Process Control of Isobutene Dimerization Plant

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The development and evaluation of the dynamic flowsheet for isobutene dimerization process is presented. The steps for developing the dynamic model, the control scheme and the controllers tuning are shown and the response of the system to different disturbances is evaluated. The results are presented in graphical form. Methods for changing the plant throughput and for controlling the product specification when the feed composition varies are presented.

Keywords: isobutene dimerization, process control, dynamic simulation, reactor-separation-recycle

Dimerization process

Isobutene dimerization became a very attractive process for producing high octane components (e.g. isooctene and further isooctane via isooctene hydrogenation) since the ban of MTBE production associated with environmental issues (e.g. groundwater contamination). Isooctene – which is a mixture of diisobutene and cross-dimers – can be easily hydrogenated to isooctane, used to replace the high octane aromatic components in the gasoline pool [1].

Similar to MTBE units, the dimerization process makes use of the C_4 fractions from FCC and Naphta Steam Cracker Units. Moreover, the MTBE units can be easily reconfigured to dimerization units [2].

In the recent years, several technologies for isooctane production were investigated: reactive distillation, reactor-separator-recycle or columns with side reactors, considering different catalysts (e.g. acid ion exchange resins, phosphoric acid) and reaction mechanisms (reaction paths and use / nonuse of polar components as selectivity enhancers) [2-7]. The main objectives were to: enhance the selectivity towards DIB because there was the likelihood of product degradation by further oligomerization reactions, to control the temperature inside the reactor in order to avoid the degradation of the catalyst and to minimize the cost of the units.

Less attention was however given to the dynamic behavior and control of the proposed flowsheets. Therefore, the current work aims to present the transient behavior and control of the dimerization process. Control structures are developed and the controllability and the transient behavior of the plant are determined.

The design of the plant was performed based on the kinetics and reactions proposed in [5]. Isobutene (IB), 1-butene (1-Bu) and 2-butene (2-Bu) react in several parallel-consecutive reactions, leading to the main products - diisobutene (DIB) and cross-dimer (cDIMER) - and by-products - triisobutene (TIB) and tetraisobutene (TEB):

$$IB + IB \xrightarrow{k_1} DIB \qquad r_1 = k_1 \cdot x_{IB}^2 \quad (1)$$

$$IB + DIB \xrightarrow{k_2} TIB \qquad r_2 = k_2 \cdot x_{IB} \cdot x_{DIB} \quad (2)$$

$$IB + TIB \xrightarrow{k_3} TEB \qquad r_3 = k_3 \cdot x_{IB} \cdot x_{TIB} \quad (3)$$

$$IB + 2\text{-}Bu \xrightarrow{k_4} cDIMER \qquad r_4 = k_4 \cdot x_{IB} \cdot x_{2\,Bu} \quad (4)$$

$$1\text{-}Bu \xrightarrow{k_5} 2\text{-}Bu \qquad r_5 = k_5 \cdot x_{1\,Bu} \quad (5)$$

The isobutene dimerization plant (fig. 1) is a reactor-separation-recycle (RSR) system consisting of: a multi-tubular catalytic reactor which is operated at high pressure, a low pressure distillation column for the separation of the heavy products from the unconverted reactants, a purge for removing the light inert components from the system, the recycle of the unconverted reactants and the mixing point of the fresh and recycled reactants. Several other columns for product purification may be used for final conditioning of the product, but they are intentionally ignored in the study because of not having any impact on the dynamics of the RSR system.

The process flow diagram of the dimerization unit together with the sizes of the main equipment – reactor, separation column, and heat exchangers – is presented in figure 1. The material and energy balance of the steady state model is given in table 1. The sizes of the reflux drums and bottom sumps are determined to allow for 5 min of liquid holdup when the vessel is 50% full, based on the total liquid leaving the vessel. Several controllers are foreseen to keep the plant within the operating window, which are presented in the following section. They can be also seen on the flowsheet, (fig. 1).

Process Control

The industrial plants are continuously facing variations of operating parameters (temperature, pressure, flow, compositions etc.) they should deal with in order to provide the required products within the quality specifications. Moreover, a safe operation should always be ensured. Therefore, control systems are designed to ensure plant safety, product specifications and profitability.

The process control activities are related to operational control and instrumented safeguarding. Operational control involves all manual and automated actions to properly operate the process and keep the process within its operating window. Instrumented safeguarding involves all unscheduled instrument actions which are designed to bring the process in a safe state if it moves towards an unsafe situation (potentially due to operational control malfunction). It consists of the protection against personal injury, equipment and environmental damage and production loss.

This paper presents the development and the evaluation of the operational control of the isobutene dimerization plant. For this purpose, the steady state Aspen Plus simulation of the dimerization unit is converted into a dynamic model, implemented in Aspen Dynamics. Control systems are therefore developed and implemented. The

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response of the plant / control system to different disturbances (e.g. flow / composition variations) is assessed through dynamic simulations.

Dynamic simulation

Dynamic modeling and simulation has proven to be an insightful and productive process engineering tool. It is used in a project to support the process and control system design. It ensures that the process is operable and can meet product specifications when the process varies from steady state design conditions [8].

Dynamic simulation of a chemical process is a useful approach for understanding the transient behaviour. The dynamic model of the dimerization plant is developed in Aspen Dynamics. The simulation is automatically initialized using the steady state Aspen Plus simulation results [9].

The performance / response of the control system depends on the process characteristics and the controllers tuning / parameters (K, T_i, T_d). The process characteristics – process gain, time constant and dead time – are determined by the design / size of the equipment. The size of the equipment should therefore be determined first and specified in the steady state model, such that it can be later used in the dynamic simulation.

For the purpose of defining the main controllers and evaluating the transient behavior of the dimerization plant in a conceptual stage, the dynamic model is developed as a flow-driven simulation. It is less demanding compared to pressure-driven simulation. No pumps or control valves specifications are required. The flowrate can be set to any desired value without any concern regarding how this is achieved [10].

Control structure

Besides safety, the control structure of the dimerization unit has to achieve two main important targets: the product purity and to keep the reactor temperature within the specified limits.

Due to the location of the dimerization plant within a refinery – downstream the cracking units – the feed stream can significantly vary. This obviously affects both the reactor performances (reactant conversion, product selectivity) and the column operation. In order to avoid catalyst degradation, temperatures higher than 120°C should be at any time avoided; therefore, the reactor temperature control loop should react fast enough to overcome the incoming disturbances.

Varying reactor yields lead to disturbances in the column feed stream. The column control structure should be able to bring it to a safe and stable state and keep the level of impurities in the product streams according to the specifications, in order to avoid off-spec product.

The following controllers are foreseen to keep the dimerization unit within the operating window:

- Reactor inlet flow controller (FC2): this controller maintains the reactor inlet flow (recycle plus fresh feed) at the desired value. Production rate can be changed by modifying the set point of the controller.

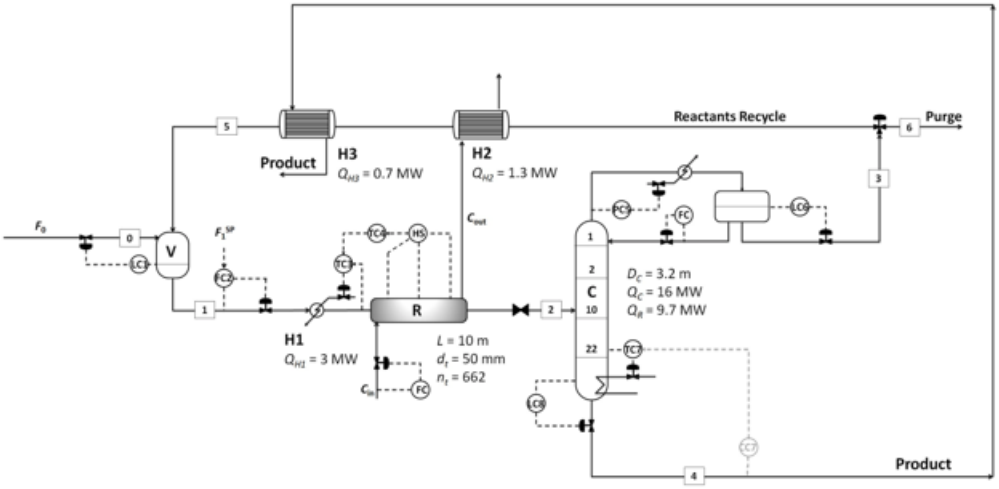

Fig. 1. Process and control diagram

Mole flow [kmol/h]	F_0	F_1	F_2	F_3	F_4	F_5	F_6
IB	173.2	266.7	98.5	98.5	0.0	93.5	4.9
DIB	0.0	1.2	53.7	1.3	52.4	1.2	0.1
TIB	0.0	0.0	4.7	0.0	4.7	0.0	0.0
TEB	0.0	0.0	0.1	0.0	0.1	0.0	0.0
2-Bu	47.3	1425.6	1457.5	1450.8	6.7	1378.2	72.5
cDIMER	0.0	0.8	49.5	0.8	48.7	0.8	0.0
1-Bu	91.7	302.5	221.9	221.9	0.0	210.8	11.1
n-C4	47.8	929.6	929.6	928.2	1.4	881.8	46.4
Total mole flow [kmol/h]	360.0	2926.4	2815.5	2701.4	114.0	2566.4	135.1
Total mass flow [kg/h]	20295	166174	166179	153557	12622	145879	7678
Temperature [°C]	100.0	77.2	54.9	54.0	155.8	73.8	54.0
Pressure [bar]	30.0	30.0	5.1	35.0	5.2	35.0	35.0
Vapor fraction	0.0	0.0	0.44	0.0	0.0	0.0	0.0

Table 1
MATERIAL AND ENERGY BALANCE

- Feed vessel level controller (LC1): the purpose of this controller is to keep the level in the buffer vessel within the specified range. In case of a disturbance in the system such as increased recycle flow or production rate change, the reverse-acting controller manipulates the fresh feed control valve such that the disturbance is rejected.

- Reactor feed temperature controller (TC3) and reactor temperature controller (TC4): in order to obtain a fast response for overcoming a temperature increase in the reactor, the reactor temperature is controlled in cascade with the reactor inlet temperature. It should be noted that high temperature increases not only the reaction rate, but also the selectivity towards formation of DIB and cDIMER (due to higher activation energies of the main reactions, compared to the secondary ones [5]). However, the temperature inside the reactor should not exceed 120°C, value above which significant catalyst deactivation occurs. Therefore, the reactor temperature is the primary controlled variable (master controller). In order to be able to measure accurately the temperature of the catalyst bed, to avoid the hot spots and catalyst deactivation, four measurement points are installed along the reactor: at 25, 50, 75% and at reactor outlet. The highest value is selected by the HS block and sent as process variable to the primary / master controller TC4, which in turn adjusts the setpoint of the secondary / slave controller TC3. When there is an upset in the feed inlet temperature, the heater outlet / reactor inlet temperature varies and the secondary controller TC3 takes corrective action, manipulating the heater duty before the temperature in the reactor changes. Note that, in order to ensure the proper control, the range of the manipulated variable (OP) of the primary controller should be the same as the range of the controlled variable (SP) of the secondary controller.

- Dual temperature control of the distillation column is not necessary since the overhead product is recycled, the purge fraction is small, the concentration of dimers in the overhead product is very low and the relative volatility between the light and heavy components is high; dimers carryover in the overhead product is unlikely to happen. The temperature profile (fig. 2) has a steep change on the last trays, demonstrating that the separation is indeed easy.

The location of the one-point temperature controller is based on the sensitivity analysis, plotting the open-loop steady state gain (K_{OLSS}) and determining its greatest variation. Open-loop steady state gain (fig. 3) is defined as

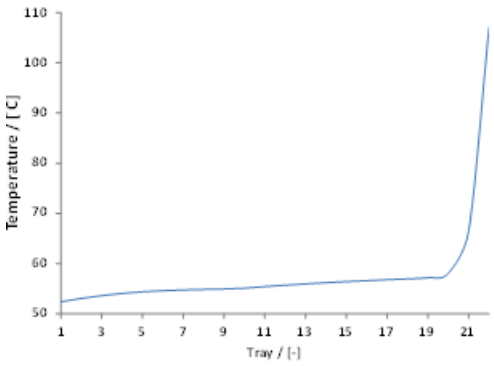

Fig. 2. Tray temperature profile

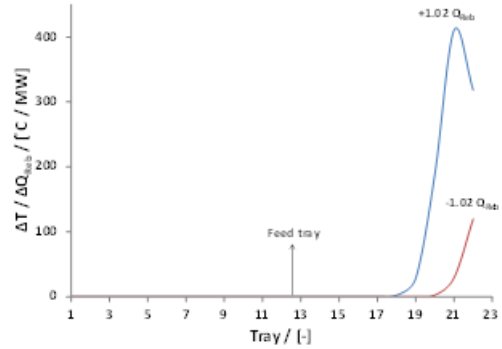

Fig. 3. Open loop steady state gain

the ratio between the change of temperature (ΔT) and the change of manipulated variable (reboiler duty, ΔQ_{Reb}). Tray 22 seems to be the proper tray for installing the temperature controller / sensor for avoiding accumulation of light products in the bottom and off-spec dimer product.

-The last controllers installed on the column are: the reflux drum level controller (LC6) which manipulates in direct action the distillate product flow, the sump (column bottom) level controller (LC8) which manipulates in direct action the bottom product flow and the overhead pressure controller (PC5) which manipulates in reverse action the condenser duty.

The set-up of the controllers is presented in the next section.

Controller tuning

The types of controllers used for the dimerization unit are proportional (P) and proportional-integrative (PI). The PID controllers are not usually used in the dynamic simulations of distillation columns. Derivative action performs better in noise-free simulations than in the real

Table 2
CONTROLLER PARAMETERS

	TC3	TC4	LC1	LC24	TC7	PC1	CC7
Controlled variable	Reactor inlet temperature	Reactor temperature	Condenser level	Sump level	Tray 22 temperature	Condenser pressure	% C4 in product
Controlled variable SP & range	100°C 80÷120°C	110°C 90÷130°C	1.6 m 0÷3.2 m	3.3 m 0÷6.7 m	66°C 46÷86°C	5 bar 4.5÷5.5 bar	7.1% 0÷14% (mole)
Manipulated variable	Heater B10 duty	SP TC3 (Cascade)	Distillate flow	Product flow	Reboiler duty	Condenser duty	SP TC22 (Cascade)
Manipulated variable nominal value & range	3 MW 0÷6 MW	100°C 80÷120°C	155 t/h 0÷310 t/h	12.5 t/h 0÷25 t/h	9.7 MW 0÷20 MW	-16 MW -32÷0 MW	66°C 46÷86°C
Control action	Reverse	Reverse	Direct	Direct	Reverse	Reverse	Direct
K_c (%/%)	1	1	1	1	1	1	0.1
T_i (min)	3	3	600	600	10	12	66
Controller type	PI	PI	P	P	PI	PI	PI

plant. Using PI controllers in the simulation the expectations for the plant are conservative [8].

The controller parameters (gain and reset time) should be determined in order to achieve the proper control. The rules of thumb provided in [10] recommend that a proper initial value for the controller gain (K_c) would be 1 (% OP range) / (% PV range). The reset time (integral time) is recommended to be in the same range as the time constant of the process. Except for one case – the composition controller added for the second case study – all the controllers are tuned following this rule. The tuning parameters of the controllers are given in the table 2.

Case studies

The proposed flowsheet with the control system implemented is subject to several perturbations to observe the transient behavior and the robustness of the proposed control structure. In the following, F_k and $Z_{i,k}$ will denote the molar flow rate of stream k (numbered accordingly to fig. 1) and the fraction of the i species in the stream k, respectively.

Initially, the column is only provided with the bottom temperature controller for the indirect control of product composition and the results are examined for feed flow and composition disturbances. The case is discussed in the next section.

Control structure 1 (CS1)

Reactor inlet flow disturbance

The first disturbance considers a decrease by 10% of the reactor inlet flowrate (F_1), achieved by closing the reactor inlet flow control valve. It is observed in figure 4 that the plant reaches relatively soon a new steady state. Since the feed control philosophy is to maintain the level in the feed vessel (V), the fresh feed flowrate (F_0) decreases as well (by ≈ 9%, fig. 4 left), to reject the disturbance. The recycle (F_5) and product flowrates (F_4) are following the perturbation and decrease with approximately 8.5% and 11.5%, respectively.

Looking to the composition profiles (fig. 4, right), it is observed that accumulation of light components into the product does not occur ($Z_{C4,4}$). Product carryover in the overhead stream is not observed at all and therefore, it is not plotted. A slight decrease of selectivity can be observed: less DIB and more C16+ are produced, which is the result of a higher isobutene conversion due to less isobutene at reactor inlet for the same catalyst amount (lower liquid hourly space velocity, LHSV). The contrary could be observed when the reactor inlet flow will be increased.

The column bottom temperature (T_{22}) is brought back to the set point relatively fast (≈2 h, fig. 5 right), by lowering the reboiler duty (Q_R), while the reactor temperature is maintained at set point (fig. 5, left).

When the reactor inlet flow (F_1) is increased by +10%, the fresh feed flowrate (F_0) increases, in order to maintain the level in the feed drum which starts decreasing (fig. 6, left). The recycle and product flowrates follow the perturbation and increase by approximately 7 and 10% respectively.

The tendency of C4 to increase in the column bottom (fig. 6 right, $Z_{C4,4}$), felt by a slight temperature decrease, is rejected by increasing the reboiler duty. The bottom temperature is brought back to the set point in less than 2

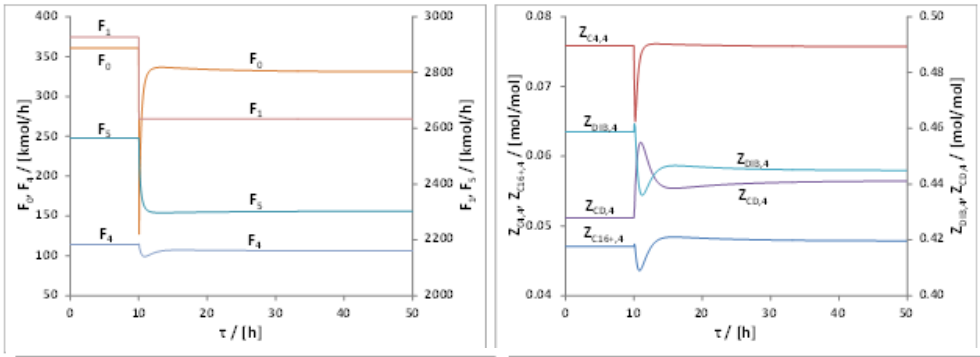

Fig. 4. Control structure CS1: Dynamic response of flow rates (left) and compositions (right), for 10% decrease of the reactor inlet flow rate

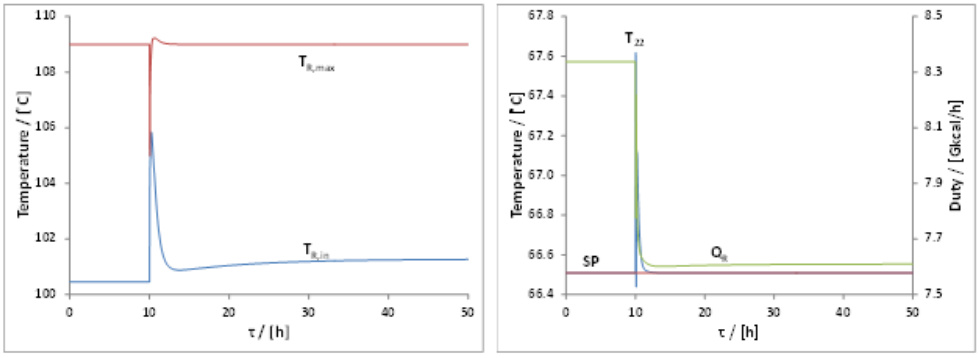

Fig. 5. Control structure CS1: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for 10% decrease of the reactor inlet flow rate

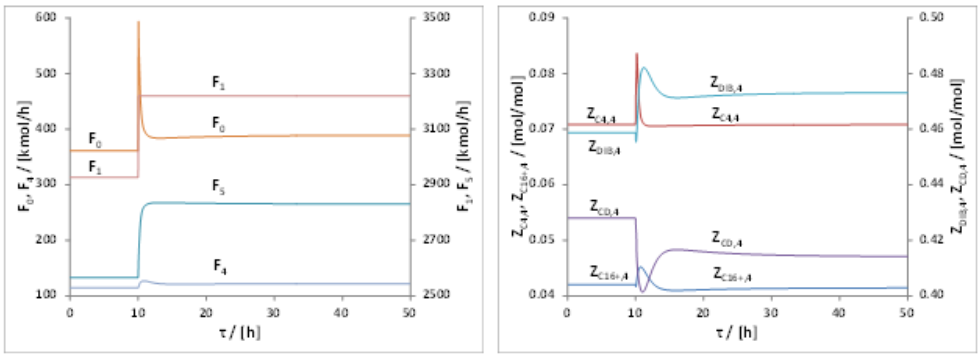

Fig. 6. Control structure CS1: Dynamic response of flow rates (left) and compositions (right), for 10% increase of the reactor inlet flow rate

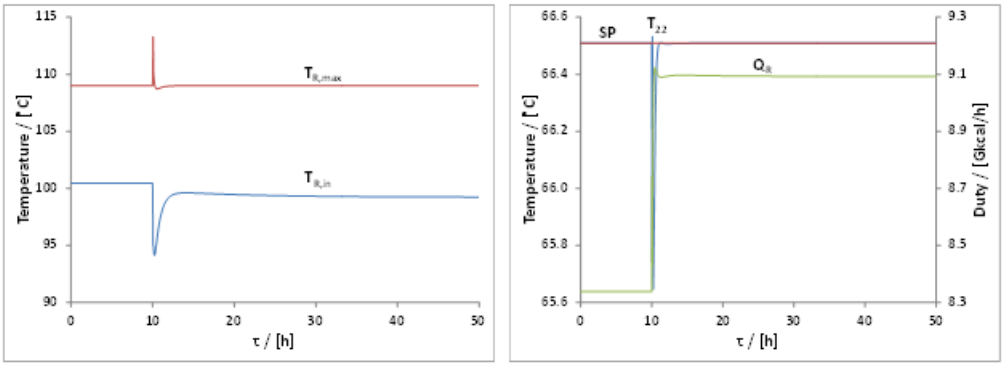

Fig. 7. Control structure CS1: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for 10% increase of the reactor inlet flow rate

h (fig. 7, right). The accumulation of light components into the product or product carryover into the overhead stream is not observed. The control structure provides a stable and smooth operation and a new steady state is reached.

The reactor temperature control loops (fig. 7, left) successfully prevent the reactor temperature exceeding the threshold and brings it back to the set point.

In conclusion, column bottom temperature control is a good solution for maintaining the product purity when disturbances in feed flow occur.

Plant feed composition disturbance

The second type of disturbance foresees a change in the plant inlet composition. The percentage of n-C4 is increased by twice of the steady state value, from 13.2 to 26.5% (table 3, disturbance D1). The rest is equally subtracted from the other C4 inlet components. The new composition is within the range of compositions found in literature for C4 streams coming from the steam crackers [2].

Although the reactor feed flow remains constant, the internal flows are changing. Less IB leads to a lower conversion (reaction rate of the main reaction is proportional with the IB concentration) and therefore to a higher recycle flowrate, which in turn causes less fresh feed to be added into the plant (fig. 8, left). The product flowrate also decreases.

When the percentage of n-C4 in the feed stream increases, the C4 composition ($Z_{C4,4}$, fig. 8, right) in the product stream decreases. Therefore, although the compositions are changing, this particular case would not be a concern for meeting the product specifications. Product carryover in the overhead stream could not be observed.

Having more n-C4 (inert) at plant inlet decreases the temperature inside the reactor, which is compensated by the control system which raises the reactor-inlet temperature (fig. 9, left). Due to the change of the composition profile along the column, it takes longer to bring the temperature back to the set-point (fig. 9, right).

Component	Initial Mole %	Disturbance, D1 Mole %	Disturbance, D2 Mole %
n-Butane (n-C4)	13.2	26.5	6.6
Isobutene (IB)	48.1	43.7	50.3
2-Butene (2-Bu)	13.2	8.7	15.4
1-Butene (1-Bu)	25.5	21.1	27.7
Total	100.0	100.0	100.0

Table 3
FEED COMPOSITION DISTURBANCES

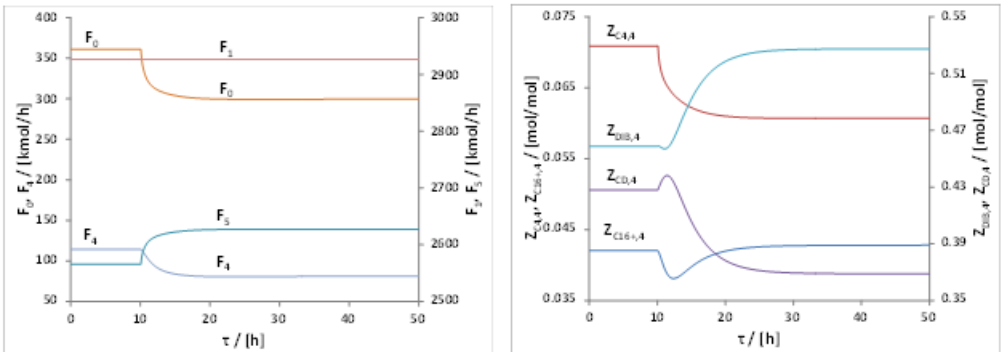

Fig. 8. Control structure CS1: Dynamic response of flow rates (left) and compositions (right), for feed composition disturbance D1

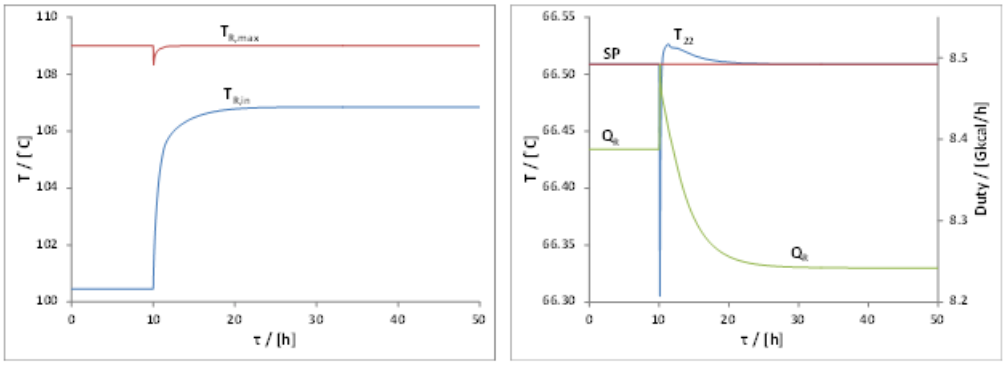

Fig. 9. Control structure CS1: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for feed composition disturbance D1

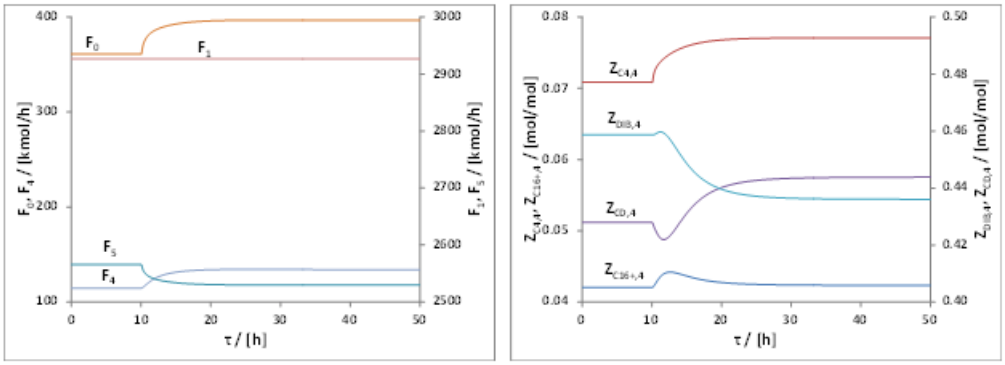

Fig. 10. Control structure CS1: Dynamic response of flow rates (left) and compositions (right), for feed composition disturbance D2

When less n-C4 is considered in the fresh feed flowrate, the percentage of n-C4 is reduced at half of the steady state value, from 13.2 to 6.6%. The difference is equally distributed to the other C4 inlet components (table 3, last column). The new composition is also within the range of compositions found in literature for C4 streams coming from the steam crackers.

Although the reactor feed flow remains constant (F_1), the internal flows are changing (fig. 10, left). Less n-C4, and consequently more IB at plant inlet, results in a higher IB concentration, which leads to a higher conversion and a lower recycle flowrate (F_5). Therefore, the plant inlet flowrate (F_0) increases (≈10%) to reject the disturbance.

It is to be noticed that, although the plant reaches a new steady state condition and TC7 brings the temperature at set point (fig. 11, right), the product purity cannot be anymore achieved just with the column bottom temperature controller installed. There is C4 accumulation in the product stream when less n-C4 and more butenes are added into the system (fig. 10, right).

In theory, if the flowrates to a distillation process are all held as ratios and the temperature on any tray is held constant, all temperatures and compositions throughout the column should return to their original values [11]. However, changing the ratio of components at plant inlet also changes the ratios at reactor outlet / column feed. In this case, the control of temperature on a tray cannot guarantee a constant composition, because in multi-component systems the temperature does not correspond directly with certain ratio between the components [11].

Less inert in the feed also results in a temperature increase inside the reactor. The reactant concentration in the reactor is higher and results in a higher conversion and more heat released. The reactor inlet temperature needs to be decreased so that the temperature inside the reactor is not increasing further (fig. 11, left).

If the levels of impurities in the product cannot be tolerated, an improved control structure should be developed. This will be detailed in the following chapters.

Control structure 2 (CS2) – Temperature-concentration cascade control

In chemical engineering industry the products should always be obtained according to a given specification. The level of impurities in the products should not exceed the specified limits. By exceeding the limits, off-spec product is obtained which leads to increased production costs by the need of reprocessing it. In figure 10 (right) it could be observed that the C4 fraction in the product increases from 7.1 to 7.8 %. In case an economic analysis leads to the conclusion that this would make the plant uncompetitive, a flowsheet containing a composition controller in cascade with the bottom temperature controller is developed, aiming to control the C4 fraction in the column bottom product.

Composition measurements alone typically have larger dead-times and lags than does temperature control [11]. Samples are taken, analyzed and the proper process adjustments are performed. The process is slow, but it drives the product purity to the desired value. In the same time, the temperature controllers are relatively fast, but as it was shown, they may not hold the product purity at desired value. The cascade composition-temperature control structure combines the advantage of both controllers: fast control while achieving the required product purity [11].

The input to the composition controller (*PV*) is the C4 fraction in the bottom product. In order to model the composition control in a realistic way, an Aspen Plus Dynamics *Discretize* operation block is added, to properly represent the concentration measurements. The samples are taken every 15 min while their analysis lasts for 10 minutes. The output (*OP*) - the setpoint of the bottom temperature controller (TC7) – is adjusted every 25 min. The output (temperature units) has the same range as the temperature controller set point.

The tuning of the composition controller was performed via a relay-feedback test (closed loop auto-relay tuning method). While running the dynamic simulation, the test is executed with the composition controller in manual mode and bottom temperature controller in cascade. In the ATV (auto-relay tuning) method (fig. 12), the controller

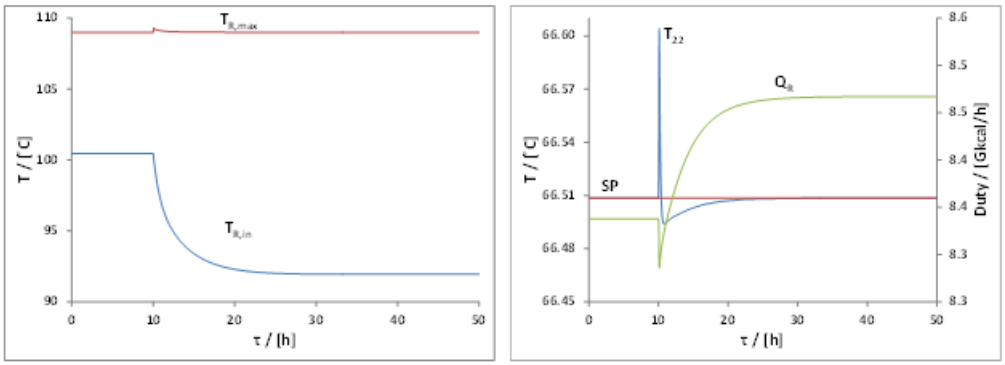

Fig.11. Control structure CS1: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for feed composition disturbance D2

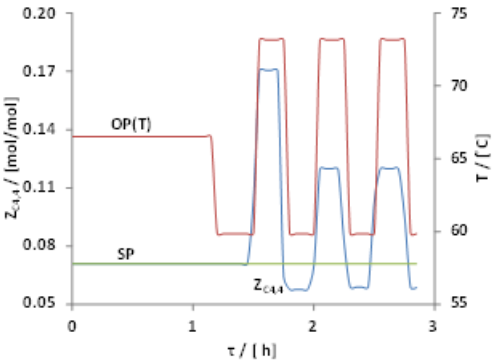

Fig.12. Relay-Feedback test

/ relay output (*OP*) is reversed each time the controlled variable (*PV*) crosses the set point (*SP*) [10]. The test provides the ultimate gain (K_U) and ultimate period (P_U), based on which, the gain and reset time of the composition controller are determined.

With the *Discretize* operation installed and the test started, the ATV method provides the ultimate gain and ultimate period (K_U = 0.298 % / %, P_U = 30 min). The controller gain and integral time are calculated with Tyreus-Luyben tuning rules:

$$K_C = \frac{K_U}{3.2} \quad (6)$$

$$\tau_i = 2.2 \cdot P_U \quad (7)$$

The result is: K_c = 0.093 % / % and τ = 66 min.

Due to high reset (integral) time, the time needed to eliminate the offset is relatively high. The controller behaves similarly to a P-only controller.

In order to observe the response of the process and the performance of the composition controller, the process is subject to several perturbations.

Reactor inlet flow disturbance

The first disturbance is a 10% decrease of the reactor inlet flowrate (F_1). It is observed that the plant reaches relatively soon (≈ 4-5 h) a new steady state. Since the feed control philosophy is to keep the level in the feed vessel (*V*) fixed, the fresh feed flowrate (F_0) decreases as well (by ≈ 9%, fig. 13, left), to compensate for the increase of level in the drum due to less reactants fed into the reactor. The recycle and product flowrates are following the perturbation and decrease with approximately 8.5 and 11.5% respectively.

The composition of C4 in the bottom product is brought back to the set point (fig. 13, right), decreasing the reboiler duty (fig. 14, right). The deviation from the steady state value is less than in the case when only the temperature controller was installed in the bottom. Product carryover in the overhead stream is not observed.

When the reactor inlet flow (F_1) is increased by +10%, the fresh feed flowrate (F_0) also increases, in order to maintain the level in the feed drum which would start decreasing. The recycle (F_5) and product flowrate (F_4) are following the disturbance and increase by approximately 10% and 7% respectively (fig. 15, left), similar as in the previous section. The accumulation of light components in the product stream ($Z_{C4,4}$, fig. 15, right) or the product carryover into the overhead stream does not occur.

The temperature inside the reactor is well maintained close to the set point by slightly decreasing the reactor inlet temperature ($T_{R,in}$), without exceeding the upper limit (fig. 16, left).

The control structure provides a stable and smooth operation and a new steady state is reached whenever a disturbance in the feed flow occurs within the range of +/ - 10%.

Plant feed composition disturbance

The change in the feed composition is a relevant scenario which is worth to be investigated. In the previous section, it was observed the difficulty of maintaining the product impurity level when the plant inlet composition was changed, just by having a simple column bottom temperature controller in place.

The first step considers a change in plant feed composition such that more n-C4 is added.

The percentage of n-C4 is increased by twice of the steady state value, from 13.2 to 26.5% (table 3, disturbance D1). The rest (up to 100%) is equally subtracted from the other C4 components. The new composition is within the range of compositions found in literature for C4 streams coming from the steam crackers.

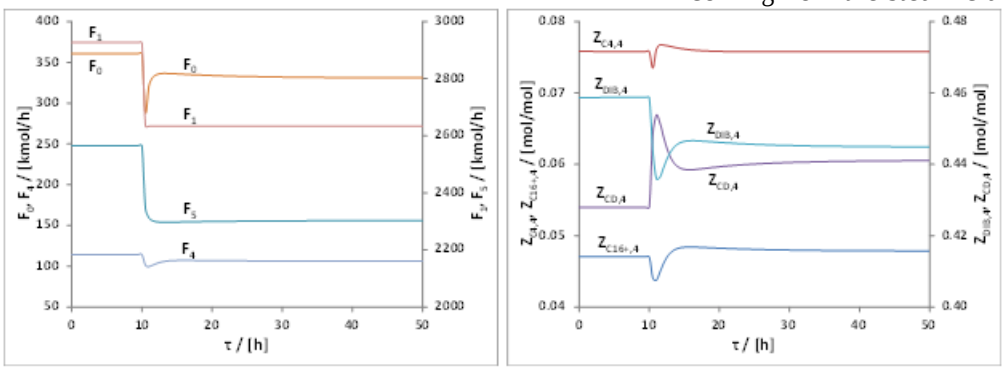

Fig.13. Control structure CS1: Dynamic response of flow rates (left) and compositions (right), for 10% decrease of the reactor inlet flow rate

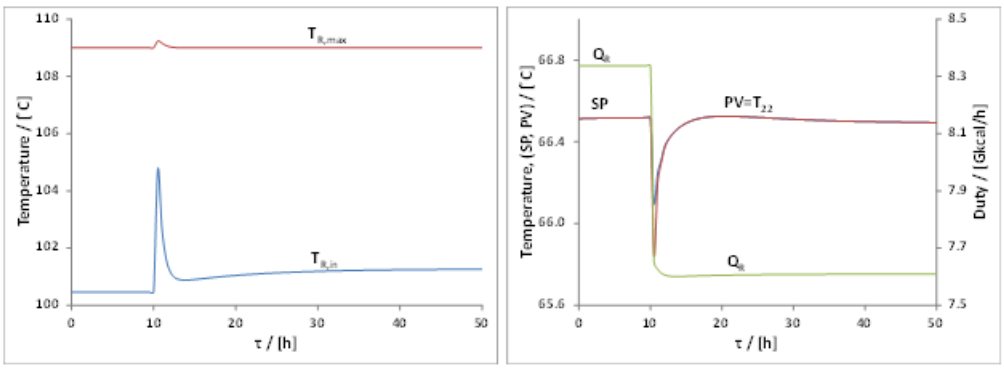

Fig.14. Control structure CS2: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for 10% decrease of the reactor inlet flow rate

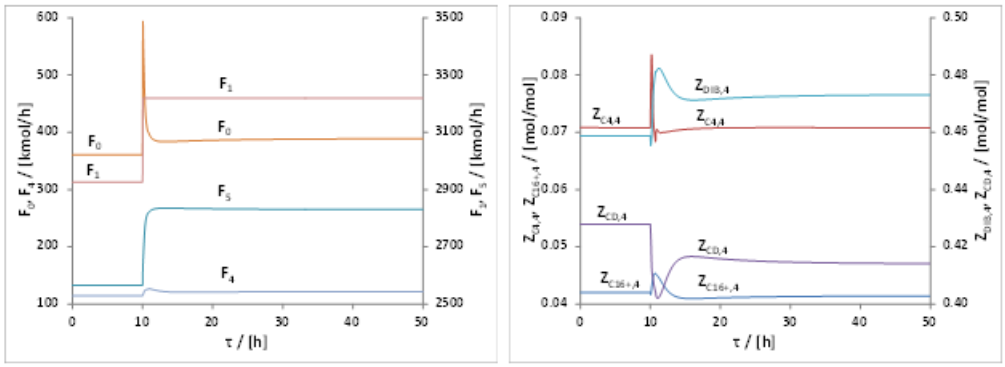

Fig.15. Control structure CS2: Dynamic response of flow rates (left) and compositions (right), for 10% increase of the reactor inlet flow rate

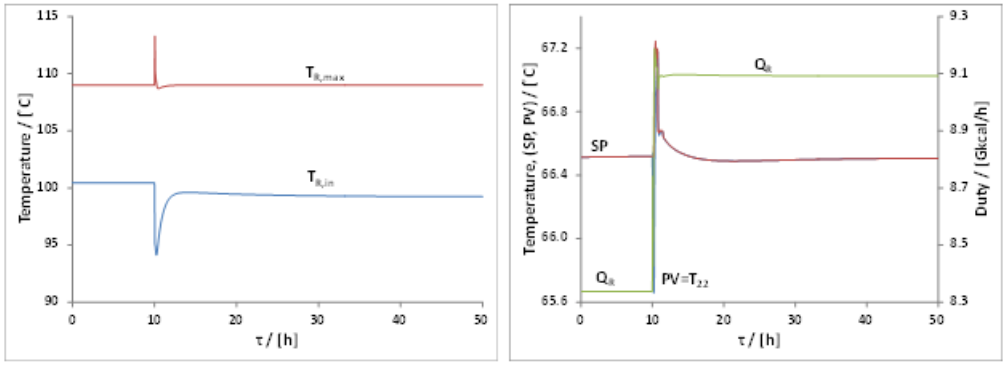

Fig.16. Control structure CS2: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for 10% increase of the reactor inlet flow rate

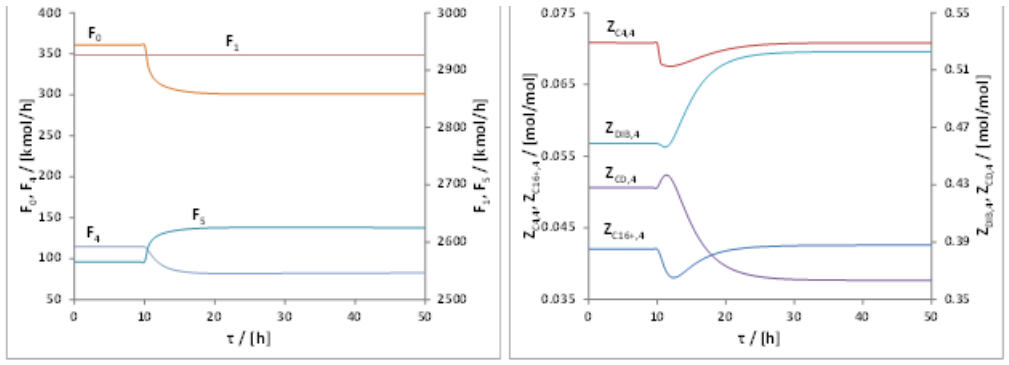

Fig.17. Control structure CS2: Dynamic response of flow rates (left) and compositions (right), for feed composition disturbance D1

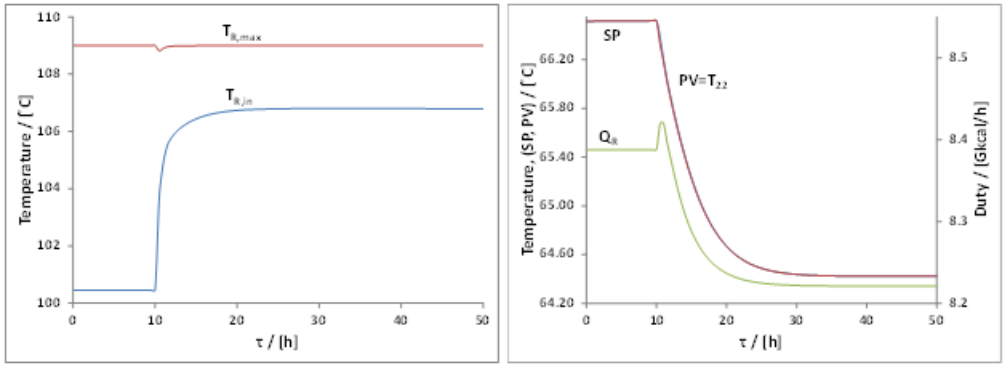

Fig. 18. Control structure CS2: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for feed composition disturbance D1

Less IB leads to a lower conversion and therefore to a higher recycle flowrate (F_5), which in turn causes less fresh feed (F_0) to be added into the plant (fig. 17, left). The product flowrate also decreases (F_4).

This scenario would not create any issues regarding the product specification, since at the time the composition of n-C4 is increased at the plant inlet, there is a decrease of C4 fraction in the product stream. However, it can be observed the influence of the composition controller, which brings back the C4 fraction to the set point (fig. 17, right). The set point of the temperature controller is not fixed anymore and it is continuously changed by the composition controller based on the C4 composition variation in the product stream (fig. 18, right).

The reactor temperature ($T_{R,max}$) is properly maintained by increasing the reactor inlet temperature ($T_{R,in}$, fig. 18, left).

The concerns appear when the concentration of n-C4 is decreased at the plant inlet and the amount of C4 in the product stream tends to increase.

When the concentration of n-C4 in the fresh feed flowrate is decreased at half of the steady state value, from 13.2 to 6.6%, the difference is equally distributed to the other C4 inlet components (table 3, disturbance D2). The new composition is also within the range of compositions found in literature for C4 streams coming from the steam crackers.

Although the reactor feed flow remains constant (F_1), the internal flows are changing (fig. 19, left). Less n-C4 results in a higher IB concentration at plant inlet, which leads to a higher conversion and lower recycle flowrate (F_5).

Therefore, the plant inlet flowrate (F_0) increases by about 10%. With the cascade concentration-temperature

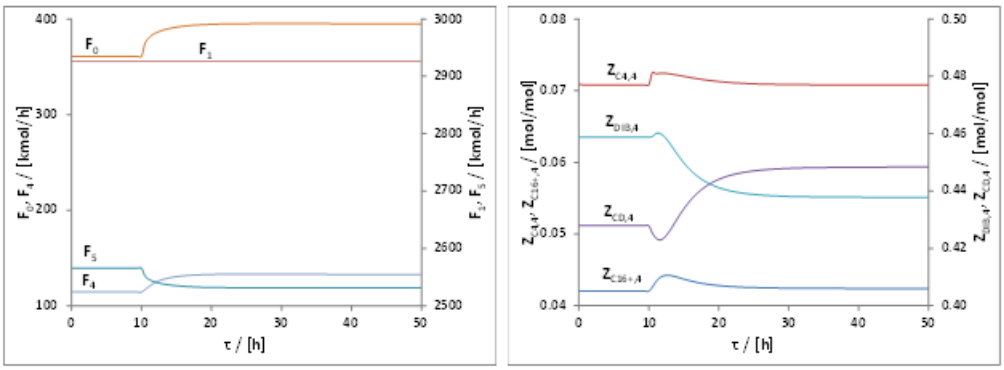

Fig. 19. Control structure CS2: Dynamic response of flow rates (left) and compositions (right), for feed composition disturbance D2

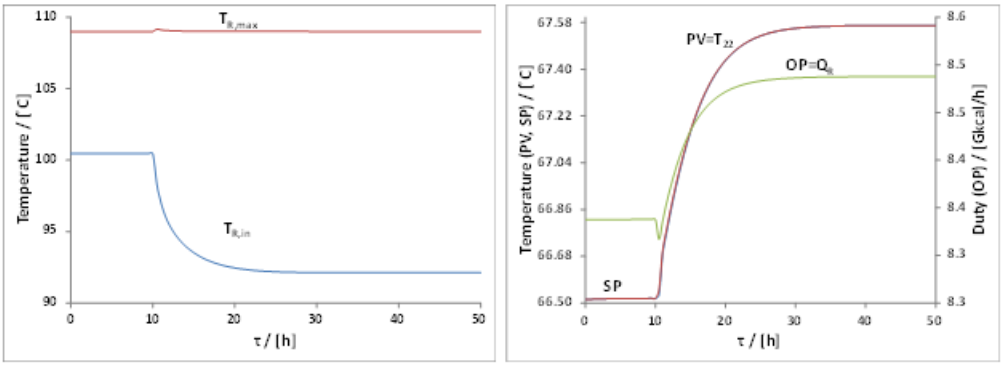

Fig. 20. Control structure CS2: Dynamic response of the reactor temperature (left) and column bottom temperature controller (right), for feed composition disturbance D2

controller in place, it can be observed that the accumulation of C4 fraction in the product does not occur and the C4 concentration is brought to the set point (fig. 19, right).

Shortly after the disturbance occurs, the C4 concentration starts to increase. The composition controller takes corrective action and starts changing the set point of the temperature controller (fig. 20, right). Increasing the set point means increasing the temperature on tray 22 (column bottom), which is achieved by increasing the reboiler duty. This action strips out the light components from the bottom product and a gradually decrease of C4 concentration in the product is observed (fig. 19, right), until it reaches the set point.

The reactor temperature, which tends to increase, is properly maintained by decreasing the reactor inlet temperature, lowering the heater (*H1*) duty (fig. 20, left).

Conclusions

The robustness of the steady state flowsheet and the proposed control system has been assessed by performing dynamic simulations and considering different disturbances: reactor feed flowrate and fresh feed composition.

The production rate could be safely increased or decreased (at least 8%) by changing the set point of the reactor inlet flow controller and feeding more (or less) fresh flow into the plant, without affecting the product purity or moving the operation of the equipment out of their operating window.

When the fresh feed composition was changed, it was observed that although the plant reached a new stable steady state, the product purity could not be maintained any more, just with a simple column bottom temperature controller installed. Therefore a cascade composition-temperature control loop was provided and properly tuned following the built-in methods of Aspen Dynamics. The product composition could then be successfully achieved.

The reactor temperature was properly maintained and prevented to reach the upper limit, by the reactor temperature control loops.

References

1. KIMURA, N., MORIKITA, T., HAMAMATSU, T., 17th Saudi Arabia-Japan Joint Symposium, Dhahran, Saudi Arabia, November 11-12, 2007.
2. KOLAH, A.K., QI, Z., MAHAJANI, S.M., Chemical Innovation, 31, no. 3, 2001, p. 15.
3. HONKELA, M., Dimerisation of Isobutene on Acidic Ion-Exchange Resins, Industrial Chemistry Publication Series, Espoo, 2005.
4. KAMATH R.S., Ind. Eng. Chem. Res., 45, 2006, p. 1575.
5. TALWALKAR, S., MANKAR, S., KATARIYA, A., ANGHALAYAM, P., IVANOVA, M., SUNDMACHER, K., MAHAJANI, S., Ind. Eng. Chem. Res., 46, 2007, p. 3024.
6. TALWALKAR, S., CHAUHAN, M., AGHALAYAM, P., QI, Z., SUNDMACHER, K., MAHAJANI, S., Ind. Eng. Chem. Res., 45, 2006, p. 1312.
7. DRAGNEA, P., BILDEA, C.S., Bulletin of Romanian Chemical Engineering Society, 1, no. 1, 2014, p. 15.
8. LUYBEN, W.L., Practical Distillation Control, Van Nostrand Reinhold, New York, 1992.
9. JANA, A.K., Process Simulation and Control using Aspen, PHI Learning, New Delhi, 2012.
10. DIMIAN, A.C., BILDEA, C.S., KISS A.A., Integrated Design and Control of Chemical Processes, Elsevier, 2014.
11. LUYBEN, W.L., Distillation Design and Control Using Aspen Simulation, John Wiley & Sons, Inc., 2006.

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