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THE POSSIBILITIES OF ADVANCING ISOMERIZATION PROCESS THROUGH CONTINUOUS OPTIMIZATION

Abstract

The process of isomerization is one among the key processes of oil generation in the production of motor gasoline of a given quality, and so, it is the purpose of every refinery for the process to be used to the fullest. To this end, there have been process advancements through the introduction of new units, such as feed prefractionation in deisopentanizer column, and separation of isomerization products through the application of molecular sieves or fractionation column. Further process advancements are based on a continuous optimization in real time, enabling the mastering and minimization of the impact of process bottlenecks, as well as maximum capacity use.

Mathematical models have been set up consisting of both dependent and independent values, for the purpose of exploring optimal working conditions, while the paper explores the possibilities of a continuous optimization in real time, the stress being on field application.

Introduction

The process of isomerization in refinery and petrochemical industry is being applied for the purpose of converting the low-octane fraction of light gasoline into high-octane fraction, for producing i-C4 for alkylation, and for producing MTBE¹.

An increasing number of refiners is faced with the fact that the process of isomerization is becoming a certain bottleneck in the production of high quality gasoline, due to stringent quality requirements through the limitation of maximally permissible share of aromatics in motor gasoline.

The goal of process advancement is the overcoming of bottlenecks, while – in the case of isomerization process, the advancement is achieved as follows:

- 1) Designing: Introducing new units enabling better use of process capacities: deisopentanizer column, deisohexanizer column, and molecular sieves,
- 2) Applying the latest generation of catalysts and the corresponding process equipment,
- 3) Advancing process control through the application of model predictive control².

The process of isomerization

The subject of the present paper is the process of isomerization at Rijeka Refinery. The process feed is a compound of light gasoline C5-85 °C from the atmospheric distillation plant and light reformat.

Given the characteristics of the isomerization reactions, the proces requires a given feed treatment, which is why the entire process may be broken down into several sections:

- 1) Prefractionation section in deisopentanizer column

For the purpose of a better plant capacity use, in deisopentanizer column there occurs feed prefractionation by the separation of high octane isopentane in column top. The product from deisopentanizer bottom, a fraction rich in n-C5 and n-C6 hydrocarbons, goes to further processing through isomerization.

- 2) Hydrotreating Section

The feed is additionally processed by hydrotreating which removes compounds of sulphur, nitrogen and oxygen, which are acting as catalyst poison on the catalysts for hydrogenation and isomerization. During hydrotreatment, apart from removing sulphur and other noxious compounds, there is also the reaction of olefin saturation.

Catalytic hydrotreating reactions proceed with cobalt-molibdenum sulfides on aluminum-oxide as bearer in a hydrogen-rich atmosphere.

- 3) Section of hydrogenation

The feed is being processed also through the section of hydrogenation, due to saturation of remaining unsaturated hydrocarbons and benzenes, which - unless removed - would react with hydrogen in the isomerization reactor and generate a lot of heat due to exothermal reactions. The reactions proceed on a catalyst Pt/Al₂O₃. Given the sensitivity of the catalyst of isomerization to moisture, the water share in the feed before introduction into the section of hydrogenation must be below 0.5 ppm mas.

- 4) Isomerization

The process of isomerization improves the applicative properties of C5 and C6 hydrocarbons, through molecule partitioning. The process causes the conversion of n-compounds, pentane and hexane, into iso-compounds and hence also an octane number increase. Isomerization is a catalytic process, with platinum used as

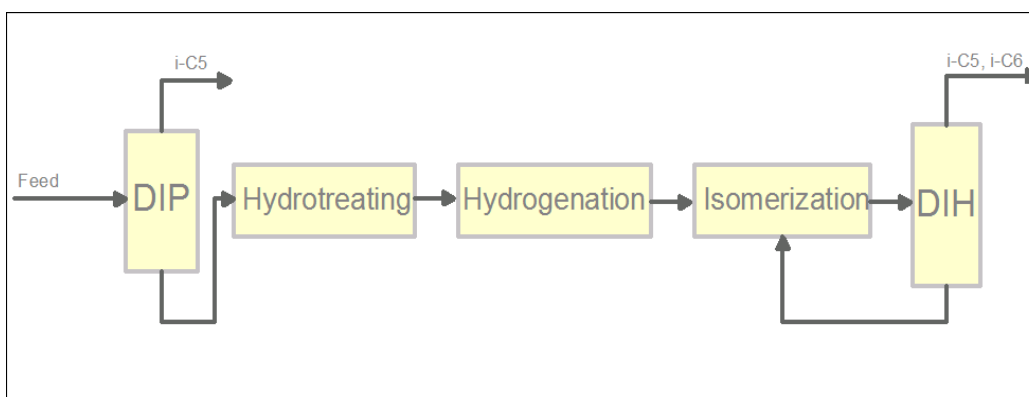
catalyst, on a solid Al_2O_3 bearer. Reactions proceed with the presence of chlorine as promotor of catalytic reactions and within a hydrogen-rich atmosphere.

5) Section of fractionation in deisohexanizer column

Section of fractionation in deisopentanizer column enables increase of the octane number of isomerisate by further 4-6 units. In deisohexanizer column, low-octane fractions are being separated from the high-octane ones, thus achieving a higher value of the product's octane number. Low-octane fractions recycle for processing in isomerization section.

A simplified outlay of the entire process is shown in Figure 1.

Figure 1: Isomerization process scheme



Approach to advancement

The present paper sets and presents the possibility of advancing process control through the application of a model predictive control and software analyzer.

Model predictive control has been developed on the basis of theoretical essentials of process control and the development of computer application^{3,4}, while - in practice - it constitutes a number of tools enabling continuous acting on the regulatory circles of the process, for the purpose of the criterion for continuous performance optimization in real time⁵. By the application of model predictive control in practise, optimal control is performed - control for the purpose of: maximizing plant capacity use, maintenance of constant quality of individual products, lowest energy consumption, etc.

Software analyzers are based on the mathematical model enabling on-line estimation of the physico-chemical properties and chemical composition. They may be applied in individual work, but also as a supplement to classical hardware process analyzers⁶.

Due to the characteristics of the process of isomerization, as well as the importance of optimal performance of the deisopentanizer column section, the deisopentanizer column is a theoretical example of applying the system of model predictive control in real time. By advancing DIP section, the entire isomerization process is advanced.

Advancing the control of deisopentanizer column section by applying model predictive control unit has as purpose:

- maintenance and advancement of yield quality,
- minimization of energent consumption,
- maximum capacity use,
- maximum yield of more valuable products,
- improved process stability and safety,
- minimal impact of disturbances on process operation.

A description of the deisopentanizer section process

The feed - a compound of light reformat and light gasoline C5-85°C - is, after pre-heating using vapour in heat exchangers E-101A/B, introduced into 40, 50, 60 and 70 column C-101 tray, where the components are separated. Top column product, fraction rich in isopentane, is conducted through air and water refrigerators EA-102 and E-103A/B into collection vessel of condensate V-101. A part of the fluids from the vessel is conducted - using pump P-103A/B - into the column as reflux, while the product, isopentane with mass concentration 90-92%, is separated as top product and forwarded for further processing. Column bottom is heated through the vaporizer E-104 using low-pressure vapour, while the bottom product - a compound of n-pentane and C6 hydrocarbons, is cooled through heat exchanger E-106 and conducted into the first catalytic section of the plant: the section of Hydrodesulfurization.

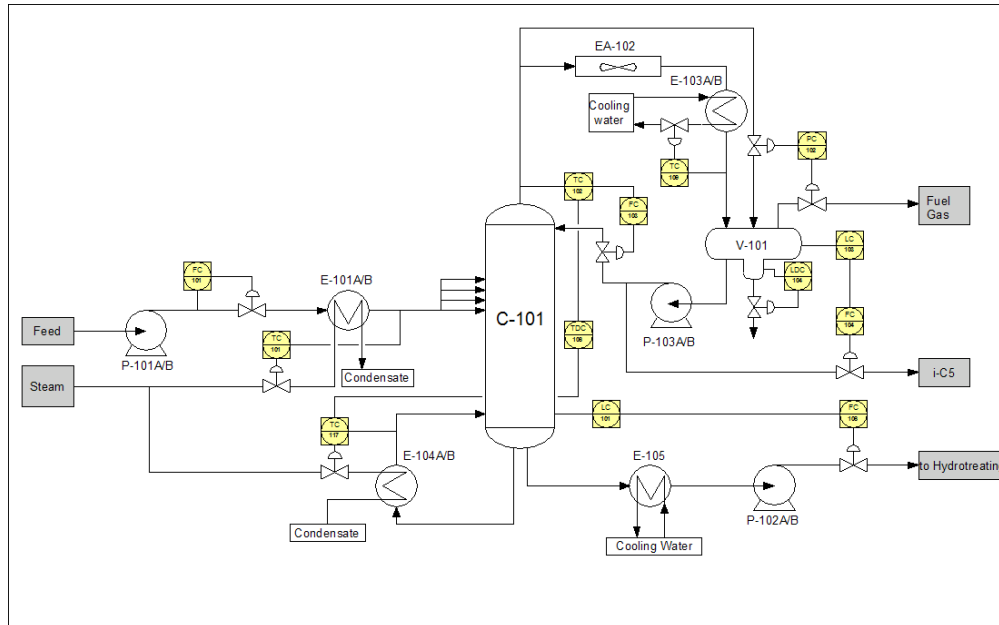
Total capacity of the section of deisopentanizer, and hence also the entire process, is regulated using flow regulation FC101, and the temperature of DIP feed - through the regulation of temperature TC101 by acting on vapour valve through heat exchanger E-101.

Temperature of top column is maintained through cascade regulation of temperature TC102, through the activity of temperature regulator TC102 on the reflux flow regulator FC103, set up in the cascade. The pressure in the column is maintained through pressure regulation PC102, through the action of the valve on the flow of top vapour into the collection vessel of reflux V-101. The level in vessel V-101 is maintained through level regulation LC103, impacting the openness of the top product flow valve, FC104.

The temperature of bottom column is maintained through the regulation of temperature TC117 by acting on the flow of low-pressure vapour through the vaporizer E-104. The difference in the temperature between top and bottom of the column is measured and regulated using TDC106, while temperature on the 120th

tray of the column is measured using temperature indicator TI104. The level of deisopentane column is regulated using the level regulator LC101, impacting product flow, placed in the cascade - the flow regulator FC106. The outline of the deisopentane section process is shown in Figure 2.

Figure 2: The deisopentane section process DIP column process scheme



An analysis of control and application of optimal process control

For the purpose of performing model predictive control and setting up the model predictive control unit, an analysis has been performed of deisopentane column control. Defined were the input and output process values, based on a systematic approach, and dependences set between the values, as set in Table 1. Due to the mutual dependence between a number of input and output values, the system for an optimal control of deisopentane column requires advanced process control, through the application of the model predictive control^{7,8}.

Also - since one among the criteria of deisopentane column control is maximum isopentane separation in the top column product, advanced control requires the equipping of the column by a top product analyzer - a software analyzer, as shown in Figure 3.

Table 1: Dependence between input and output values

		Output values										
		TC101.OP	PC102.OP	FC103.OP	FC103.PV	FC104.OP	TC109.OP	TC117.OP	FC106.OP	TDC106.PV	TI104.PV	AI101.PV
Input values	FC101.SP	Model	Model	Model	Model	Model	Model	Model	Model	Model	Model	Model
	TC101.SP	Model	Model	Model	Model	Model	Model	Model	-	-	Model	Model
	PC102.SP	-	Model	Model	Model	Model	Model	Model	Model	Model	Model	Model
	TC102.SP	-	Model	Model	Model	Model	Model	Model	Model	Model	Model	Model
	TC109.SP	-	-	Model	Model	Model	Model	-	-	-	-	Model
	TC117.SP	-	Model	Model	Model	Model	Model	Model	Model	Model	Model	Model

Based on the analysis performed and the set input and output values, a system of model predictive control was established, through the application of the appropriate program system. Given the impossibility of performing an experimental research of the plant, the research was performed on the basis of engineering know-how and practice, as well as through the application of the statical mathematical model of the process in question⁹.

Obtained were mathematical dynamic models of the dependence of input and output values, together with the set criterion of optimization, constituting a model predictive control unit.

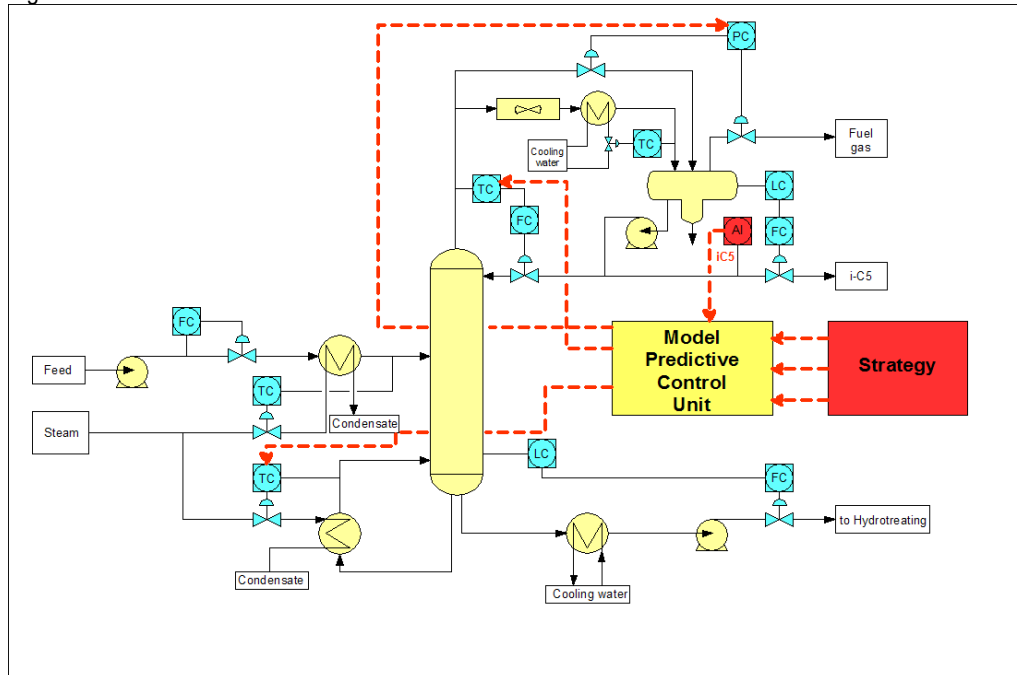
Criteria for the optimal control of deisopentanizer column are as follows:

- maximum separation of isopentane in top column,
- minimal energy consumption,
- minimal disruption impact on column performance.

Criteria of optimal control of deisopentanizer column have been set in order to impact the advancement of the entire process, for the following purpose:

- maximum capacity use of the entire process,
- extended catalyst service life,
- more stable operation of the entire plant.

Figure 3: DIP column with MPC unit scheme



An example of the possibility of advancing deisopentanizer column through optimal control application

The criterion of optimization: minimizing energent consumption

The activity of a model predictive control unit has been graphically described through the outline in Figure 3. As a criterion of optimization in the described example, defined was the minimization of energent use. Through the activity of a model predictive control unit, the criterion of optimization is being performed on-line, in real time, acting each minute on the key regulation circles, i.e. input values: top column pressure, PC102.SP, temperatures of the top and bottom of deisopentanizer column, TC101.SP i TC117.SP, other input values. The key value for estimating column operation is the mass isopentane share in the top product. Since there is no on-line monitoring of the chemical composition of the top column product, for the purpose of a better control of the DIP column, the advancement by elaborating a software analyzer for determining isopentane in top product is suggested. Apart from isopentane share in top column product, the model predictive control unit obtains response from other output values, which is the basis for a further performance of the criterion of optimization within the set permissible limits of input and output values.

Figure 4: MPC Unit actions

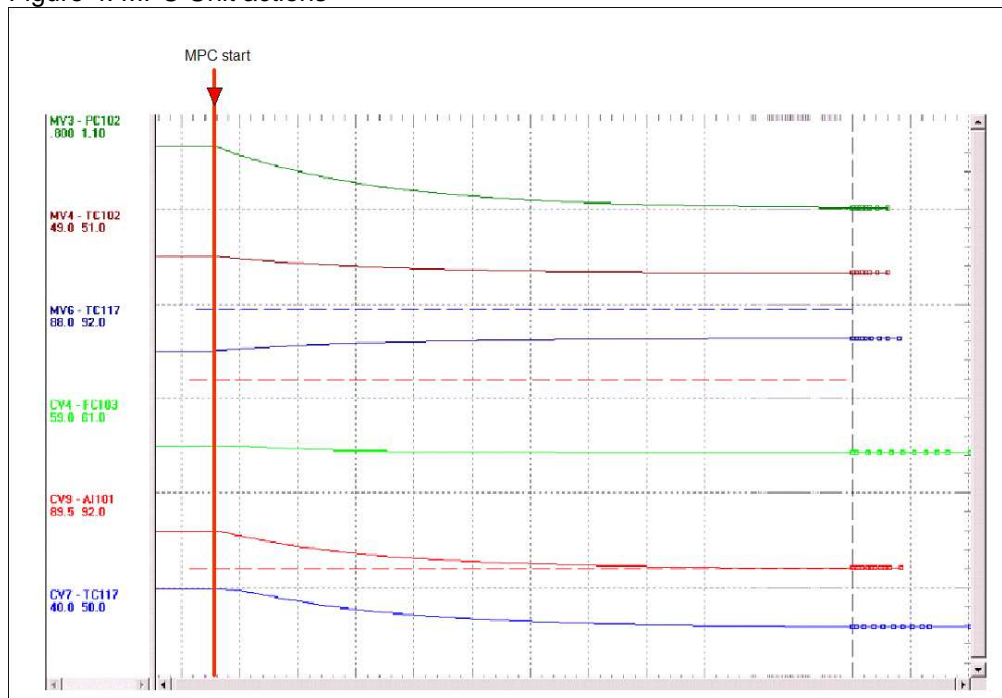
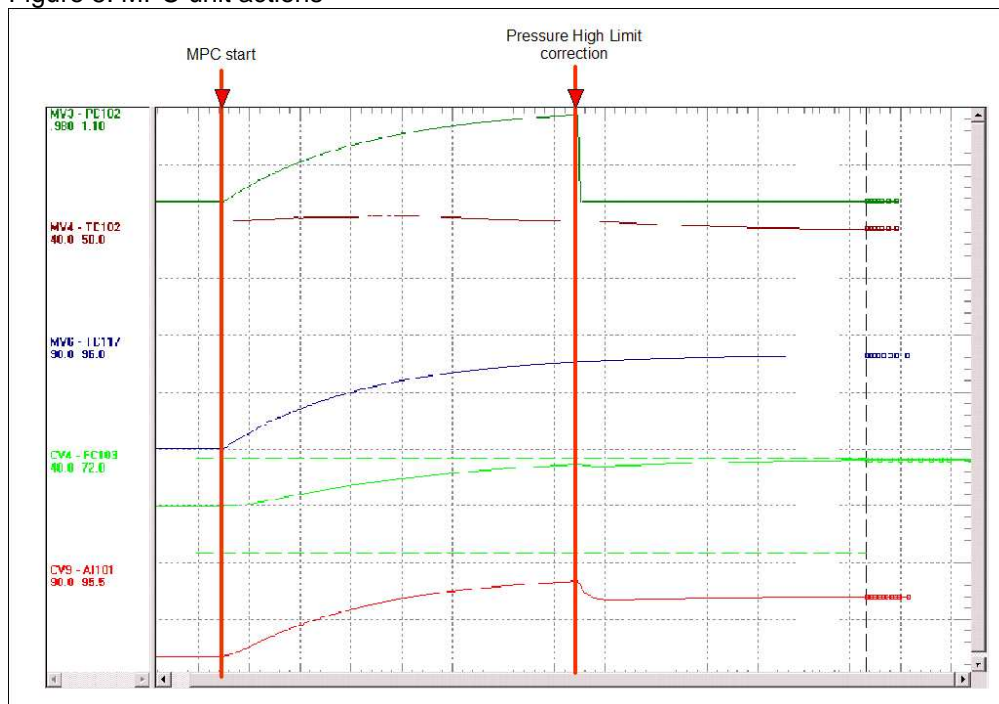


Figure 4 presents the action of the model predictive control unit on the key input and output values. The presented graph reveals that minimal energy consumption is achieved through minimal pressure in the column up to the set bottom limit, as well as minimal top column temperature TC102. This results in a mild increase of the bottom temperature due to a reduced reflux flow through the column, FC103.PV, but also achieved is a reduced consumption of the bottom column heating medium by closing down the valve, TC117.OP. The key value setting the bottom limit of pressure decrease is the share of isopentane in the column product, set at 90 mas%. By reaching the minimal permissible limit of isopentane share, a further minimization of energent consumption is limited.

As a criterion of optimization, one may also set the maximum isopentane share of top column product. The results of the unit's activity on optimal process control are as shown in Figure 5. The unit for optimal control causes the increase of pressure and temperature throughout the column, in order to achieve as high as possible a share of isopentane in top product. The second step is the limiting of the activity of the model predictive control unit by reducing top pressure limit. After pressure limitation, the model predictive control unit finds the optimal solution under momentary process conditions in keeping with the current process limitations.

The purpose of introducing a model predictive control unit is the on-line performance of all the required criteria of optimization and determining an optimal solution each minute, depending on the current process conditions. The advantages of such process control over classic control lies in the fact that key process values: input and output values, are observed on-line each minute, enabling impacting the input values each minute. Changes are made in small steps without additional introduction of disturbances into the process. In this sense, the application of optimal control is superior to the classic way, based on human possibilities, thus excluding the capability of processing such an amount of information within a single minute. On-line process control also enables operators and process engineers to devote more time to the economics of the process by defining bottom and top amounts of the input and output values, as well as criteria of optimization. The basis for the decision on the criteria of optimization should be daily planning.

Figure 5: MPC unit actions

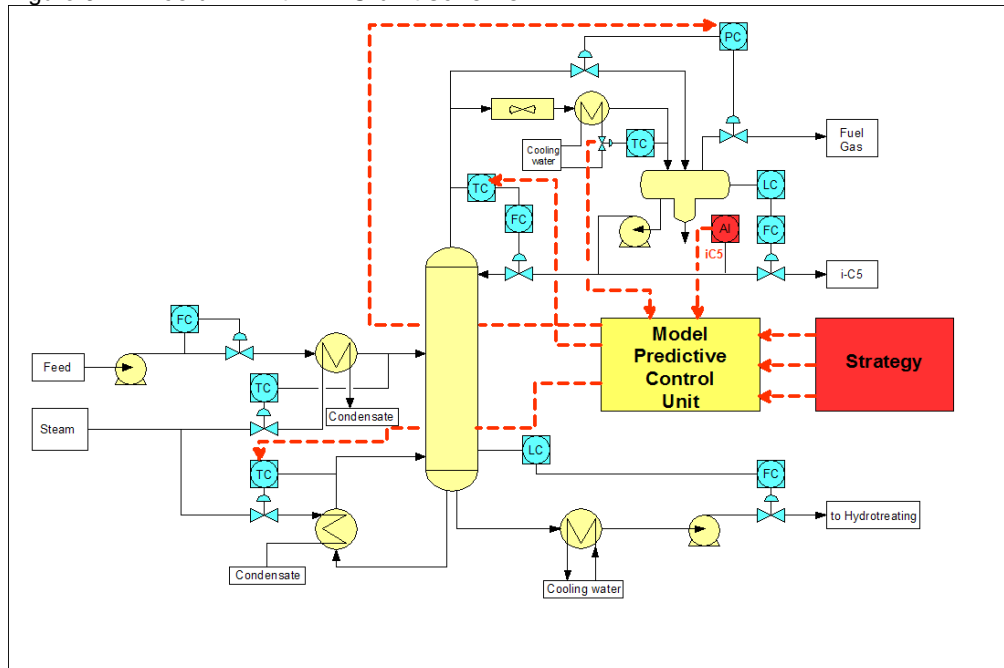


An example of the possibility of advancing deisopentanizer column by optimal control application

Criterion of optimization: minimizing the impact of disturbance on column performance

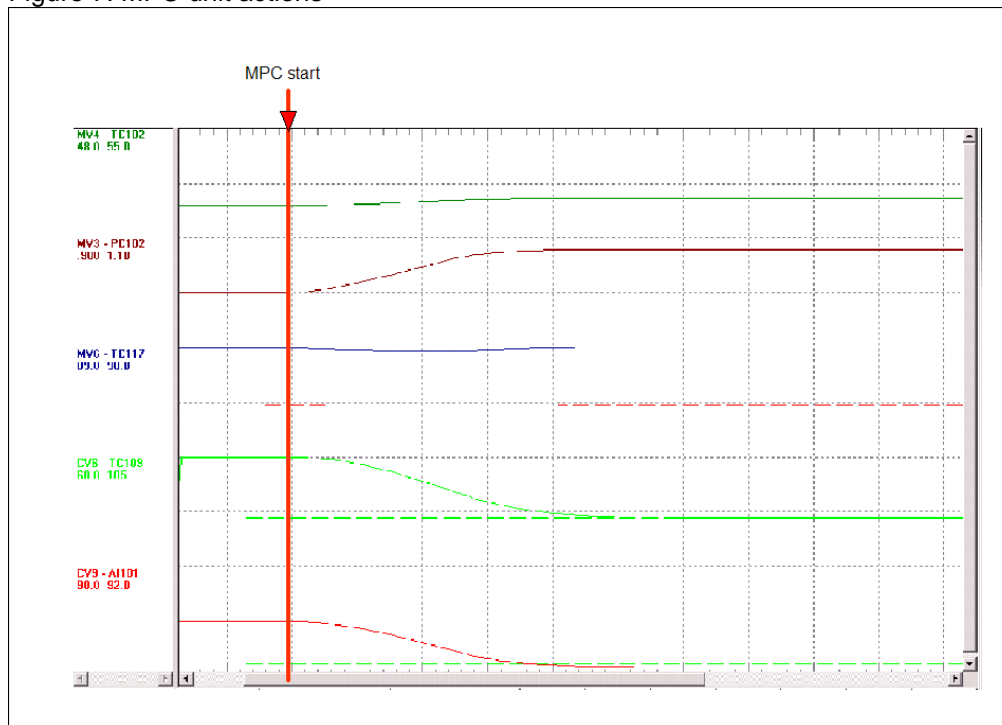
One among the more frequent disturbances in the operation of every column may be the impossibility to adequately cool the column top over summer months. By introducing the optimal process control unit, the problem cannot be entirely dismissed, but it can be reduced by introducing an optimal process control unit, through on-line acting on input values, as shown in Figure 6.

Figure 6: DIP column with MPC unit scheme



According to results shown by Figure 7, it may be observed that the unit for optimal control uses pressure increase, PC102.SP in order to mitigate the disturbance impact, causing the closing down of the cooling water valves TC109.OP, but also reduction of the isopentane share in the top column product.

Figure 7: MPC unit actions



Conclusion

On the example of isomerization process deisopentanizer column, the possibility of process advancement by applying optimal control in real time is demonstrated. In the above examples, the following criteria of optimization have been applied:

- minimal energetic consumption per feed unit,
- maximum top column isopentane share,
- minimal disturbance impact.

The same criteria of optimization may be applied on the entire process of isomerization, and also be expanded to include the following criteria of optimization, relevant to the isomerization process:

- maximizing octane number,
- maximizing capacity use of the entire process of isomerization,
- process control for the purpose of maximizing catalyst life,
- stability and safety of process.

The above examples substantiate the fact that dynamic optimization & model predictive control is today one of the most frequent and most applied methods of process optimization in the world - both in oil-petrochemical industry, and in its related process industries.

UDK	ključne riječi	key words
.001.53	gledište mogućnosti unapređenja procesa	Process Improvement Opportunity (PIO)
665.6.011	analiza i optimizacija procesa	process analysis and optimization
66.012.7	viševeličinsko optimalno prediktivno vođenje	multivariable optimal predictive control

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