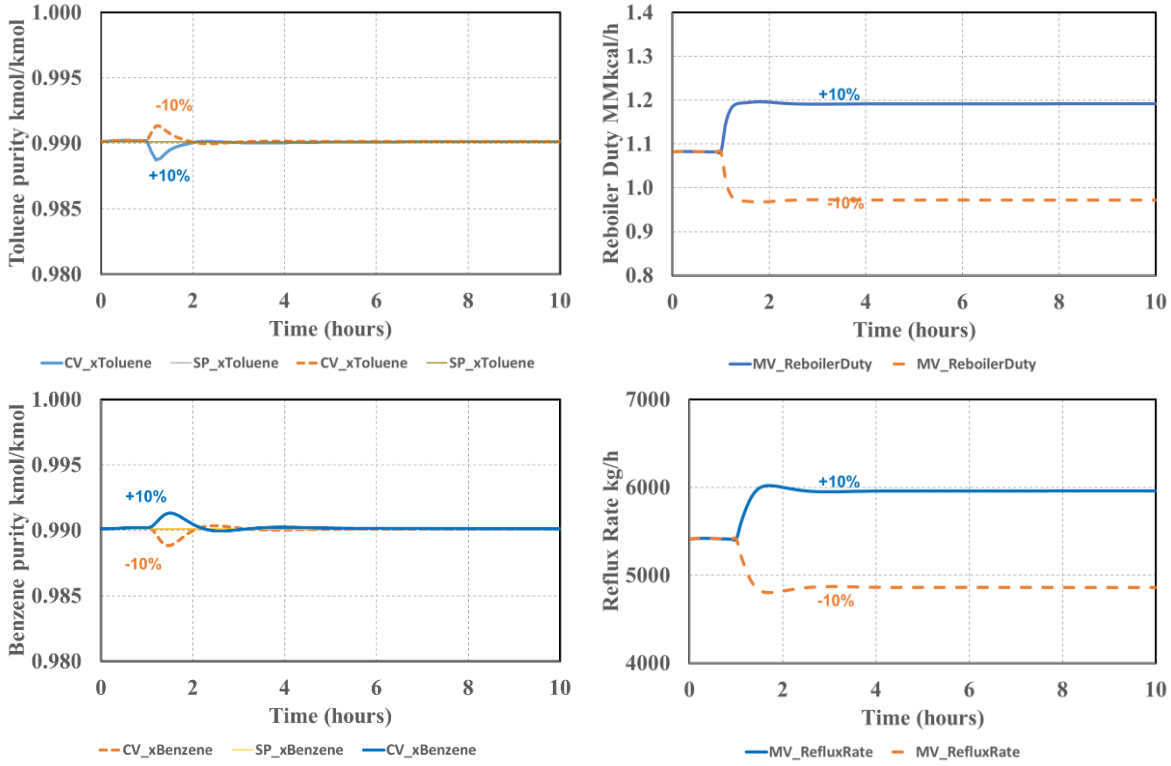


Figure 7. Dynamic response of benzene-toluene distillation column for ±10% of feed flow disturbance (MPC by Aspen Dynamics linearization)

Performance evaluation between conventional control and Model Predictive Control

In Figure 8 through Figure 11 the dynamic responses for each of the five (5) control structures are compared with respect to the product purities.

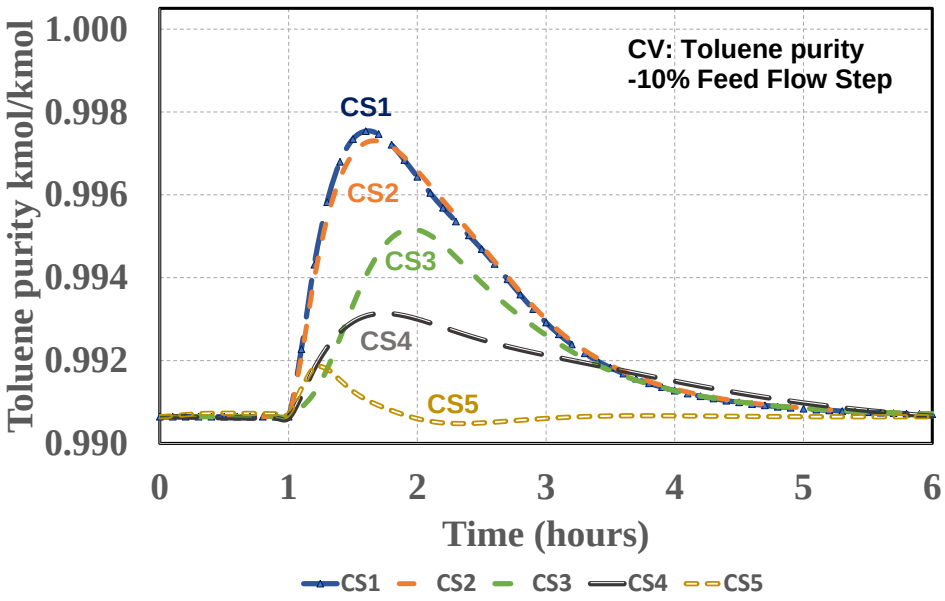


Figure 8. Results of dynamic responses for toluene purity at -10% feed flow step change

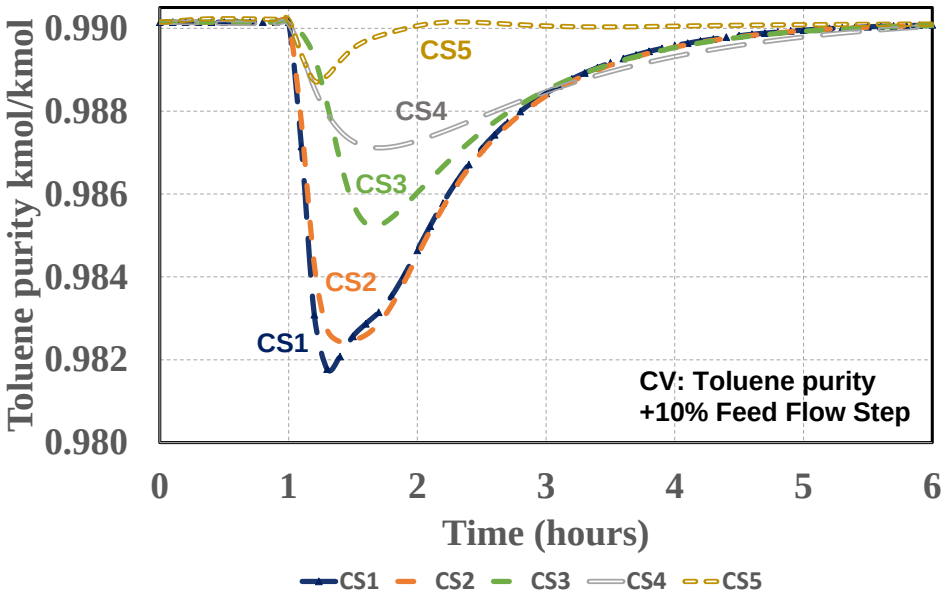


Figure 9. Results of dynamic responses for toluene purity at +10% feed flow step change

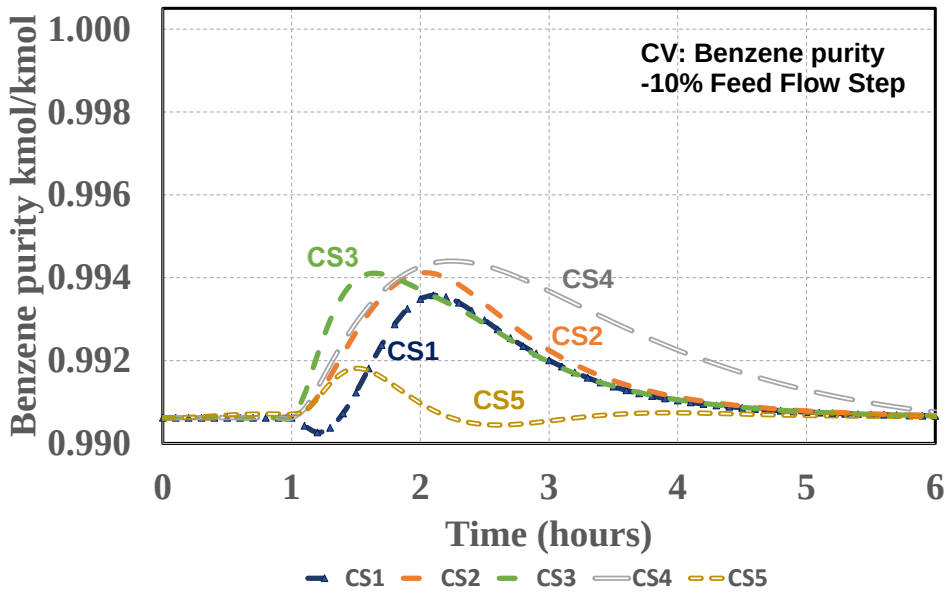


Figure 10. Results of dynamic responses for benzene purity at -10% feed flow step change

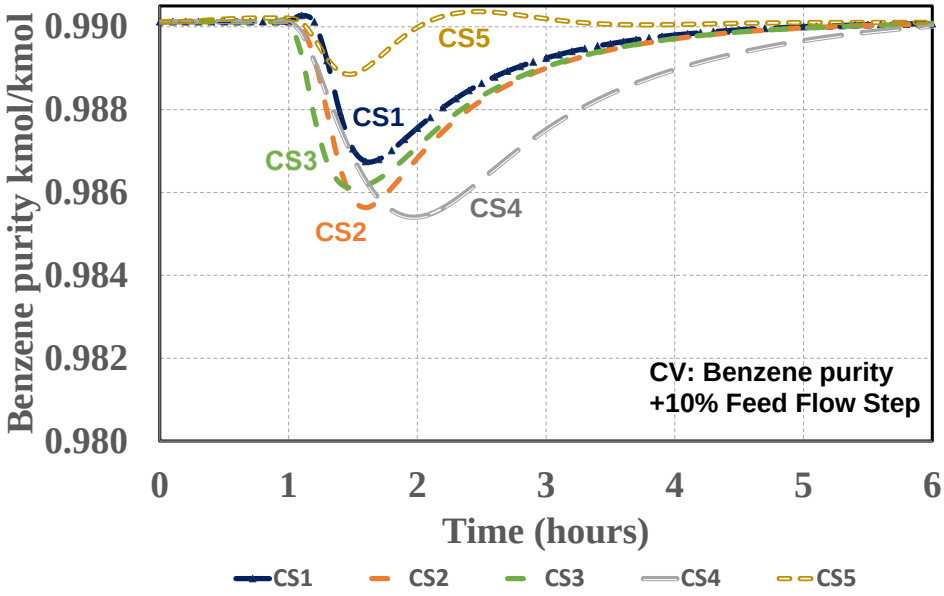


Figure 11. Results of dynamic responses for benzene purity at +10% feed flow step change

The results from the dynamic responses of toluene purity with respect to feed variation show a progressive improvement in the control structures from conventional PI to the more advanced control structures. Somehow unexpectedly, the dynamic responses of benzene purity do not reflect the same performance as for toluene, and seems to illustrate a more performant control in adjusting the benzene purity with the simple implementation of conventional PI (CS1) in comparison with the other three control strategies (3), (e.g., CS2, CS3, CS4). In both cases, the MPC designed with the model linearization from Aspen Dynamics, represented by CS5, proved to be the most efficient.

The control structures mentioned above are evaluated by employing several calculation methods for characterizing the system performance and identifying the most performant control structure.

The mean square error loss (MSE) is calculated for the product purities with respect to each control structure to illustrate the performance and control response for the same feed disturbance, hence ±10% of feed flow. The control performance is assessed using the MSE for each individual control structure.

The mean square error loss represents the sum of the squared difference errors between the predicted and actual output values, in this case the product purities, divided by the number of data points.

The integral square error (ISE) represents another measure of evaluation of the system performance by integrating the square system error over the sample time (fixed interval of time).

In industrial practice, since is highly important to maintain the product qualities and not overshoot or even worse to generate off-spec product, the control performance is evaluated by the maximum deviation for the controlled variables, here denoted peak error, PE.

Although, the maximum peak error, PE, identifies the maximum deviation, no information related with the fluctuations or ability to achieve the set point is provided, hence one other common method to evaluate the control response and accuracy is given by, the integral absolute error, IAE.

The IAE determines the sum of areas above and below the target (set point), such as it penalizes all errors equally regardless of direction.

Table 2. Control performance results for toluene purity specification (time=20 h)

Toluene	CS1		CS2		CS3		CS4		CS5	
	+	-	+	-	+	-	+	-	+	-
MSE x 10^{-5}	0.25	0.28	0.27	0.25	0.10	0.11	0.065	0.065	0.003	0.003
ISE x 10^{-5}	5.20	5.70	5.53	5.10	2.20	2.25	1.30	1.30	0.05	0.05
PE x 10^{-2}	0.69	0.83	0.77	0.67	0.49	0.46	0.30	0.25	0.12	0.12
IAE x 10^{-2}	1.20	1.15	1.15	1.20	0.79	0.84	0.76	0.73	0.12	0.15

Table 3. Control performance results for benzene purity specification (time=10 h)

Benzene	CS1		CS2		CS3		CS4		CS5	
	+	-	+	-	+	-	+	-	+	-
MSE x 10^{-5}	0.04	0.04	0.08	0.07	0.07	0.07	0.15	0.15	0.003	0.004
ISE x 10^{-5}	0.87	0.88	1.58	1.41	1.50	1.42	2.92	2.92	0.068	0.077
PE x 10^{-2}	0.30	0.34	0.45	0.35	0.40	0.35	0.30	0.38	0.125	0.121
IAE x 10^{-2}	0.50	0.46	0.62	0.64	0.62	0.64	1.00	1.03	0.124	0.159

The same results are determined mathematically, as illustrated also graphically in Figure 8 through Figure 11. The most performant control structure proved to be the model predictive controller (CS5) designed with Aspen Linearization model.

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Design of 2-butene metathesis unit

As a response to higher demand for propylene, alternative solutions for conversion of low-value by-products to high-value olefins are of interest. Albeit the well-known processes for obtaining propylene, naphtha steam cracking and fluid catalytic cracking, another viable alternative is represented by olefin metathesis.

The 2-butene byproduct, produced from fluid catalytic cracking unit was used as feedstock for the olefin metathesis. On a conceptual design basis, process synthesis by hierarchical approach was applied for several process alternatives for determining the “best” economical process flowsheet, which returned the highest revenue for a fixed flow rate of raw material.

Economical optimization of the unit is investigated, organized in two parts, namely for the preheat section and for the distillation section. The objective function for optimization is the total annual cost, TAC.

Conceptual design of 2-butene metathesis unit

This chapter presents the conceptual design of an olefin metathesis process from 2-butene derived from a FCC unit. This fraction is a low-value by-product, typically, sent to the LPG pool for blending purposes, however in this case; it could be upgraded to a more valuable product. The basis of design related to the feed characterization, stoichiometry, kinetics and thermodynamics will be discussed. The metathesis reaction can be carried on in the presence of tungsten oxide catalyst, converting butenes to valuable olefin products ranging from C2 to C6, particularly propylene.

Several alternative flowsheets of the olefin metathesis process for propylene production will be identified. These alternatives shall be economically assessed using a hierarchical approach. Finally, detailed design of the most cost-effective and promising alternative will be presented.

Identification of flowsheet alternatives

In this case study a low-value feedstock nBB fraction from the FCC unit is considered, composed of 70 mole % 2-butene and 30 mole % n-butane, the latter being an inert species. A feed flow rate of 5.7 t/h C4 fraction was used for all process alternatives evaluated.

The first type of flowsheet evaluates the recycle of un-reacted raw material here denoted as Unit Structure 1 (US1). Several configurations from this group are considered mostly driven by the way the inert is removed. The study of the structure US1a revealed that achieving a high conversion and using a large amount of purge fraction led to higher returns. Consequently, the second category here denoted, Unit Structure 2 (US2) includes alternatives where high conversion levels are targeted, however separation and recycle of the reactant is not pursued due to large costs.

In the following figures, the PRODUCTS stream consists of a group of valuable and market attractive components such as: ethylene, propylene, pentene, hexene; the stream denoted as INERT consists mainly of n-butane. The stream denoted PURGE contains a mixture of butenes and n-butane; the stream BY-PRODUCTS represents a C4 fraction containing butenes without or with inert (Figure 12 and Figure 13, respectively).

Flowsheets with recycle (US1)

In the ***Reactor – Separation - Recycle (US1a),*** the reactor effluent is routed to a separation section. Here, the most valuable components (ethylene, propylene, pentene, hexene) included in PRODUCTS stream are separated and removed from the plant, whereas the reactant is recycled. However, it should be noted that the separation between 2-butene /n-butane (relative volatility 0.9) appears difficult. Specific for structures with recycle, purging a fraction of the recycle containing the inert represents the simplest solution to avoid accumulation of n-butane. (Figure 12)

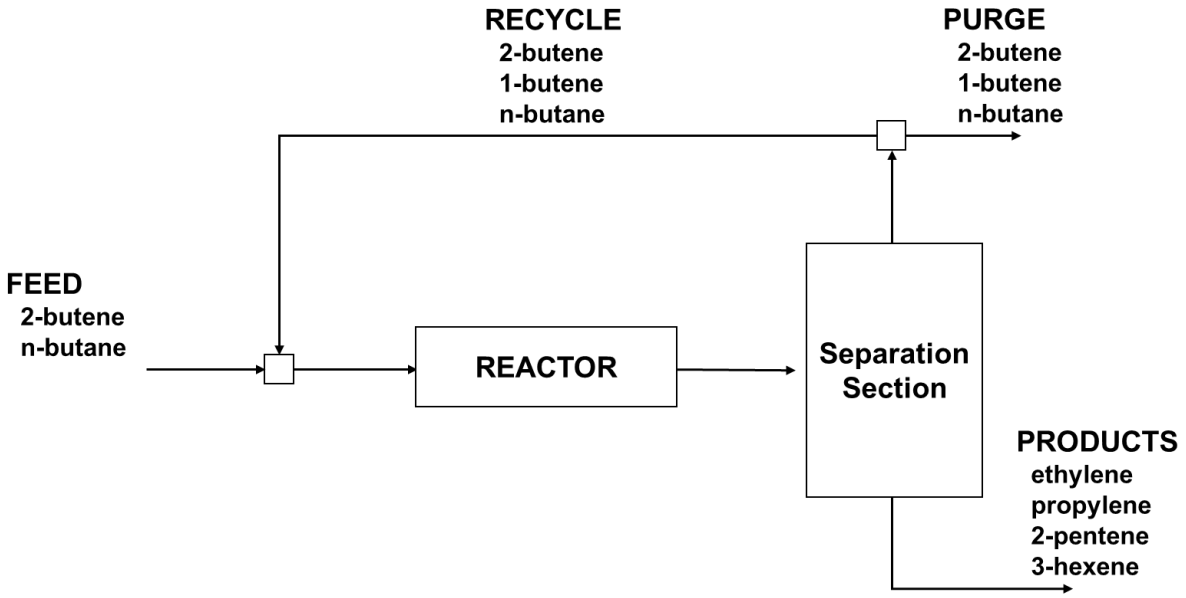


Figure 12. Reactor – Separation – Recycle, with purge (US1a).

One solution to process the useful reactant in the purge is to separate the reactants namely, 2-butene and 1-butene from the inert n-butane. Two possible options are proposed for this separation, as it can be carried out either within the recycling loop or before the recycling loop in the upstream process (Figure 13 and Figure 14).

Reactor – Separation – Recycle (US1b) structure consists in adding a separation unit in the recycle loop to remove the inert from the system (Figure 13).

Reactor – Separation – Recycle (US1c) structure ensures the inert is removed prior entering the plant (Figure 14) and inert accumulation is avoided.

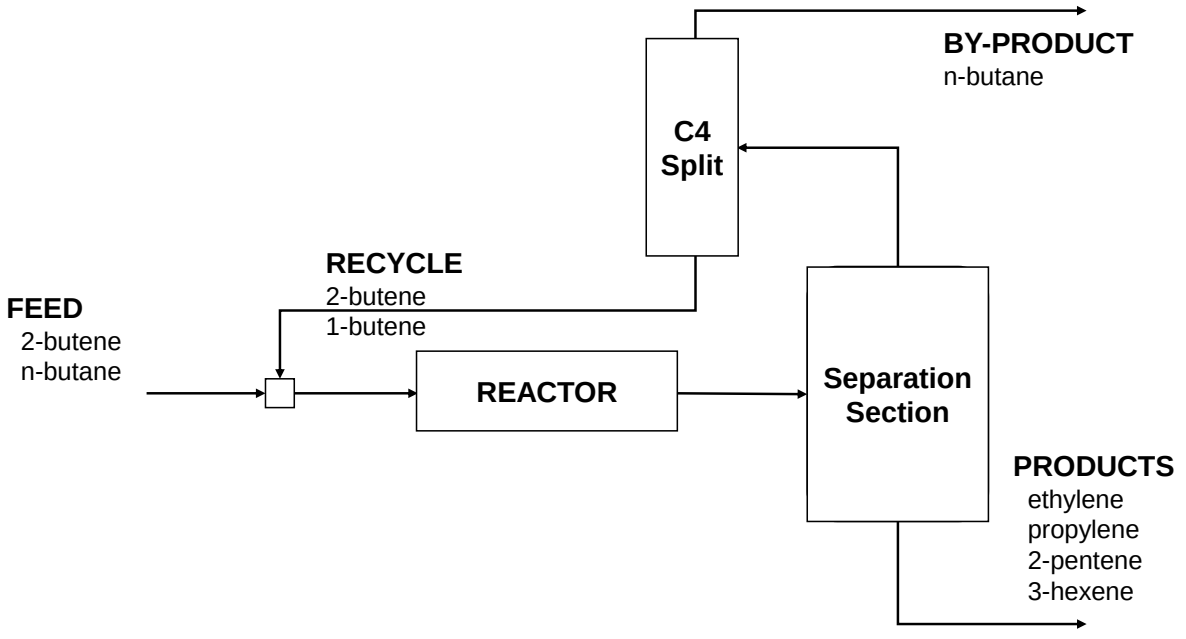


Figure 13. Reactor – Separation – Recycle. The inert is separated and removed downstream of reactor (US1b).

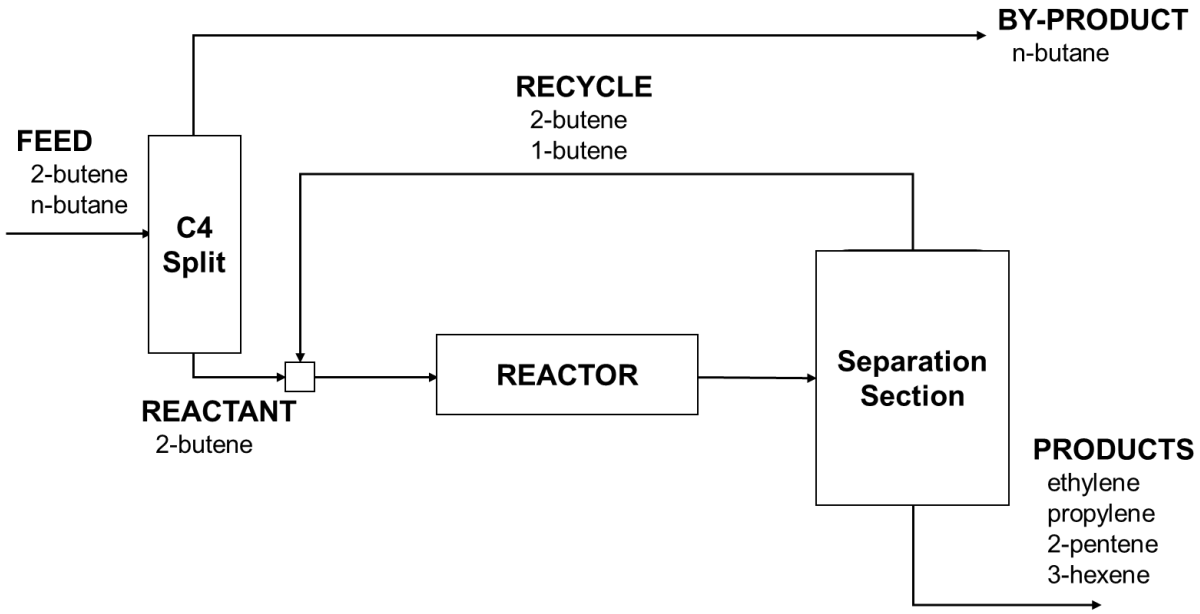


Figure 14. Reactor – Separation - Recycle. The inert is separated and removed upstream of reactor (US1c).

Flowsheets without recycle (US2)

Two alternatives were evaluated for unit structures without recycle (US2).

Reactor – Separation (US2a) structure consists in a simple configuration where the inert is separated upstream of entering the reactor, in this way, overloading the reactor and separation sections is avoided (Figure 15). Regardless of the high cost associated with separation of the inert, this alternative might be economically sound due to the attractive price of the high-purity n-butane (see **Error! Reference source not found.**) and the lower cost of downstream units

Reactor – Separation (US2b), where the inert is passed through the reactor (Figure 16). This is the simplest process alternative.

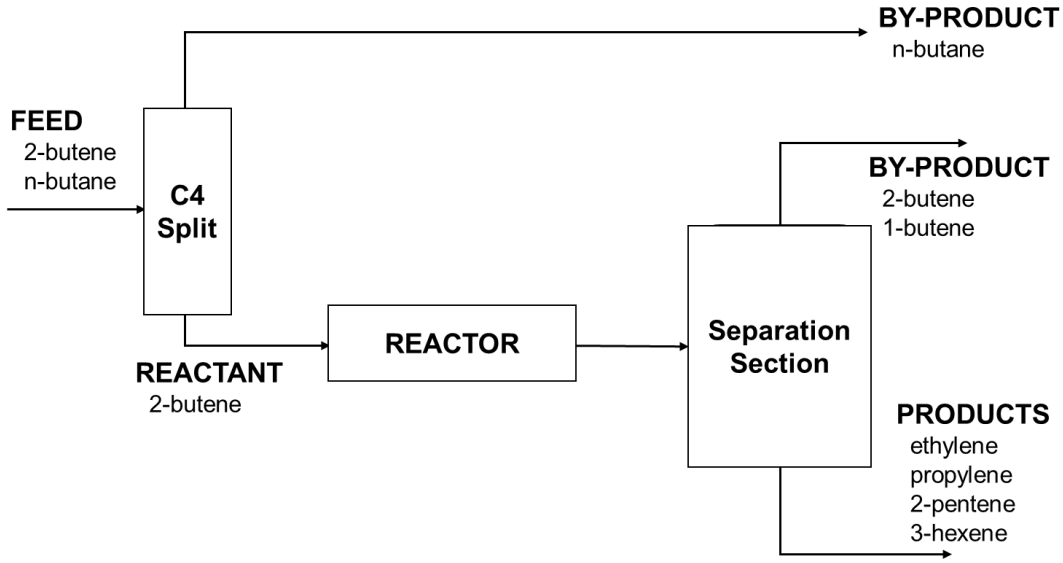


Figure 15. Reactor – Separation, the inert is removed upstream of the reactor (US2a).

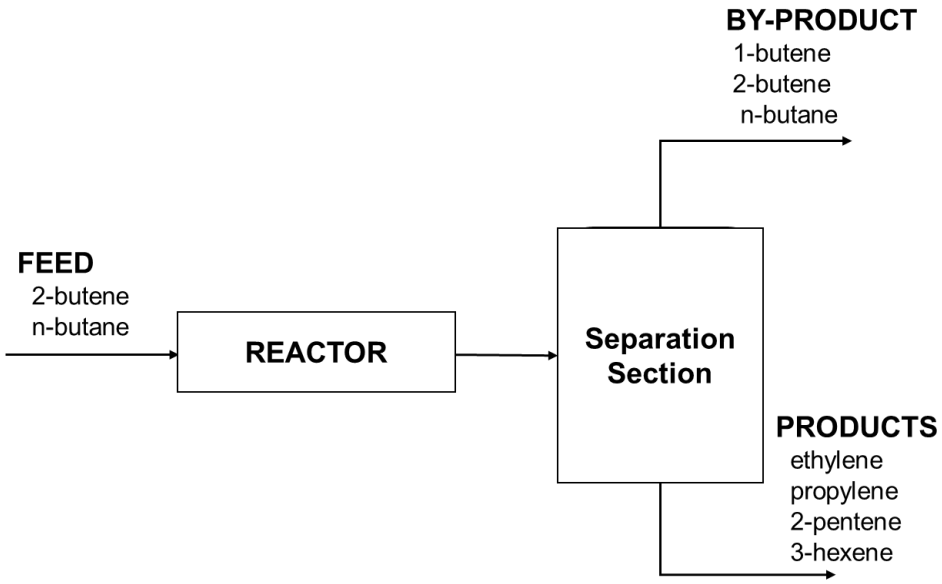


Figure 16. Reactor – Separation (US2b).

Economic evaluation of process alternatives

The first level of screening detail, namely, the input-output analysis revealed that the process could be profitable, since the revenues from selling propylene, the most expensive product, exceed the cost of raw material. When the selectivity of the chemical transformation and the costs associated with the reactor were considered by means of a kinetic reactor model, the optimal conversion value of the reactor was obtained. As expected, the optimal conversion is high, in the range of 90%. Obviously, this value reduces the loss of fresh material with the purge. However, results at this level of analysis were not conclusive enough to allow choosing one alternative. Further details were required by considering the investment and operating costs related to the separation equipment.

Results of economic evaluation of flowsheet alternatives

The process alternatives were assessed in a hierarchical approach (Dimian et al., 2014), in order to determine the most cost-effective solution, the condition was the economic potential EP.

The hierarchical approach scope is to reject the alternatives with low economic potential, in the early stages of conceptual design, focusing consequently only on the most promising alternatives.

Flowsheets with recycle

US1a: Typical Reactor – Separation - Recycle (A + B + I)

Sensitivity study was done for a fixed reactor temperature at 550°C and pressure of 1 bar with constant reactor diameter of 3 meters. As the kinetic parameters were determined in a range of

temperature between 350÷550°C and a pressure of 1 bar, no extrapolation beyond the maximum temperature/ pressure was done. A variable purge fraction, denoted P, was introduced to establish the optimum design with respect to economic potential. The results show, that at given reactor length, higher reactant conversion is obtained by increasing the purge fraction (Figure 17). This can be explained by the fact that the recycle (containing large amounts of inert) decreases both the reactor residence time and reactant concentration.

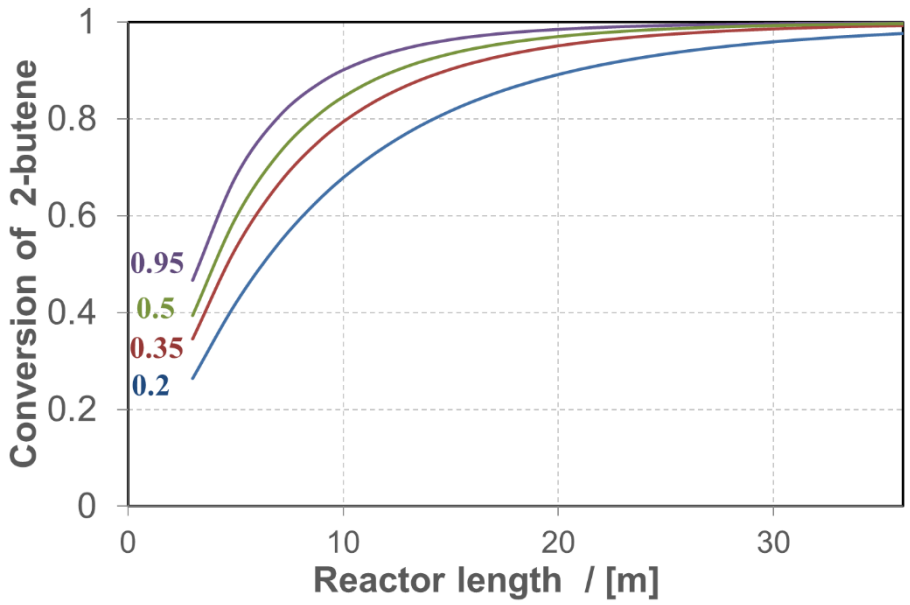
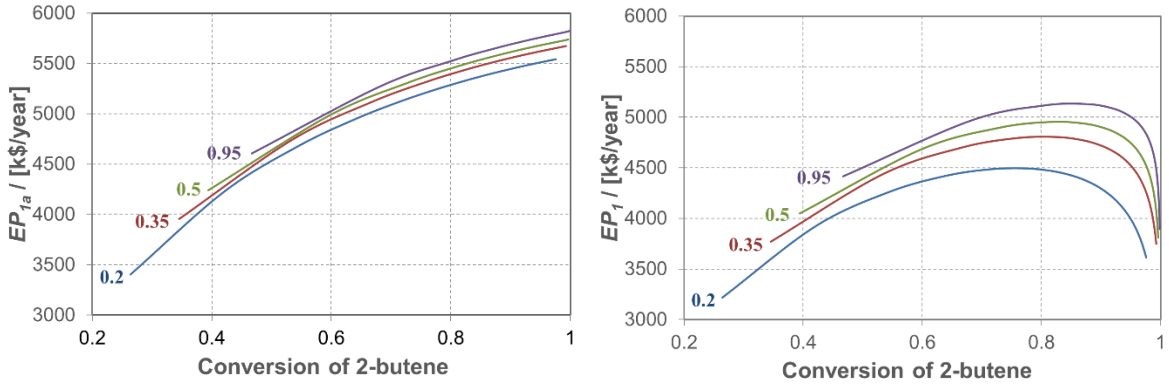


Figure 17. Conversion of 2-butene vs. reactor length (diameter = 3 m), for different values of the purge fraction P.

As more inert is recycled, larger reactors are required to achieve a certain conversion level, with a negative effect on capital expenditures (CAPEX) and operating costs (OPEX). The results from Figure 18 reveal that as purge fraction P is increased the unit is becomes more profitable. One interesting remark was that at the next levels of analysis, the economic potential decreases by more than 50% of the initial EP1a.



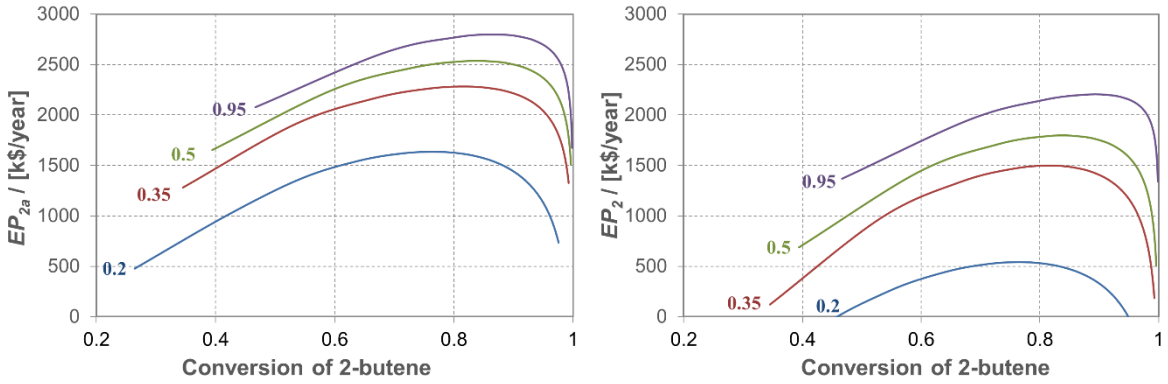


Figure 18. Economic potential versus conversion, at different purge fractions, for US1a

The optimum design with a large purge fraction, P=0.95, returns an economic potential of EP2 = 2250 k$/year while the 2-butene conversion is X_A= 90% for a reactor length of D = 3 m, L_R= 9 m (63.6 m^3). However, for a smaller purge fraction (for example, P = 0.2), the profit reduces considerably from an initial EP1 = 4500 k$/year to EP2 = 500 k$/year at the most detailed level. In other words, the process alternative went from an economical solution to a barely-profitable design.

US1b: Reactor – Separation - Recycle (A+B) with inert separation downstream of reactor

The second alternative assumes the separation of the inert (n-butane) from the reactants in a distillation column downstream of the reaction section. Additional costs for OPEX and CAPEX are expected for this distillation column because the volatilities of the key components are very close. Although the price of the high purity n-butane exceeds the cost of the raw material, the n-butane / 2-butene separation is so difficult that the associated costs exceed the benefit. Results are presented in Figure 19.

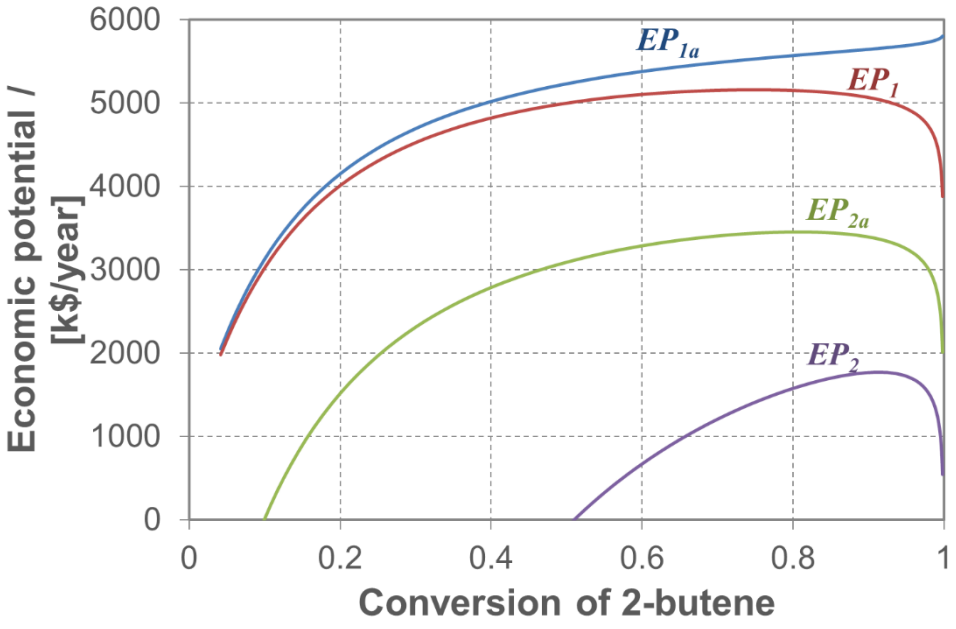


Figure 19. Economical potential vs conversion of 2-butene for US1b

The sensitivity analysis reveals that the addition of another distillation column involves higher costs and affects the final economic potential EP2. The separation of inert (n-butane) and recycling only the reactants (2-butene, 1-butene) does not have a positive effect on overall plant cost, compared with the previous alternative US1a. The optimal design uses a reactor with length L_R= 9 m and diameter D = 3 m, achieving a conversion of X_A=87%. The most detailed level returns a lower economic potential with approximately 21%, (EP2 =1773 k$/year).

US1c: Reactor – Separation – Recycle (A+B), with inert separation upstream of reactor

Compared to the other two options presented above, this case is interesting because the initial separation of inert upstream of reactor could have a positive effect, relieving the following equipment of useless circulation of inert. However, it is also challenging because the separation n-butane / 2-butene is very difficult due to their similar volatilities. When the economic potential was determined for different values of conversion, it was found out (Figure 20) that the structure US1c returns a maximum economic potential (EP2) of only 273 k$/year. The explanation is that the separation of the inert n-butene from 2-butene is very difficult (because of low relative volatility), demanding a large column and high utility consumption.

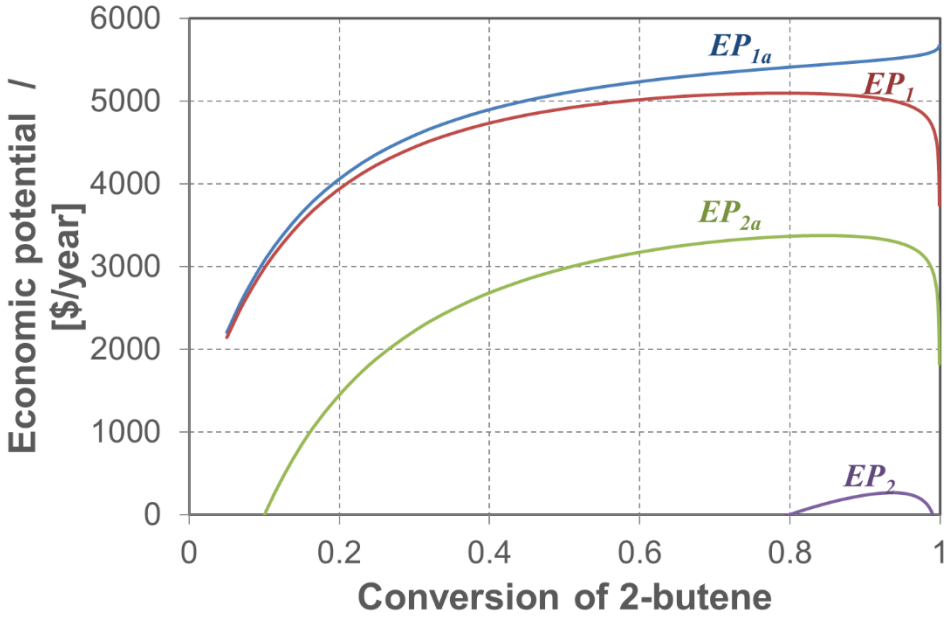


Figure 20. Economical potential vs. conversion of 2-butene for US1c

Flowsheets without recycle

US2a: Reactor - Separation with inert removal upstream of reactor

The process alternative US2a, returns an economic potential (EP2=288 k$/year) similar with the one observed for US1c (273 k$/year). The reason consists in the optimum design for US1c corresponding to a rather large value of the conversion, causing a small recycle which has a low

impact on the revenue. The results are illustrated at different evaluation levels (Figure 21) and show a very comparable outcome with the process alternative US1c.

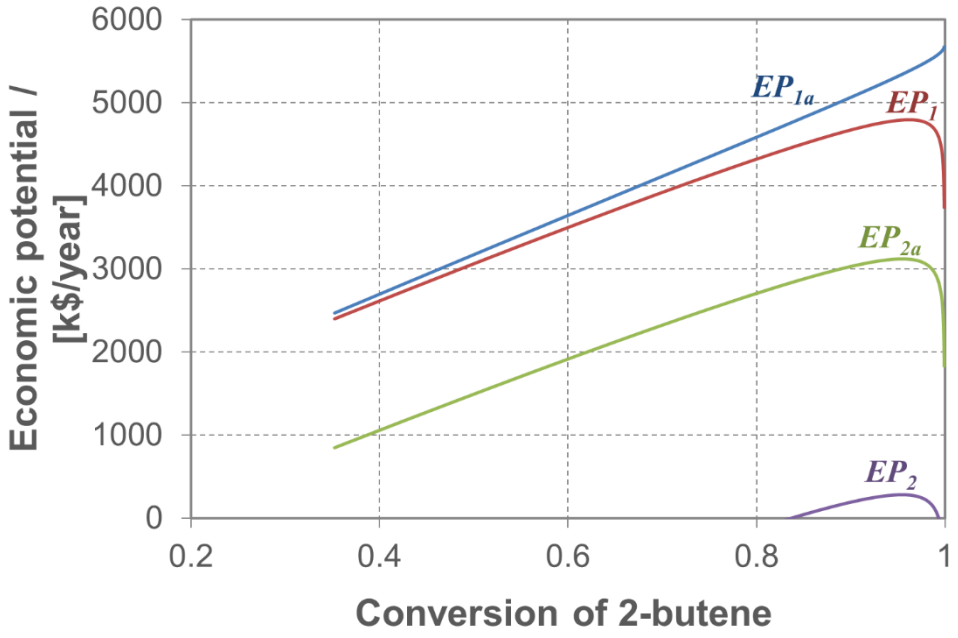


Figure 21. Economic potential vs conversion of 2-Butene for US2a

US2b: Reactor - Separation

For the once-through configuration without recycle, the economic potential at different decision levels was plotted on a single graph (Figure 22) to reveal the impact of various costs. The decline of economic potential is progressive and steady for EP1, and EP2a similar with the other alternatives already described. The largest impact is when the cost of separation equipment is taken into account in the economic analysis, with almost 50% reduction of revenue. Finally, adding the utilities results in a reduced economic potential, which is reflected in EP2.

Somehow unexpectedly, it turns out that this process alternative is the most profitable one, giving 2300 k$/year. Note that this value is consistent with the value obtained for alternative US1a (Reactor – Separation – Recycle) where the inert was removed by means of an extremely large purge (95% purge fraction).

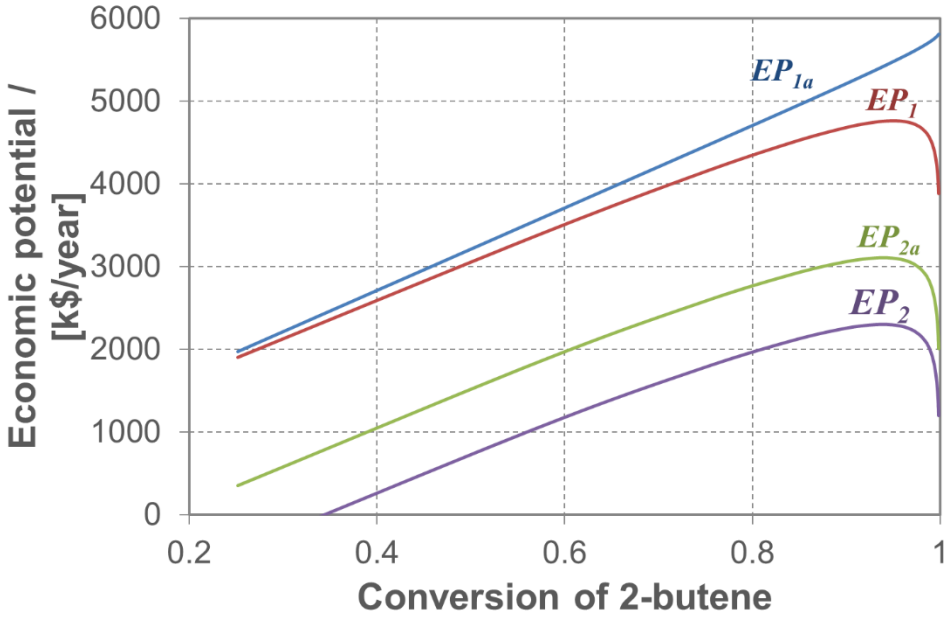


Figure 22. Economic potential vs conversion of 2-butene for US2b

The rate of return of investment (ROI) was calculated to express the annual profit generated by the capital invested.

$$\%ROI = \frac{Annual\ net\ profit}{Invested\ capital} \cdot 100\% = \frac{EP2}{CAPEX} \cdot 100\% \qquad (0.4)$$

The summary with the optimum points from the economic analysis for the five different flowsheet alternatives studied are presented in Table 4. The largest ROI (35%) is returned by the Reactor – Separation flowsheet US2b.

Table 4. Results of the optimal flowsheet solutions for the olefin metathesis process

	US1a (P = 0.95)	US1a (P = 0.2)	US1b	US1c	US2a	US2b
Optimal conversion XA	90%	80%	87%	92%	96%	93%
Economic potential EP2 / [k$/year]	2250	500	1773	273	288	2300
Return of investment ROI	32%	7%	26%	4%	4%	35%

Details of the Reactor – Separation flowsheet

The simplified process flow diagram (Figure 23) for the most economical solution US2b reveals the major equipment considered in the process synthesis analysis by hierarchical approach. A preliminary sizing was performed for the main equipment considering process guidelines and technical literature. The unit mass balance is reported in Table 5.

Table 5. Mass balance for "best" process alternative US2b

OLEFIN METATHESIS PROCESS – MASS BALANCE									
Stream	U.M	S1	S2	S3	S4	S5	S6	S7	S8
Temperature	°C	40	450	550	511.7	149.7	50	207.8	50
Pressure	bar	7	6.5	1.2	1.15	1.05	1.05	31	31

Vapor Frac		0	1	1	1	1	1	1	0
Mole Flow	kmol/hr	100	100	100	102.5	102.5	102.5	102.5	102.5
Mass Flow	kg/hr	5671	5671	5671	5671	5671	5671	5671	5671
Mole Fractions									
2-Butene		0.7	0.7	0.7	0.065	0.065	0.065	0.065	0.065
1-Butene					0.042	0.021	0.021	0.042	0.042
Propylene					0.242	0.259	0.259	0.242	0.242
2-Pentene					0.191	0.209	0.209	0.191	0.191
Ethylene					0.1	0.117	0.117	0.1	0.1
3-Hexene					0.07	0.092	0.092	0.07	0.07
n-Butane		0.3	0.3	0.3	0.29	0.29	0.29	0.29	0.29

OLEFIN METATHESIS PROCESS – MASS BALANCE									
Stream	U.M	S9	S10	S11	S12	S13	S14	S15	S16
Temperature	°C	-15	140	40	154	40	112.7	40	40
Pressure	bar	32	34.2	25.5	25.5	6.5	7.5	2.5	3.5
Vapor Frac		0	0	0	0	0	0	0	0
Mole Flow	kmol/hr	12.0	90.5	26.5	64	32.8	31.2	21.74	9.42
Mass Flow	kg/hr	337	5334	1118.2	4215.3	1901.3	2314	1520.9	793.1
Mole Frac									
2-Butene		<0.01	0.01	<0.01	0.014	0.019	<0.01	<0.01	<0.01
1-Butene		<0.01	0.024	<0.01	0.034	0.067	<0.01	<0.01	<0.01
Propylene		<0.01	0.294	0.99	<0.01	<0.01	<0.01	<0.01	<0.01
2-Pentene		<0.01	0.236	<0.01	0.335	<0.01	0.687	0.99	<0.01
Ethylene		0.99	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
3-Hexene		<0.01	0.104	<0.01	0.147	<0.01	0.303	<0.01	0.99
n-Butane		<0.01	0.331	<0.01	0.469	0.913	0.01	<0.01	<0.01

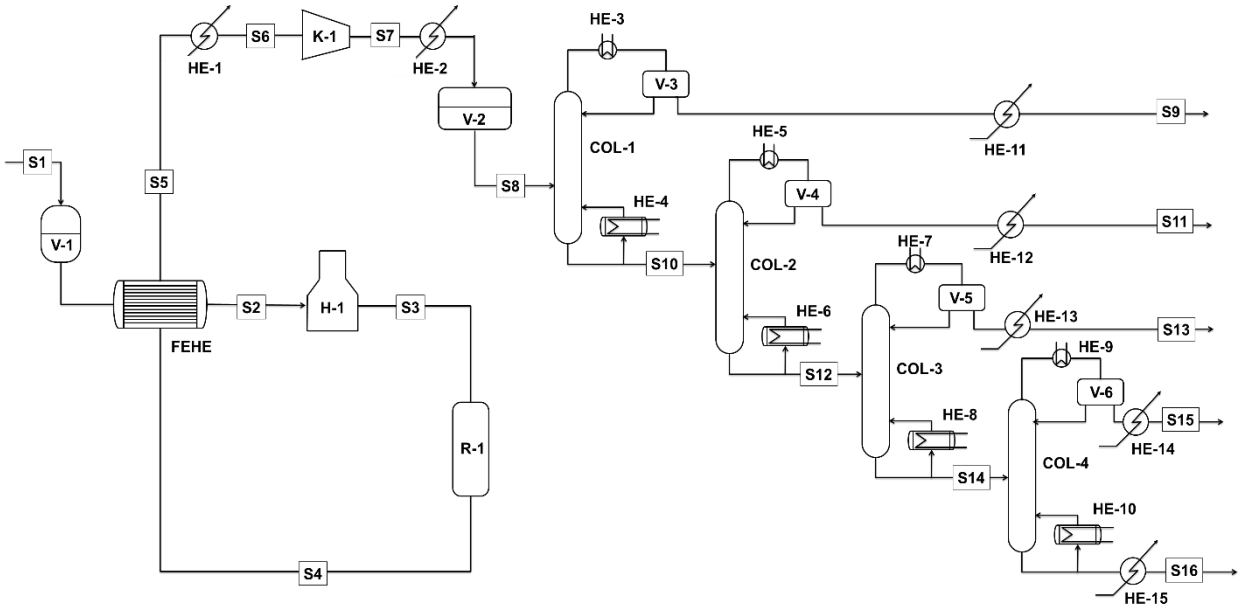


Figure 23. Process for metathesis of 2-butene, flowsheet US2b

Economical optimization of the unit

Firstly, the feed preheat section is evaluated, consisting in feed effluent heat exchanger (FEHE), furnace heater and reactor for selecting the most economical inlet temperature in the heater with respect to total annual cost, TAC. For the system comprised of feed effluent heat exchanger (FEHE), furnace (H1) and reactor (R1), the objective was to select the most economical inlet temperature of the heater with respect to total annual cost, TAC. The same concept for payback period applies, that is 3 years.

Typically, in engineering companies the payback period is set considering the investment value required for the project. For projects below 10 million of U.S dollars the payback period is set to 3-5 years. Particularly, for this case, the conservative payback period of 3 years was set considering several factors that might augment the total annual cost of the unit above the calculated (estimated) TAC. These additional costs consist in constructions activities, instrumentation and control, piping, commissioning activities etc.

The variables for optimization are the heat transfer area of the FEHE and the duty of heater, which involves two effects, one on the capital expenditures regarding the size of the heater and FEHE, and the other one on the operating expenditures reflected in the fuel gas consumption

The sensitivity calculations were determined in Aspen Plus with cost equations edited in FORTRAN. It turns out that the minimum total annual cost of TAC= 305 k$/year is achieved for an inlet furnace temperature of T_{in}= 450°C.

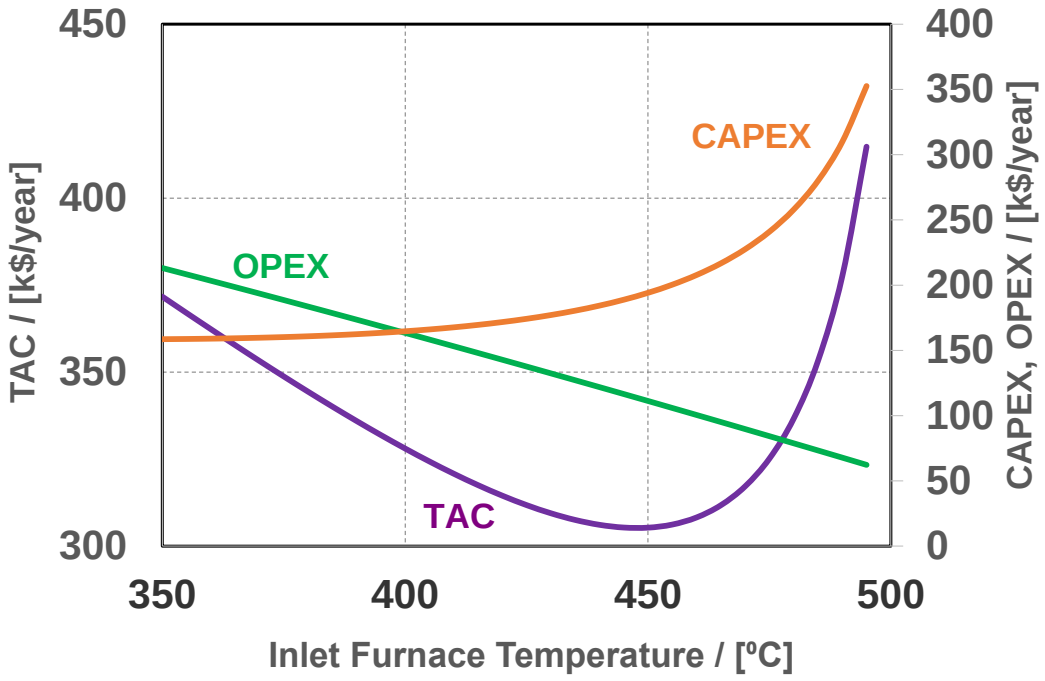


Figure 24. Furnace inlet temperature versus TAC, OPEX, CAPEX

Secondly, the optimization study is shifted towards the highest energy consumers namely, the high purity distillation columns. The simplified process flowsheet (Figure 25) shows the sections considered for the optimization study. The column optimization consisted in determining the minimum TAC with respect to several targets such as: column overhead pressure, feed temperature, number of stages for distillation column, feed location, side

condensing or side reboiling. Cost equations implemented in FORTRAN from Aspen Plus supported the economic calculations.

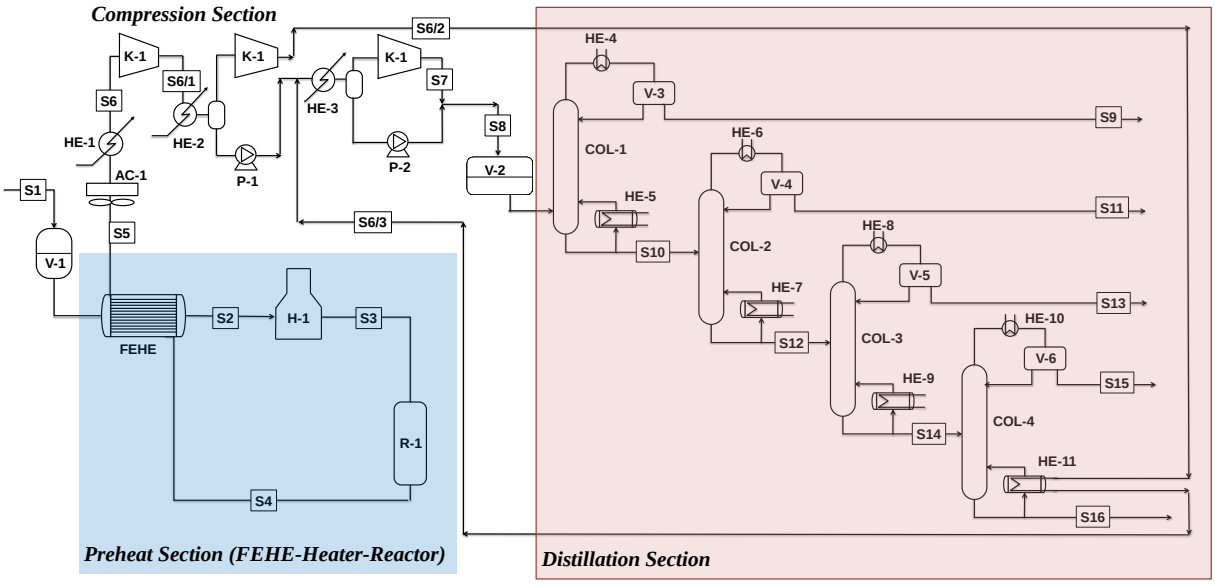


Figure 25. Simplified flowsheet of 2-butene olefin metathesis process

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Process control of 2-butene olefin metathesis

This chapter presents the assessment of the dynamic behavior and the control system response of the 2-butene olefin metathesis process, using flow-driven dynamic simulation performed in Aspen Dynamics. Two different control strategies are applied on the 2-butene olefin metathesis unit, namely, conventional feedback control and model predictive control. The steps for developing the control structures and the controllers tuning are discussed. The transient behavior of the reactor-separation plant to throughput variations of +/-10% is evaluated for the conventional feedback control. The results are presented in a graphical form.

The linear model predictive controller (LMPC) is configured on a supervisory level acting directly on the regulatory controllers via the co-simulation between Aspen Dynamics and Simulink/ MATLAB. The performance of the model-based control strategy is compared with open-loop response from the dynamic unit through several efficiency indexes (MSE, ISE, PE and IAE). The product flow targets for the most expensive products (e.g., ethylene and propylene flow) are adjusted by LMPC. The linear model predictive controller outperforms the feedback controller.

Conventional process control

Control structure description

The dynamics and control of the plant was assessed using flow-driven dynamic simulation from Aspen Dynamics. The basic controllers were automatically added from Aspen software, however for good control of the unit, other controllers were added to improve the controllability of the plant. The feed mixture consists of one single stream, routed to the reaction section, passing by the feed effluent heat exchanger (FEHE) and furnace. The reactor inlet temperature is adjusted in reverse action by the heater duty via a temperature controller. Since the reaction conditions require a low pressure and high temperature, namely P=1.0 bar and T=550ºC, the effluent stream is entirely in vapor phase; hence, a compressor is required to ensure the flow of reactor products to the separation section. Similar with other typical designs, part of the reactor effluent heat is recovered by preheating the feed stream, with the FEHE, and subsequently further cooled to ensure safe temperature condition to the inlet of the compressor. That being said, a temperature controller is positioned upstream of the air cooler of the compressor, to maintain a proper inlet temperature by adjusting the duty of the air cooler and water cooler in reverse action. Prior reaching the separation section, the heat resulted from the power of compression is partially recovered in the de-pentanizer reboiler (HE-11), outcome resulted from the heat integration analysis. This amount of heat duty provided to the reboiler is constant. The compressed reactor effluent is routed to the distillation section for purification purposes.

In the distillation section, each column contains one pressure and two-level loops for inventory control; thus, all four columns are equipped with pressure controller on the condenser and level controllers for sump and reflux drums. All reflux drums and column sump are sized to provide sufficient holdup when level is at 50% full in steady state conditions. As expected, the pressure is controlled in reverse action by the condenser duty, whereas the liquid hold-ups are maintained in direct action by their corresponding level controllers via the product flowrates. This approach for level control is best suited for relatively small reflux ratios (L/D) and boil-up ratios (V/B) (Skogestad, 2007).

The first distillation column is designed to separate the ethylene from the reactor effluent, on the overhead. The specification of the ethylene product is kept by indirect composition control, hence via a temperature controller provided on Tray 7, which manipulates the reflux rate in direct action. It should be noted that the location for all temperature-control trays is based on the “sensitivity criterion”, where the largest change in temperature for a change in the manipulated variables is observed, either reflux ratio or reboiler duty.(Luyben, 2006).

Since there are four distillations columns in series, and each of the distillate flows requires a relatively high purity product, it is imperative to prevent the light product carryover in the bottoms flow. A combination of cascade control via a composition control (XC) and temperature control (TC) is employed. Similarly, to industrial practice, the composition controller inherits a 10 minute delayed response from the process, in the form of a dead time, and the results are displayed once at 10 minutes. The temperature controller is responding faster

at any change of composition on the distillation column tray in reverse action on the reboiler duty to maintain the impurity level to the desired value, until the composition controller (XC) receives the new set of data and updates the set point of the TC accordingly. In this way is prevented any alteration of the bottoms composition such that the subsequent distillate composition remains on specifications.

Particularly, the HE-11 reboiler duty from COL-4, receives a constant heat duty from the compression work generated for the pressure increase of the reactor effluent and the remainder through low-pressure steam.

The same control strategies is applied for the remaining distillation columns.

The simplified flowsheet of the unit with control valves is illustrated below and discussed in the next chapters.

The algorithms employed for the controllers are conventional PI, except for the level loop. All level controllers, for the reflux drums, the sumps of the columns, the feed vessels and the reactors are P type controllers with a gain of 1 %/%. The ranges for the controlled and manipulated variables for level controllers were set to twice the nominal value.

The general rules of thumbs are applied, with controller gain values (KC) for most of the loops of 1%/% (%OP range / % PV range). The integral time, Ti is recommended to be in the same range as the time constant of the process (Dimian A., 2004).

Composition controllers are tuned by running relay-feedback test, with the Tyreus-Luyben tuning rule.

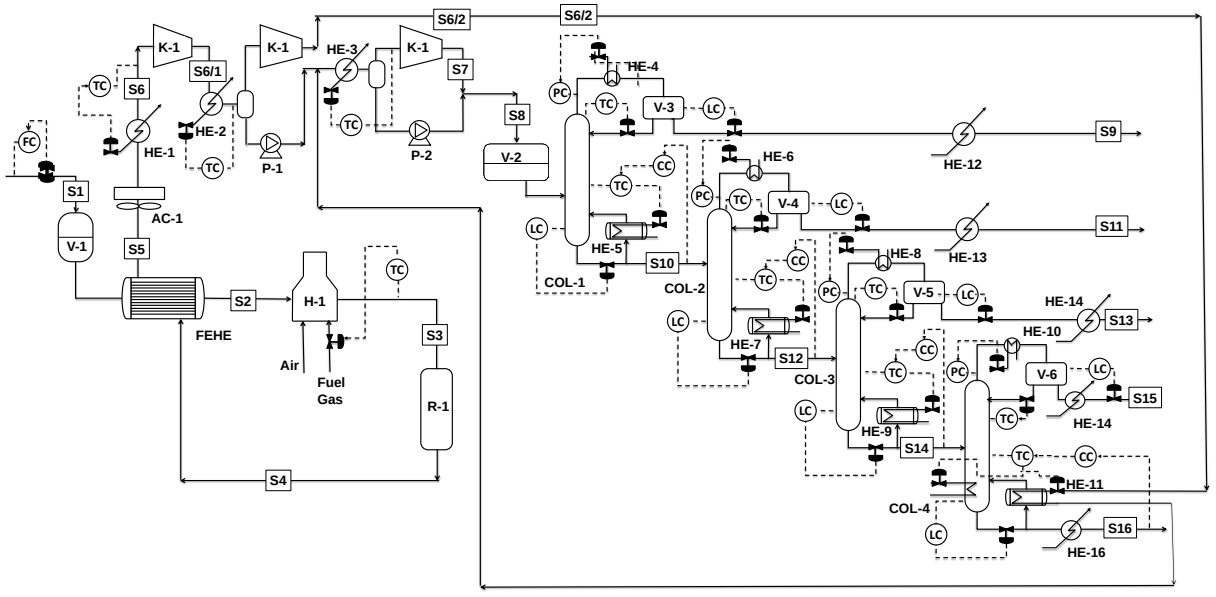


Figure 26. Metathesis process of 2-butene – flowsheet and plantwide control

Plantwide dynamic response of the unit

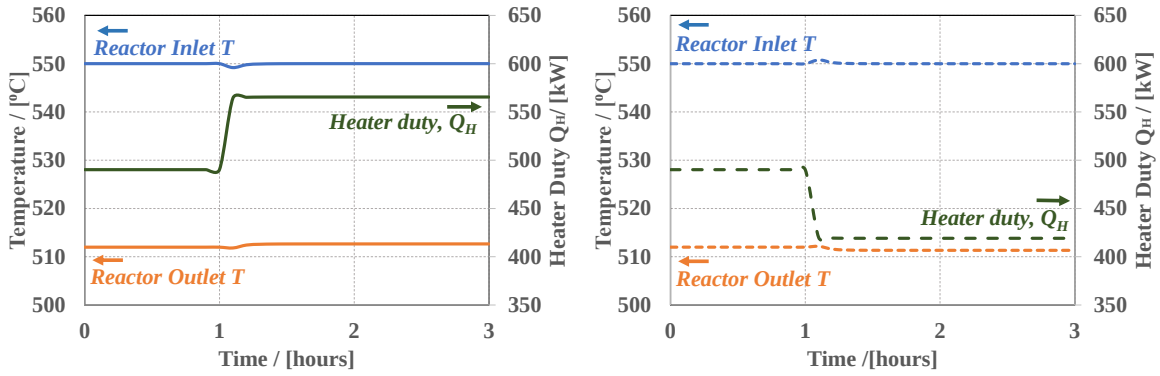
The dynamic controllability and flexibility of the plant was investigated by considering the molar feed flow as disturbance.

The reactor dynamic response and stability was investigated to feed flow (FF) variations of ±10%. Results are shown in Figure 27 where the solid lines represent 10% increase in feed flow and the dashed line are 10% decrease of fresh feed flow. The nominal steady state was kept for 1 hour, and then the feed flow disturbance followed. The reactor inlet temperature (550ºC) was maintained nicely by the TC loop adjusting the heater duty accordingly. It can be remarked that the control system was capable to bring the process to a new-steady state in a couple of minutes since the disturbance, with a reactor outlet temperature variation of less than 1ºC at +/-10% feed flow variation with the same reactor inlet temperature. As expected, the 2-butene conversion initially at $x_{2B/P}$ =90.4% increased to 92.2% with lower feed rate (e.g., -10%FF) and reacted in the opposite direction at higher feed rate (e.g., +10%FF) with the same conversion deviation, hence 88.5%.

The variation of yield (η) was studied considering propylene (C3) as the product of interest, and 2-butene as reactant.

$$x_{2B} = 1 - \frac{F_{2B,in}}{F_{2B,out}}$$
$$\eta_{C3/2B} = \frac{F_{C3}}{F_{2Bin}} \qquad (1.1)$$

Where, $F_{2B,in}$ and $F_{2B,out}$ represents the 2-butene molar flows at the inlet and outlet of the reactor, and F_{C3}, represents the reactor effluent molar flow of propylene. More fresh reactant ($F_{2B,in}$) fed into the system decreases the yield ($\eta_{C3/2B}$) with approximately 0.5%, with the reverse effect for the reduction of fresh reactant.



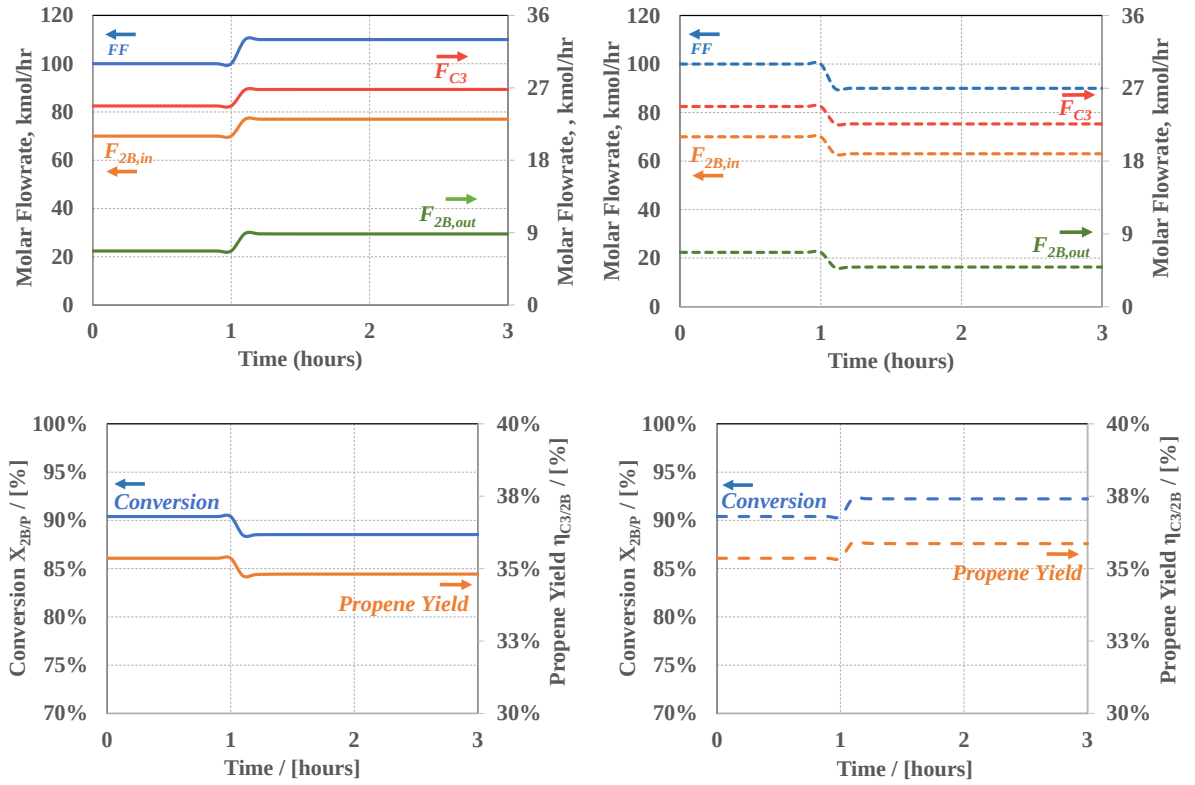


Figure 27. Reactor dynamic stream results and performance for feed flow disturbance (solid lines +10%FF and dashed lines -10%FF)

Since the reaction is endothermic, the objective was also to investigate if any possibility of reactor "quench" effect exists. Fortunately, no such problem was revealed, and of course, no problem concerning temperature excursions or run-away reactions was evaluated, effect characteristic to exothermic reactions. The variables studied for the feed disturbance were heater duty, reactor inlet and outlet temperature.

Another important factor is to reflect the dynamic response and separation control on the product specification since the variation of feed flow influences the yield distribution and conversion.

The first column COL-1 separates ethylene on the overhead, and the rest of the products consisting of C2+ olefins in the bottoms. The steady-state condition was maintained for 1 hour, after which the feed flow of 100 kmol/hr was varied with +/- 10%. The plant reached a new steady state in less than five hours, and so the distillate flow D1, while the composition of the ethylene in the overhead x_{D1}, was well maintained at 99.9% mole fraction with no noticeable oscillations. The ethylene impurity in the bottom of the column x_{B1} was very well maintained with negligible effect on the bottoms compositions. It could be remarked that the dual-composition, temperature and composition controller performed very respectably.

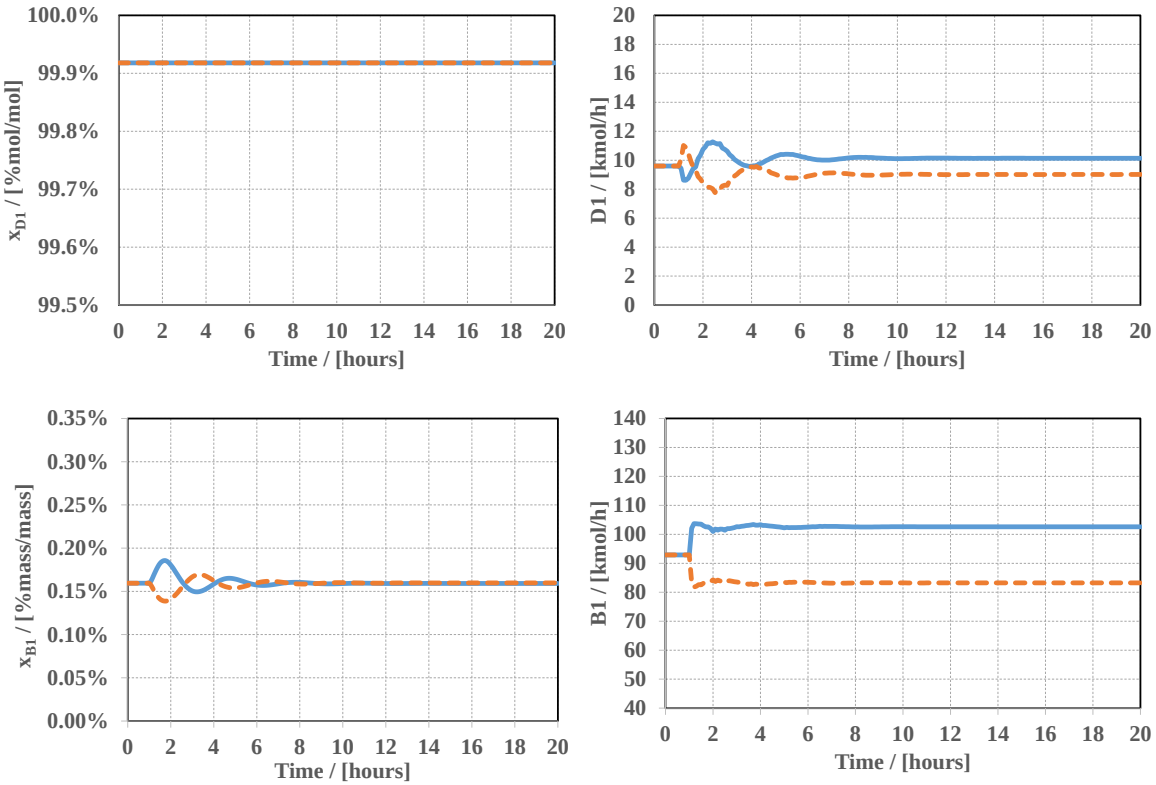
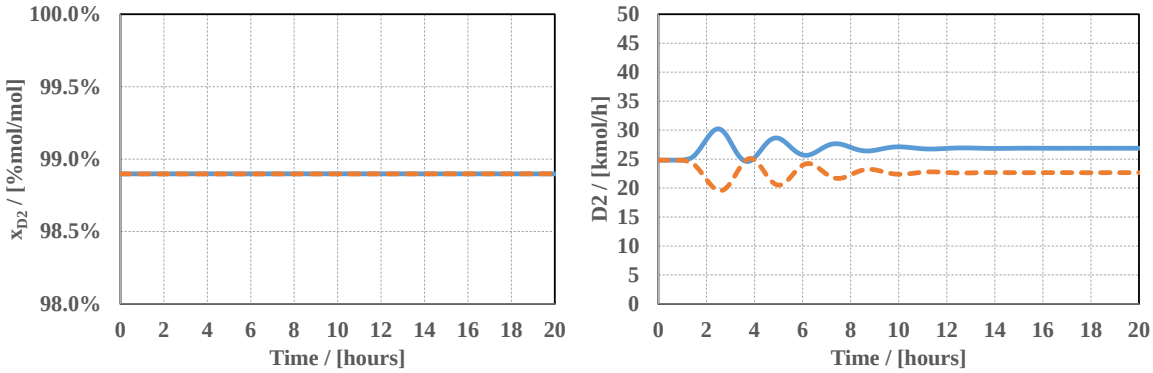


Figure 28. Feed disturbances for COL-1 with feed step changes (solid lines +10%; dashed line -10%)

In the second distillation column, COL-2, propylene product is separated on the overhead. The propylene purity x_{D2} specification of 99% mole fraction was well maintained with no visible effect on the propylene purity. The distillate and bottom flows (D2, B2) showed minor oscillations. The propylene carry-over to the bottoms was negligible due to the good performance of the composition controller cascaded with temperature.



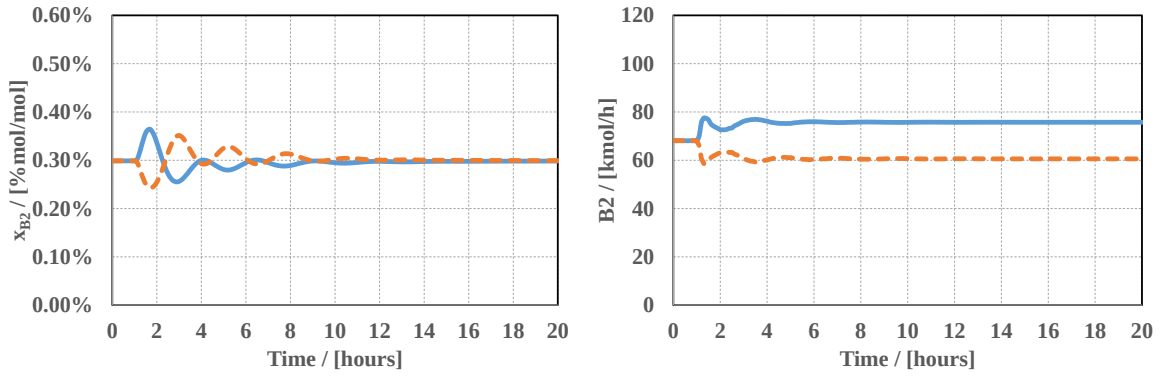


Figure 29. Feed disturbances for COL-2 with feed step changes (solid lines +10%; dashed line -10%)

As expected, the retention time in each vessel influences and adds on a larger time-span for the subsequent columns for adjusting. For distillation column, COL-3, a new steady state condition is reached after approximately 6 hours since the feed variation initiated at 1 hour. The distillate flow D3 consists of a C4 mix (2-butene, n-butane, and 1-butene) and the impurity concentration is maintained in distillate, to avoid contamination with heavier products (e.g., pentene C5). The impurity in distillate is well maintained with the temperature controller, showing insensitiveness to the feed variations. The bottoms composition is controlled via the composition – temperature controller set on minimizing the concentration of 2-butene in the bottom column COL-3, x_{B3}. The bottoms composition is adjusted reasonably fast for a distillation column, in 6 hours, with minimum product give-away.

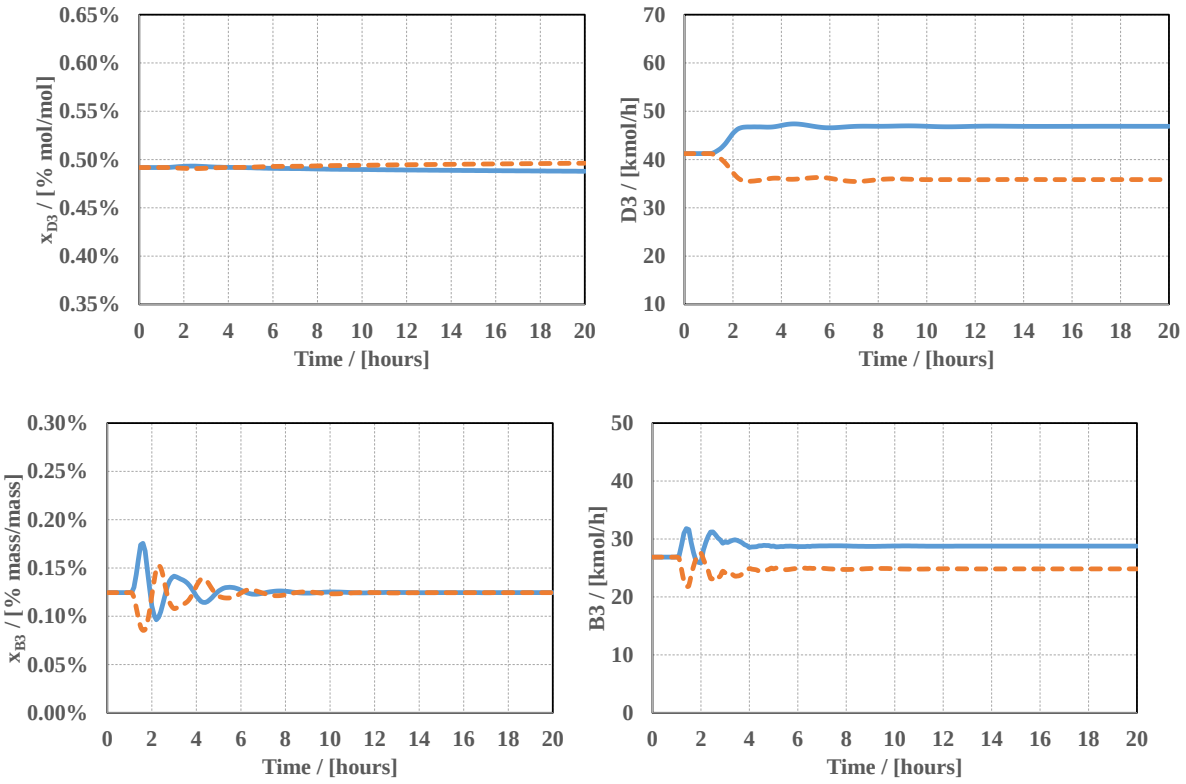


Figure 30. Feed disturbances for COL-3 with feed step changes (solid lines +10%; dashed line -10%)

The dynamic behavior of COL-4 shows good performance even though the time until it reaches steady-state condition is around 9-10 hours, mostly due to disturbances coming from upstream column COL-3. The composition of C5 in the overhead column, xD4, is kept fairly constant at 99% mole fraction, in the meanwhile the composition of hexene C6 in the bottom product exhibits oscillatory waves which after several hours are returned to the specification of 99% mole fraction.

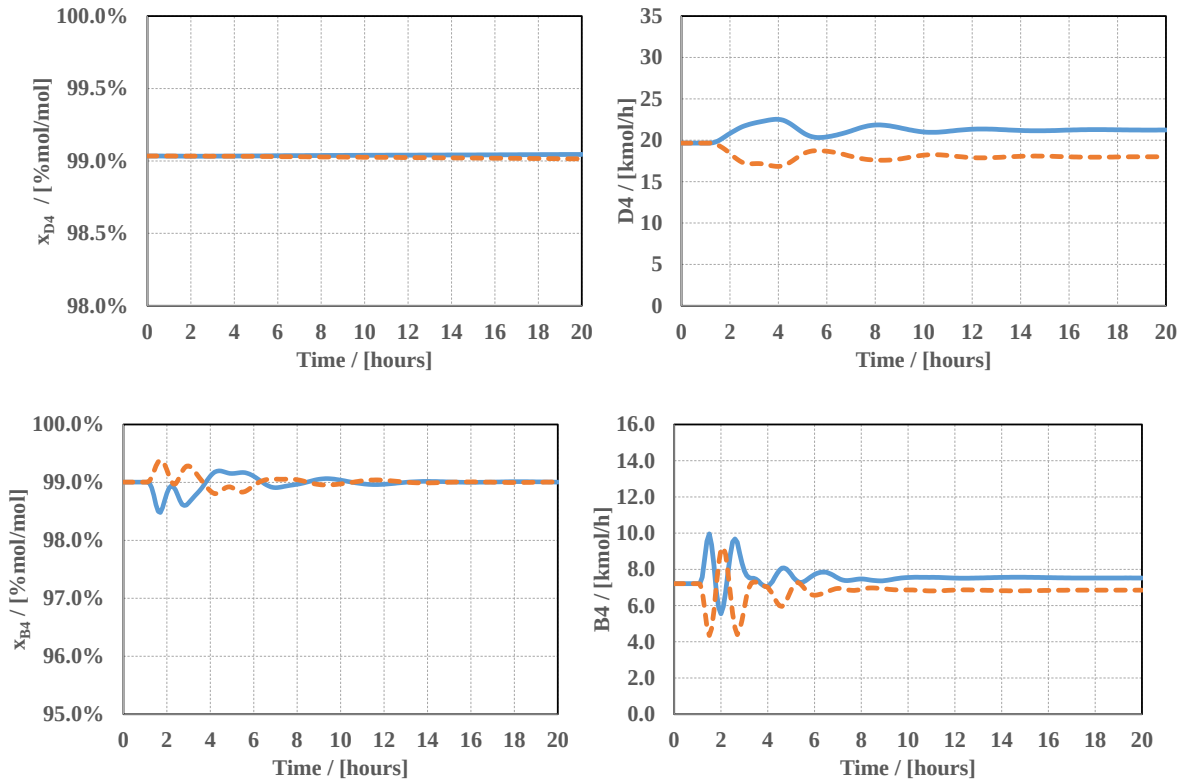


Figure 31. Feed disturbances for COL-4 with feed step changes (solid lines +10%; dashed line -10%)

Model predictive control

Linear MPC description

MPC is an optimization-based control approach that uses the model to predict and optimize future process responses. The MPC algorithm is described by the following optimization problem:

$$\min_{\Delta u(k)\ldots\Delta u(k+m-1)} \sum_{i=1}^{p} \|\Gamma_i^y([y(k+1)\,|\,k) - r(k+1)]\|^2 + \sum_{i=1}^{m} \|\Gamma_i^u([\Delta u(k+l-1)\|^2$$

subject to

$$\dot{x}(k+1) = Ax(k) + Bu(k)$$

$$y(k) = Cx(k) \qquad (1.2)$$

$$\Delta u = \{\Delta u \,|\, \Delta u_{\min} \le \Delta u(k) \le \Delta u_{\max}\}$$

where Γ_i^u , Γ_i^y are weighting of each component of input (u) and prediction output (y), respectively. The matrices A, B, and C are the state-space matrices of the linear model around a nominal operating point. The MPC predicts the behavior in the future of the process output (y) to minimize error for reference setpoint (r) as a function of the future control moves (Δu). The number of prediction horizon (p) and control horizon (m), respectively, determines the prediction of y and Δu. Recommended values for the prediction and control horizon are provided by several references (Agachi et. al, 2006; Gariga et al., 2010). Prediction horizon values are between 10-30. Higher values provide less aggressive control action and slower response with more computational effort. Prediction horizon can be reduced, however lower values may lead to instability and more aggressiveness of the control action. Control horizon values between 1-4 or 1/3 of the prediction horizon, ensure a good control performance with reduced computation effort and robustness.

Particularly for this MPC, the prediction horizon is set to ten (10) and the control horizon is set to two (2) with the output weight set to the nominal value for each variable.

In this work, the LMPC controller is configured on a supervisory level with direct action on the conventional process control. The scope of MPC is to control the production flows of ethylene and propylene to the required targets by adjusting the setpoints of the two manipulated variables, feed flow (MV1) and reactor inlet temperature (MV2). The user sets the required production targets. The 2x2 MIMO (multi-input multi output) system has significant coupling between the manipulated and controlled variables, however due to their multivariable nature, advanced control strategies – such as model predictive controller allow the control problem to be addressed globally (S.Agachi, 2006). One other alternative may be subsystem partitioning, dividing the unit in reaction section and separation section, such to design for each one a separate linear model predictive controller (Chinpraasit, 2019). Alternatively, coupling linear and nonlinear MPC controllers by decomposing the plant into linear and nonlinear subsystems was investigated (Zhu et al., 2000).

LMPC design and tuning

Model predictive control systems are designed based on a mathematical model of the plant. The model to be used in the control system is a state-space model developed by process identification. The plant model is developed by open-loop identification from input-output generated from the Aspen dynamic simulation data. Space-state model formulation and validation is performed in MATLAB and co-simulation environment between Aspen Dynamics and MATLAB/ Simulink is used to facilitate the connection between the dynamic simulation and Model Predictive Controller block from Simulink.

In industrial applications, step tests in opposite directions (bump tests) are typically executed on the operating unit to identify a valid process model required for designing the model predictive controller. Herein, the dynamic simulation from Aspen Dynamics, acts as the “live” unit to extract the necessary process data to configure and then apply a 2 x 2 MPC system by co-simulation of Aspen Dynamics and MATLAB/ Simulink. Particularly, for this study, bump tests are performed for two input variables with open-loop responses, feed flow and reactor inlet temperature, respectively, referred as manipulated variables (MV). The bump cycle

method alternates the step change in opposite directions, e.g., +/-10%. The ethylene and propylene flow are the output or controlled variables (CV); these production targets are controlled/ set by the user through the LMPC. The list of manipulated and controlled variables for the supervisory level are shown below. LMPC implementation is carried out in a two-layer structure, namely the layer of "traditional" decentralized PID loops stabilizing the main process variables, and MPC layer adjusting the set points of the basic regulatory loops.

Table 6. Input / Output values in engineering units

Input/ Output	Nominal value	Minimum	Maximum	Dimensionless Nominal value	Type
Feed flow / [kmol/h]	100	75	125	50	Manipulated variable (MV1)
Reactor inlet temperature / [ºC]	550	450	650	50	Manipulated variable (MV2)
Ethylene flow / [kmol/h]	9.6	4.8	14.4	50	Controlled variable (CV1)
Propylene flow / [kmol/h]	24.5	16.1	33.5	50	Controlled variable (CV2)

The response of the two outputs is recorded, and a state space model is obtained from the input-output simulation data. Subsequently the two state-space models are concatenated into one single final state-space model using MATLAB. The order of the model identified is 24 and stability verification is carried on; particularly, the eigenvalues of matrix A are verified. In Figure 32 the results from the identified model and simulation data are displayed, where the bump cycle method by alternating the step change in opposite directions with +/-10% of the input variable.

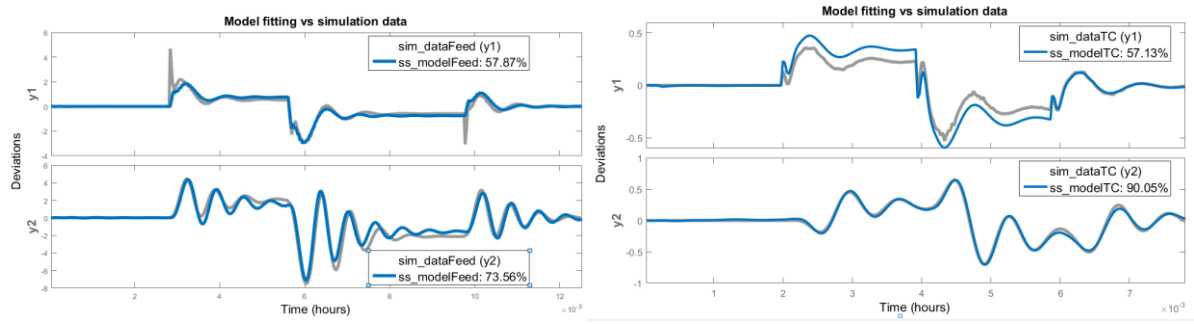


Figure 32. Model fitting vs simulation data (left – temperature model, right – feed model)

The models are developed based on deviations from the nominal values in order to simplify the complexity of the process model and consequently the model-based controller. The results show a good accuracy between the model estimates (ss_modelFeed and ss_modelTC) and the process simulation data output (sim_dataFeed and sim_dataTC).

Simulink environment is used for this study in co-simulation with Aspen Dynamics to facilitate the connection between the dynamic simulation and the model-based controller configured in MATLAB/Simulink. MATLAB calls process simulators using ActiveX automation server and enables connection through the Simulink environment and Aspen Dynamics. Compatibility issues between the two software, MATLAB and Aspen Dynamics, respectively, should be carefully considered, otherwise the communication is not achieved.

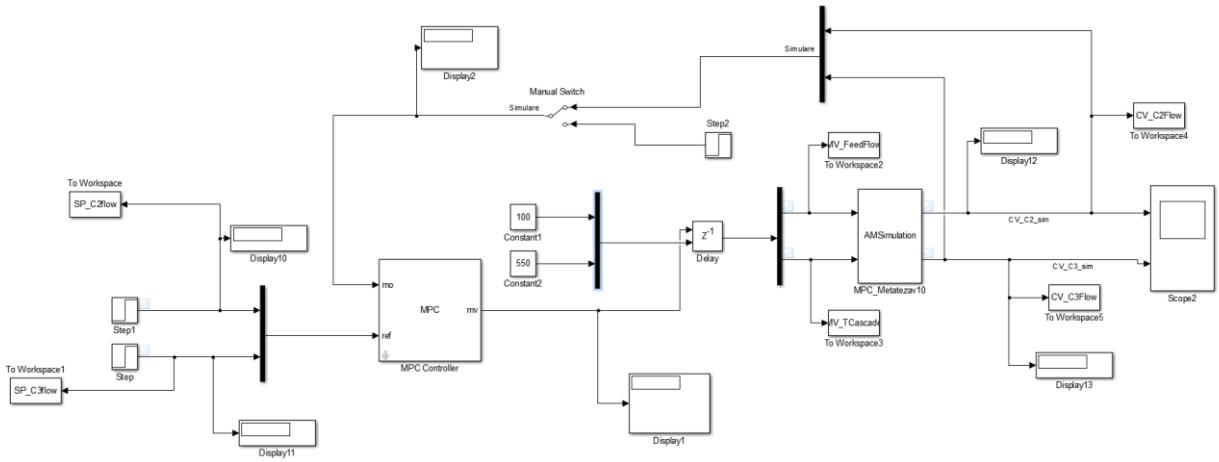
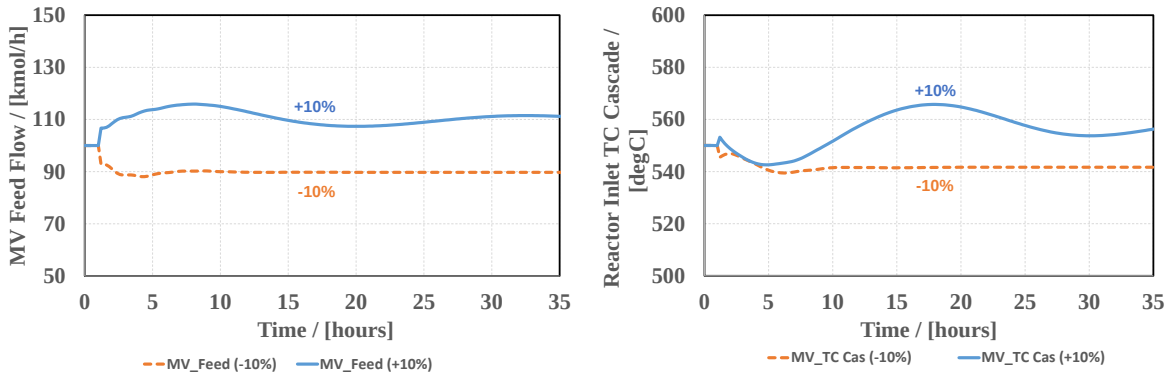


Figure 33. Simulink flowsheet of MPC connected with Aspen Dynamic Simulation

Plantwide dynamic response performance

The control performance of MPC controller is evaluated through regulatory tests of step disturbances applied on the controlled variables, generated after 1 hour of steady state. Two sets of data are generated, for a step change +10% (continuous solid blue line) applied simultaneously on both controlled variables (e.g., ethylene and propylene flow) and another test consisting in a change of -10% (dashed orange line) on the same two (2) CVs, ethylene flow and propylene flow, respectively. The performance of the MPC is compared with the open-loop response from the dynamic simulation data. In the open-loop test, the manipulated variables, feed flow and reactor inlet temperature, are modified by applying a step such that the output variables (C2 flow and C3 flow) are equivalent with +/-10% of their steady state values. In this way, the two control strategies could be assessed by index performances such as, Integral Square Error (ISE), Mean Square Error (MSE), Integral Absolute Error (IAE), Peak Error (PE) or overshoot, in order to evaluate the performance.



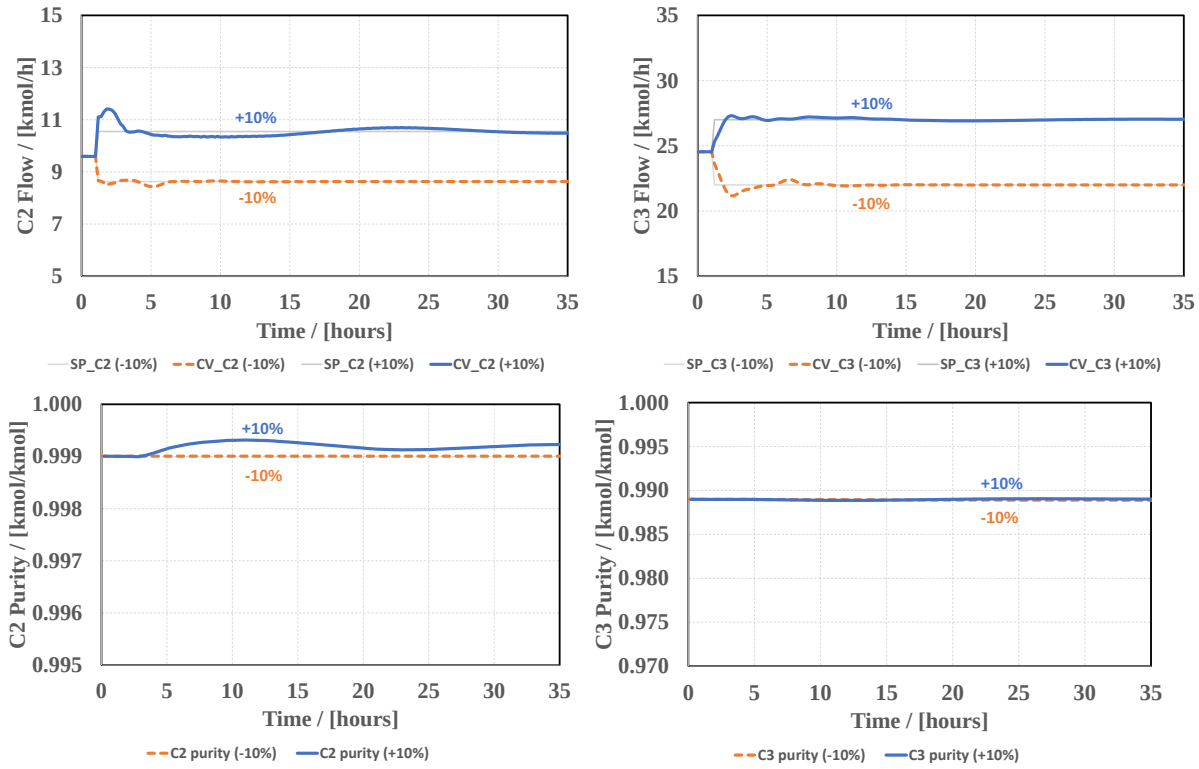
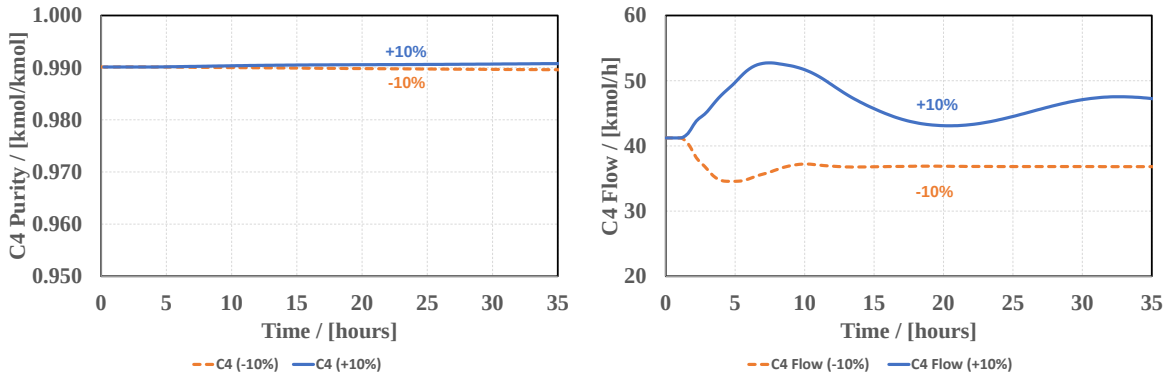


Figure 34. MPC - Profiles of control variable flowrates and purities, feed rate and reactor inlet temperature

In Figure 34, the advanced controller shows a stable and rapid attainment of the target production rates in a reasonable duration (<5 hours). The overshoot of the flow set points is negligible, confirmed also by proper control of product purities of ethylene and propylene. Oscillations of feed rate and reactor inlet temperature are expected since these variables are modified by the MPC to reach the new production rates targets. It can be observed that for a +10% step change of production flows, the model drives the initial reactor inlet temperature MV in an opposite direction and after some couple of hours, the MPC corrects this MV in the right direction, such that both controlled variables targets are reached.



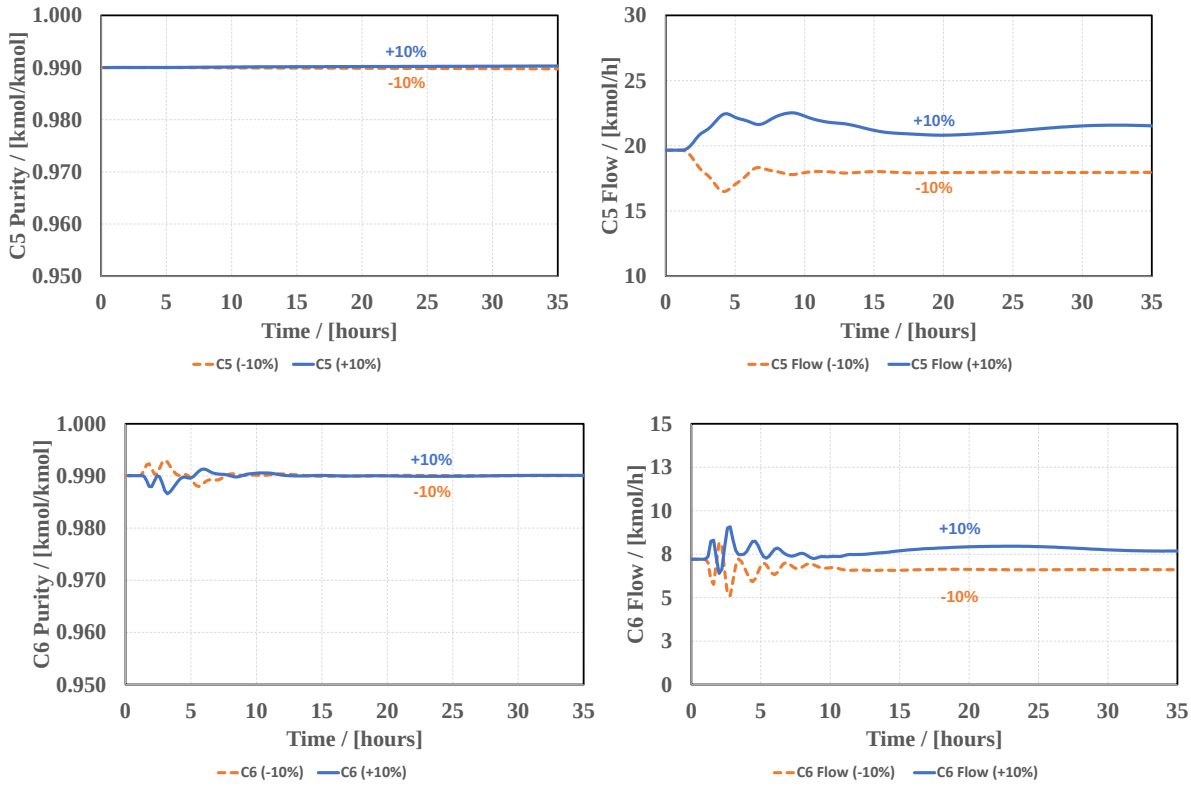


Figure 35. MPC - Profiles of product flowrates (C4, C5, C6) and purities

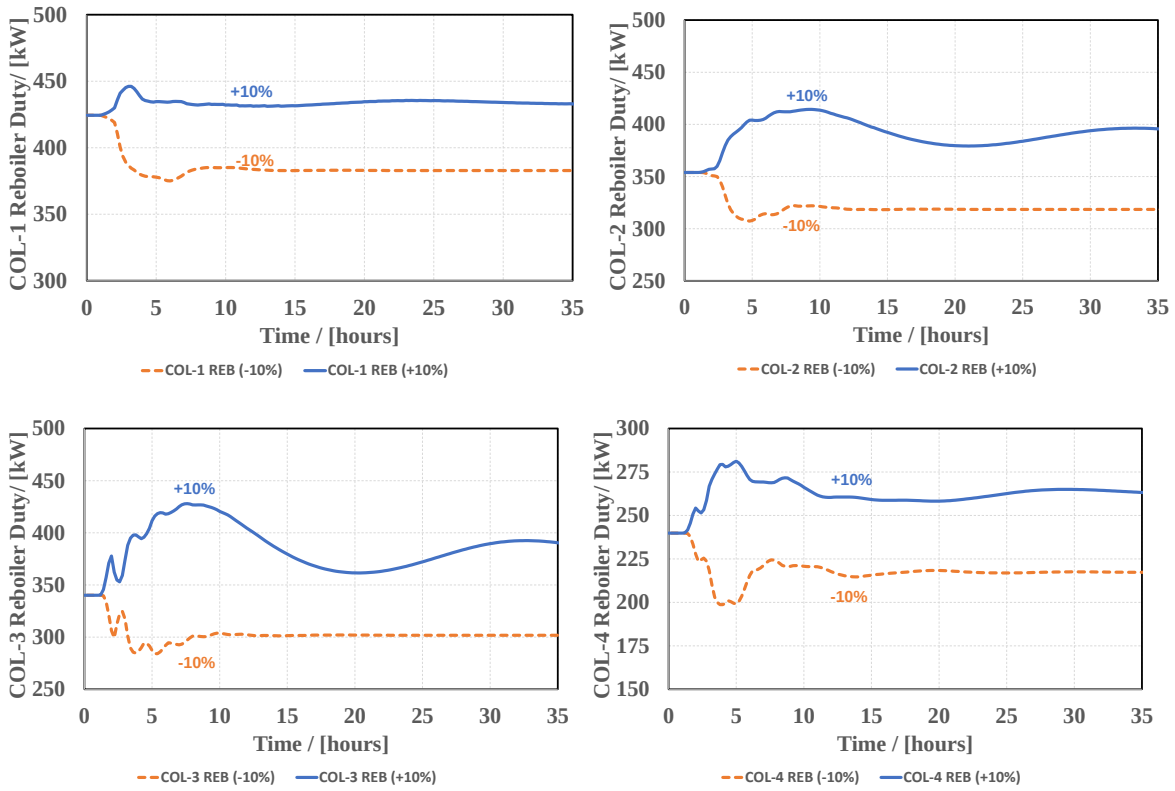


Figure 36. MPC - Profiles of columns reboiler duties

Notably, the response to the -10% step change (represented by the orange dashed line) is faster compared to the +10% step change. This indicates that it is easier to decrease the production rate.

The performance of the LMPC is compared with the open-loop response using the dynamic simulation data. In the open-loop test, the manipulated variables, feed flow set point and reactor inlet temperature set point, are modified by applying a step such that the output variables (C2 flow and C3 flow) change by +/-10% of their steady state values (as in the LMPC tests). In this way, the two control strategies could be compared by means of performance indexes such as, Integral Square Error (ISE), Mean Square Error (MSE), Integral Absolute Error (IAE), Peak Error (PE) or overshoot. Results are presented in Figure 37 and Figure 38.

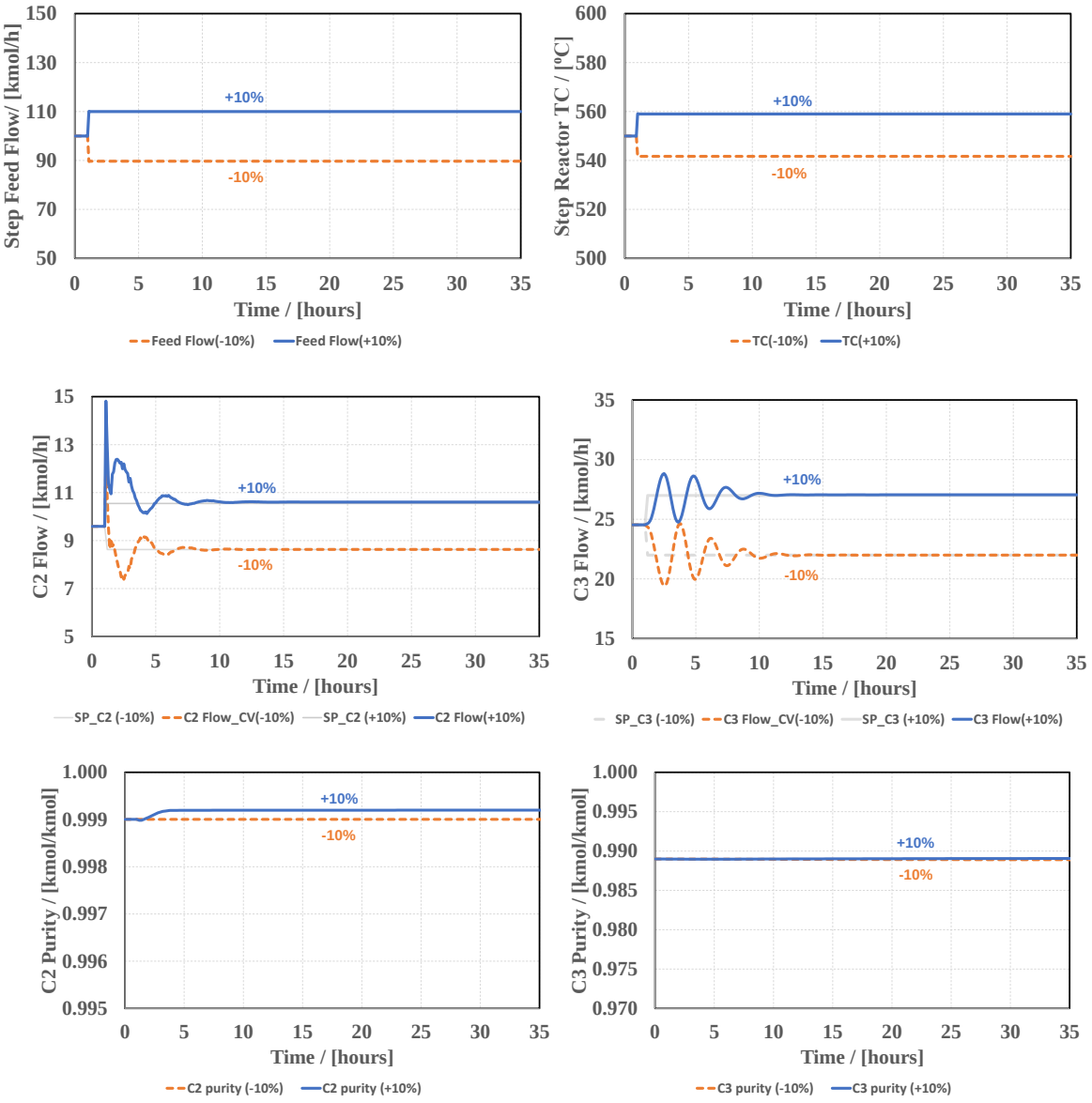


Figure 37. Open loop - Profiles of control variable flowrates and purities, feed rate and reactor inlet temperature

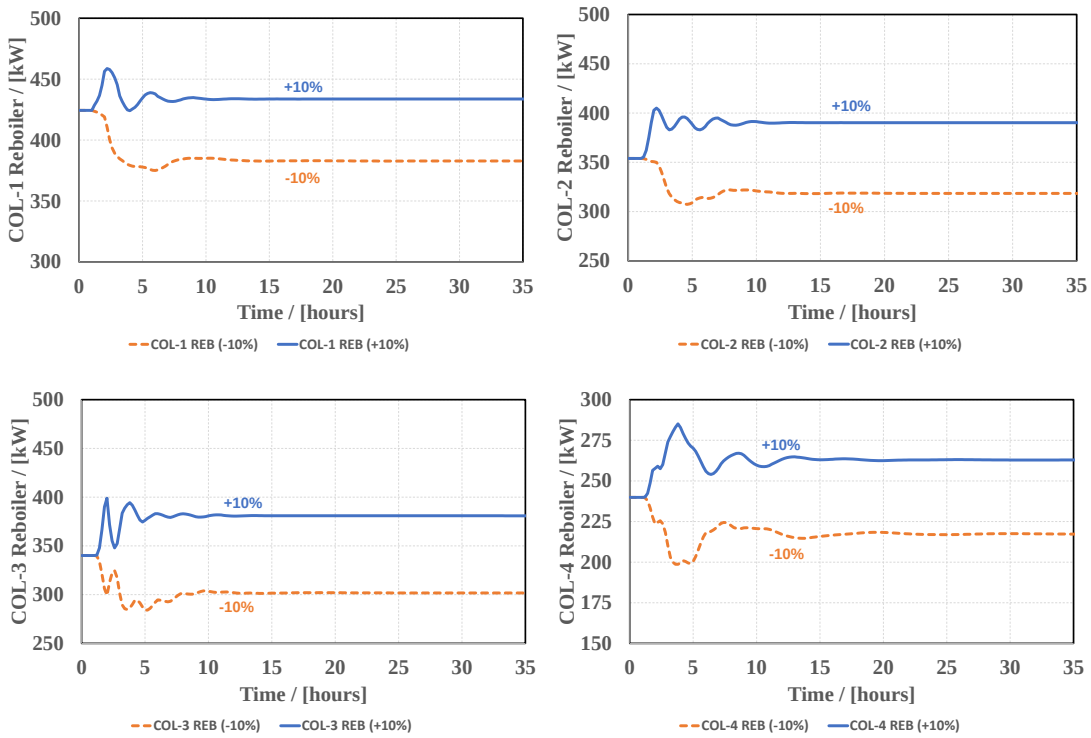


Figure 38. Open loop - Profiles of columns reboiler duties

In Figure 37 and Figure 38 the open-loop responses demonstrate reasonable control with some oscillations until reaching the production flow targets after approximately 15 hours, followed by a steady-state regime. The ethylene flow exhibits an overshoot of approximately 50% compared to the set point value; however, the feedback controllers efficiently adjust and swiftly reduce the error. Throughout these tests, the feedback controllers effectively maintain the product purities of ethylene and propylene at their respective set points for both control strategies. Albeit the nonlinearity of 2-butene olefin metathesis unit, the results show that the linear model predictive controller outperforms the open-loop response.

To characterize system performance and identify the most effective control structure, several performance indexes are considered. The mean square error loss (MSE) is utilized to illustrate the performance and control response for the same step change of +/-10% in production flow over a period of 30 hours. The MSE represents the sum of squared differences between predicted and actual output values, divided by the number of tested hours.

Additionally, the integral square error (ISE) is employed as another measure to evaluate system performance, calculated by integrating the square of the control error over the same period (by applying the trapezoidal rule, with a fixed 0.2 hours step). In industrial practice, the control performance is often assessed based on the maximum deviation of the controlled variables, referred to as peak error (PE). However, while PE identifies the maximum deviation, it does not provide information about fluctuations or the ability to achieve the set point. Therefore, the integral absolute error (IAE) is commonly used to evaluate control response and accuracy. The IAE calculates the sum of areas above and below the set point, penalizing errors equally regardless of direction.

The results presented in Table 7 consistently indicate that the LMPC exhibits significantly better performance compared to open-loop responses, demonstrating its superior control capabilities.

Table 7. Index performances of control strategies

Method	U.M	Controlled variable 1: C2 Flow (y_1)				Controlled variable 2: C3 Flow (y_2)			
		MPC -10%	Open Loop -10%	MPC +10%	Open Loop +10%	MPC -10%	Open Loop -10%	MPC +10%	Open Loop +10%
ISE	$(kmol/h)^2 \times h$	0.05	3.16	1.34	6.19	1.7	15.8	1.3	10.6
MSE	$(kmol/h)^2$	0.01	1.05	0.22	2.06	0.3	5.3	0.2	3.5
IAE	(kmol/h) ×h	0.50	5.63	4.80	9.35	2.8	20.8	3.3	16.2
PE	kmol/h	0.20	3.57	0.86	4.26	1.6	2.7	1.7	2.4

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Andrei, A.M., Bildea, C.S., Linear Model Predictive Control of Olefin Metathesis Process, PROCESSES, vol 11, issue 7, article number 2216, 2023. IF 3.5, Q2 Engineering, Chemical.

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