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Dynamic Simulation Step to Advanced Process Control Implementation

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Abstract

Paper presents detailed description of the proposed methodology for challenging the control problem of propylene/propane splitter within FCC Gas fractionation unit. Based on this methodology it was proposed that the simulation software HYSYS to be integrated with DMC Plus controller as alternative platform for step testing, being the most cumbersome task in each APC project with very long settling times in association with propane propylene splitter HYSYS dynamics was recently used in real APC projects to overcome challenges like: the need to obtain long time settling accurate response drowned by process disturbances, capture the effect of random movement in feedforward variables. Authors detailed factors that contributed to prepare best practice APC development using this alternative methodology based on dynamic simulation.

Key words: *dynamic simulation, splitter column, APC control, process disturbances*

Introduction

Heat integration, process recycles and minimum hold-ups are typical design features. Whilst such designs optimize steady state operation, they present particular challenges to plant control and operations considering dynamic behavior [1].

Dynamic simulation of refinery and chemical processes based on first principles models has also become a mature technology. This technology is commonly used for design and revamps studies, operator training, testing of DCS configurations and the development of operating procedures.

Paper searched dedicated procedure applied for the real APC implementation using DMC multivariable controller over the process unit. In order to avoid real step tests within refinery units it has been studied the possibility to apply HYSYS simulation software considering their dynamic simulations facilities and compatibility to DMC Plus Software supplied by Aspen. Both software were available within a Romanian refiner already having Aspen APC facilities implemented. Virtual step tests were used to design step curves used for tuning of dynamic compensators, such as PID regulators and lead/lag blocks within a feedforward or decoupling scheme. Using Hysys – DMC Plus integration, no real Gas Fractionation Unit step-tests were needed in the real plant.

The simulation software HYSYS was integrated with the DMCplus controller as an platform in order to develop the step testing, specific task in an APC project with very long settling times, like Propylene/Propane splitter of 232 trays with a settling time of 2 or 3 days.

The steady state simulation model was obtained by incorporating parameters from a case-study supplied by a Romanian refiner. Hence, it may be claimed that the model developed and used in this study provides a better match to industrially observed behavior. It has the following features:

1. Our model considers a feed consisting of four components: Ethane (traces), Propylene, Propane and n-Butane (also traces). The benchmarked model did not consider the off-key components Ethane and n-Butane found in feed in traces and so effectively treated this as a binary system. It is worth noting that when studying inferential control applications in distillation columns, it is essential that one considers situations where a direct one-to-one relationship between tray temperature and tray compositions is absent. Hence, binary systems do not provide a true test for inferential control strategies.

2. In the steady state model, the vapor liquid equilibrium (VLE) was calculated using a relative volatility that was a quadratic function of liquid phase propylene mole fraction. The quadratic coefficients were linear functions of pressure. Hence the tray temperatures aren't functions of the tray compositions. In other words, the benchmarked model is inadequate for inferential control studies. In our model, the Peng Robinson Equation of State (PR-EOS) is used to determine the bubble point temperature and vapor compositions.

3. Simulated column characteristics are presented within table 2. Also feed components physical and thermodynamic property data are indicated within table 1.

4. Our model considers a Murphre tray efficiency of 90% while the benchmarked model's trays are 85% efficient. This difference in tray efficiencies and thermodynamic calculations are responsible for the large differences in the number of trays required for similar degrees of separation.

5. Our model uses a linear wier equation to describe the liquid dynamics with a hydraulic time constant of 3 seconds which is the same as that used in the benchmarked

Table 1. Physical and thermodynamic property data for C3/C3` splitter

Component index	Ethane	Propylene	Propane	n-butane
	1	2	3	4
Molecular weight (MW)	30.07	42.081	44.097	58.124
Critical Temperature (Tc)	305.42	364.76	369.82	425.18
Critical Pressure (Pc)	4880.1	4612.6	4249.2	3796.9
Accentric factor (ω)	0.099	0.1424	0.1516	0.1931
Specific gravity (Sp. Gr.)	0.548	0.612	0.582	0.579

$$P = \frac{RT}{V - b_{mix}} - \frac{a_{mix}(T)}{V(V + b_{mix}) - b_{mix}(V - b_{mix})} \tag{1}$$

Bubble point temperature calculation using the PR-EOS is performed as follows. First, the following pure component quantities for each component q are evaluated [2,3,4]:

$$\left.\begin{aligned}\kappa_q &= 0.37464 + 1.54226\omega_q - 0.26992\omega_q^2\\ b_q &= 0.07780R\tfrac{T_{c,q}}{P_{c,q}}\\ ac_q &= 0.45724R^2\tfrac{T_{c,q}^2}{P_{c,q}}\\ a_q &= a_{c,q}\left(1+\kappa_q\left(1-\sqrt{\tfrac{T}{T_{c,q}}}\right)\right)^2\end{aligned}\right\} \tag{2}$$

The Van der Waals one-fluid mixing rules are used to calculate the parameters for the mixture and the EOS of the mixture in terms of the compressibility.

$$\begin{aligned}a_{mix} &= \sum_{i=1}^{4}\left(\sum_{j=1}^{4}(x_i x_j\sqrt{a_{i,i}a_{j,j}(1-k_{i,j})}\right)\\ b_{mix} &= \sum_{i=1}^{4} x_i b_i\\ A &= \frac{a_{mix}P}{(RT)^2}\\ B &= \frac{Pb_{mix}}{RT}\end{aligned} \tag{3}$$

The following cubic equation is solved for the compressibility roots using Cardano's method. All imaginary roots are set to zero. The largest root is the vapor compressibility (Zv = Zmax) while the smallest one is the liquid compressibility (Zl = Zmin) [4].

$$Z^3 + (B-1)Z^2 + (A - 3B^2 - 2B)Z + (-AB + B^2 + B^3) = 0 \tag{4}$$

$$ln\left(\frac{f_i}{x_i P}\right) = \frac{(Z-1)b_i}{b} - ln(Z-B) - \frac{a\left(\frac{2\sum_{j=1}^{4}(z_j\sqrt{a_i a_j}(1-k_{i,j})}{a} - \frac{b_i}{b}\right) ln\left[\frac{(Z+(1+\sqrt{2}B)}{(Z+(1-\sqrt{2}B)}\right]}{2\sqrt{2}bRT} \tag{5}$$

The procedure consists of two nested iteration loops. The inner loop iterates on the vapor phase composition until the vapor phase species fugacities (fv s) are equal to the liquid phase species fugacities (fl s) for every species within a prespecified tolerance. Once the inner loop converges, the outer loop iterates on the temperature until the vapor phase mole fractions sum to 1 within a prespecified tolerance. When the outer loop iteration is done, the final temperature and vapor composition are the Bubble point temperature and vapor composition.

Table 2. Physical and thermodynamic property data for propane/propylene splitter

Item No.	C3/C3` splitter		
	Characteritics	U.M.	Values
1	Number of trays	-	232
2	Feed tray location	-	64
3	Feed flowrate	kg/s	13.41
4	Lighter than light key component	fr. mol	0.02
5	Light key component C3`	fr. mol	0.42
6	Heavy key component C3	fr. mol	0.56
7	Factor times minimum reflux	-	1.3
8	Column diameter	m	3.96
9	Overhead pressure	atm	15
10	Overhead product impurity	%mol	0.3
11	Bottoms product impurity	%mol	1.0
12	Overhead flowrate	kg/s	9.21
13	Overhead temperature	0C	34.7
14	Bottom flowrate	kg/s	4.21
15	Bottom temperature	0C	42.3
16	Reboiler vapor flowrate	kg/s	131.18 kg/s
17	Reflux ratio	-	12.6
18	Feed quality	-	saturated

Figure 1 shows the process flowsheet along with the controller pairings for the base control system. The Base control system consists of the Reflux-drum level being controlled by the distillate flow rate while the bottom column-level is being controlled by the heat input to the Reboiler. If analyzers for the composition of the top and bottoms streams are available, then the distillate composition can be controlled using the Reflux-flow rate while the bottoms composition can be controlled using the bottoms flow rate.

This arrangement is typical of situations involving a high boil up ratio (i.e. high V/B) and is known as the “L-B” configuration. It should be noted that such an arrangement has the potential for inverse response. Table 3 provides the controller tuning parameters used. Real plant Step-Tests present some challenges [5,6]:

- The need to excite sufficiently to obtain clear responses may produce off-spec product;
- Long settling time responses are drowned by other process disturbances;
- They must be of sufficient duration to capture the effect of random movement in feedforward variables. HYSYS dynamics has served as a simulation platform to experiment with new control technologies for oil refining process units.

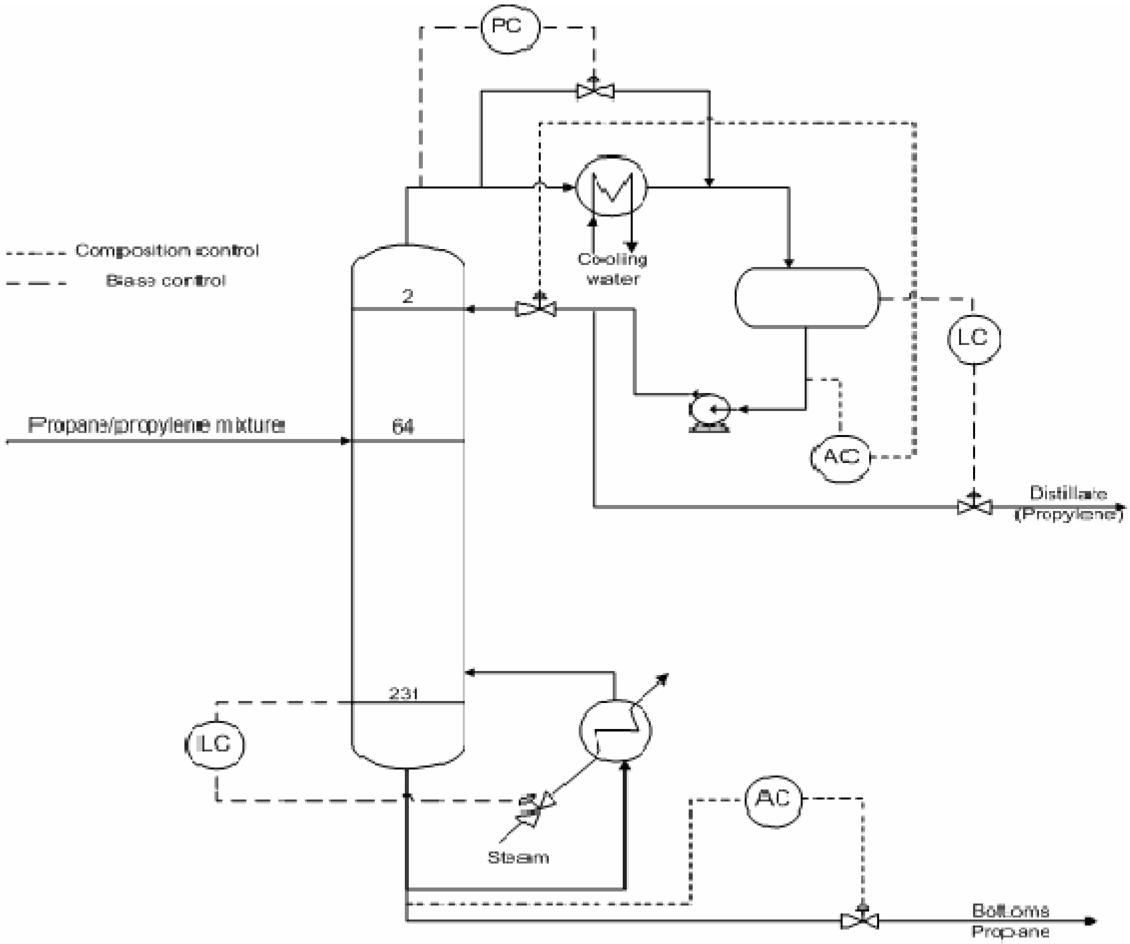

Fig. 1. The Superfractionator (C3 Splitter) with its base control system

Table 3. Control structure, parameters, setpoints and steady state values for propane-propylene splitter

Loop No.	Controlled variable		Manipulated variable		Type	Ke	TR (min)
		SP	Stream (physical state)	SS time			
1	$\%C_3H_6$ in distillate (xT(2))	0.954	Reflux flowrate (LR)	8	PI	0.5	60
2	$\%C_3H_6$ in bottom	0.046	Bottom flowrate (LB)	7.5	PI	20	30
3	Condenser drum level (LT)	50%	Distillate flowrate(LD)	1.2	P	1	-
4	Column bottom level (LB)	50%	Vapor flowrate (VB)	1.6	P	1	-

Dynamic DMC control model

A simulation rigorous model, which may reflect well the actual plant conditions, is a different exercise from producing a rigorous model when designing a new plant. Models of plants to be built by off line simulation don't need to be any historic plant data directly extracted from the historian database. Authors adopted within this study the followed modeling methodology indicated in figure 2.

In a classical control design procedure, control engineers obtain dynamic response information by a series of plant step tests from which empirical models of the process are identified.

Quality of the step test data represents the most important factor determining the success of a multivariable control application. Unfortunately, obtaining good quality step test data can be very difficult. The main issue is that the process must be excited sufficiently such that the process response signals to be represented clearly above the process noise. An acceptable signal to noise ratio may cause not acceptable disturbance to the process and risk off-specification product. In some cases, the time it takes for the process to respond may be so long that the response to the imposed step change becomes drowned by other process disturbances. On-line model-based controllers have been implemented with minimal [2] or no plant testing [3]. The advantages of conducting step tests on a desktop simulation compared to live plant are obvious. No plant testing is required, the test data is free of noise and valve cycles, all feedforwards can be stepped and engineering time and effort can be minimized especially for processes with many variables and/or long settling times [6].

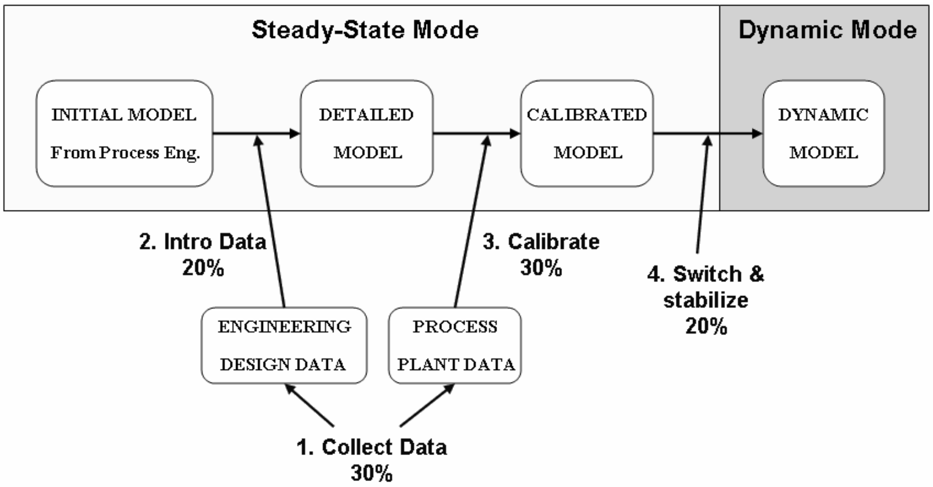

Fig. 2. Prepare dynamic plant model

Percentages indicated also in the figure 2 shows the estimated spent time for every step; for the Propylene/Propane splitter. To obtain a dynamic model which reflects realistically the plant behavior, there are a couple of factors that the engineer must consider:

Hysys integrator step-size and tray residence time: In order to run the simulations fast (70 real-time factor), integrator step-size of Hysys pressure-flow solver was initially set to 6 seconds. This step-size seemed to be right for most of the units and controllers, either if it seemed the cause of the very long response times of the column. Hysys could be manually adjusted manually for the execution rate of the Pressure Flow Solver (considered 1), the energy balances (considered 2), the controllers (also 1) and the composition and flash calculations (10 is default value).

Hold up of trays: The tray model has to represent the amount of liquid inside the column, since it has an effect concerning the response times of the overall column (more mass = more inertia). The manufacturer’s column design data has to be introduced into the model, and the simulator calculates the hold- up in each tray for a given internal liquid flow.

Main parameters influencing tray liquid hold-up are: column diameter, weir height and total weir length. Distillation column classic configuration (tray liquid hold up) is indicated in figure 3.

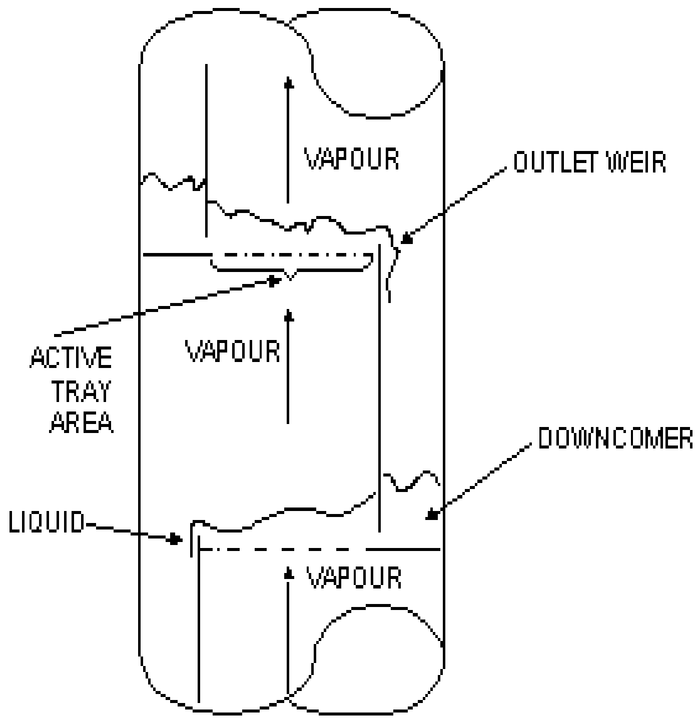

Fig. 3 Distillation column liquid holds up

In the case of the propylene/propane splitter, may not be possible to gather reliable plant step test information on which to base a controller design mostly for the following reasons:

1. Tight quality specifications prohibit steps of sufficient magnitude to achieve a signal to noise ratio reasonable for model identification.
2. Long settling times and frequency of daily disturbances blocks the plant the unit to achieve a real steady state.
3. DCS operator considers that any deviation from the current philosophy of running the tower at constant high reflux and reboil may destabilize tower operation.

Process functions of the propylene propane splitter

Primary control objective is propylene quality (C3 in splitter`s top ≤ 0.5 mole %). The secondary control objective is propane quality (propylene composition in bottom ≤1%). The optimization objective is to increase propylene yield versus power reboiler energy consumption. The unit constraint is tower flooding.

The steady state model was used to generate the relationship between the refluxes and product qualities. The results of such analyze has been shown in figure 5. Both top and bottom qualities are shown to be highly non-linear in the composition region of interest. Some improvement in linearity is observed when a logarithmic transform is applied. Logarithmically transformed quality variables are therefore used for the remainder of this study [7,8].

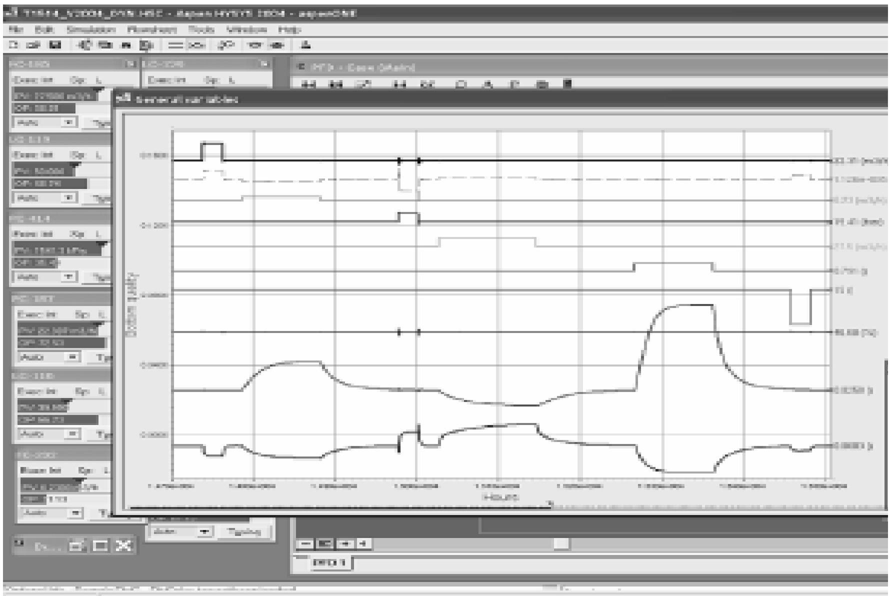

Fig. 4. C3/C3` step test developing using Hysys

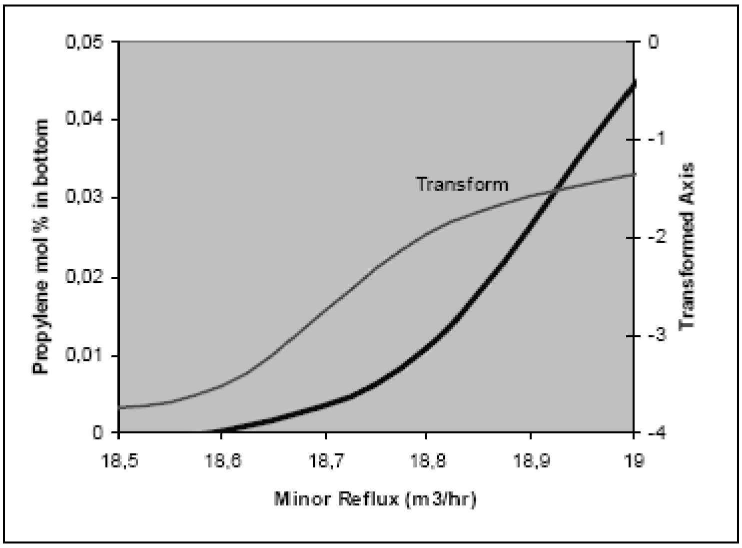

Fig. 5. Unit response to reflux changes

Starting from the steady state model, a dynamic simulation was built in HYSYS by specifying additional engineering details including pressure/flow relationships and equipment dimensions. In addition, all basic controllers were included in the model and configured exactly as they are in the plant. The dynamic model was checked for consistency and calibrated against process data. A dynamic simulation of this size and complexity is numerically intensive. At best the simulation could run 70 times faster than real time on the experienced PC with 2.4 Ghz CPU and1GB RAM due to the facilities Hysys offers [8].

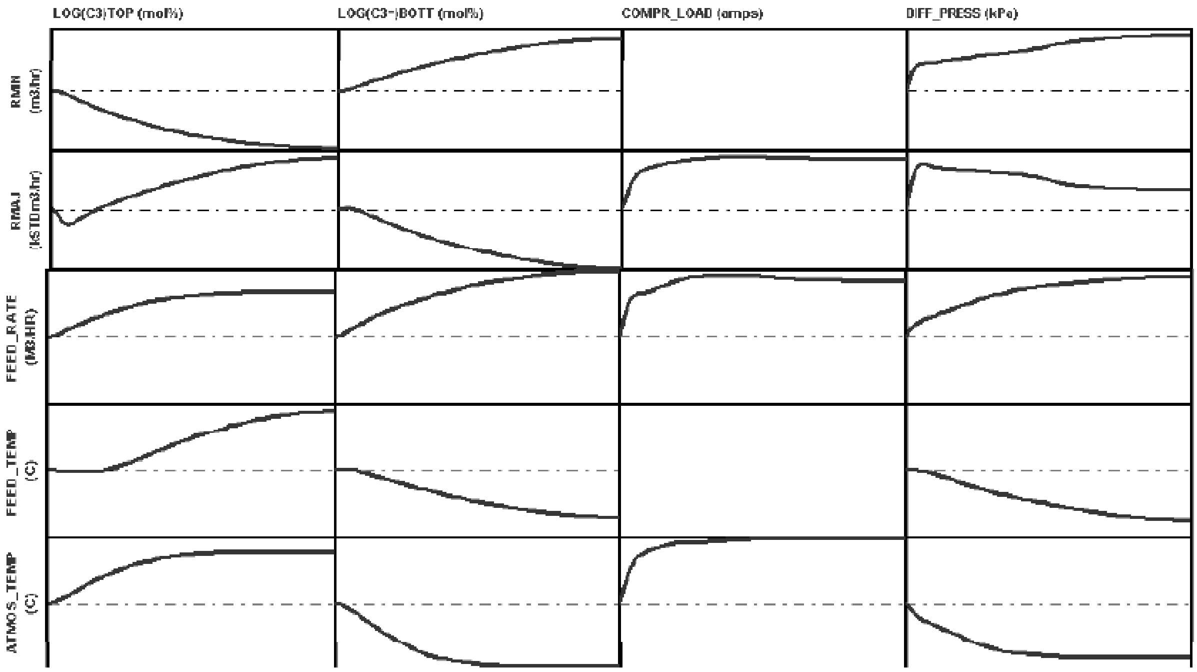

Fig.6. Dynamic matrix generated by using step test data

Data recorded during the step test were exported to Aspentech´s DMCplus Model identification package using the specific Aspen DMC ".clc" file format, convenient between HYSYS environment and Aspen. Logarithmic transforms could be applied to composition vectors. Subspace models may then be generated from the step data. Given that the step data is noise free, the identified models were observed to be very clean. Figure 6 shows a typical dynamic matrix generated by this analysis in which scales have been removed for clarity.

APC model based on Dynamic Matrix Control (DMC)

The original work developing dynamic matrix control was developed by Cutler and others. DMC control is based on a discrete time step response model that calculates a desired value of the manipulated value that remains unchanged during the next time step. Details of the derivation of the formulae are derived in the course. The new value of the manipulated variable the value that gives the smallest sum of squares error between the set point and the predicted value predicted values of the controlled variable. The n umber of time steps the DMC uses for its prediction is called the "Prediction Horizon". The dynamic model used to predict the future values of the controlled variable is represented by a vector, A, whose elements are defined as [8, 9]:

$$a_i = \frac{\Delta y(t_i)}{\Delta u(t_0)} \tag{6}$$

where:

$\Delta y(ti) = y(ti) - y(t0)$

$y(t)$ = the value of the controlled variable at time t

$\Delta u(t0)$ = the change in the manipulated variable at t_0

Thus, the response of a process to a step change, Δu, in the manipulated variable at t_0 ($\Delta u(t0)$ is given by:

$$\begin{bmatrix} \Delta y(t_1) \\ \Delta y(t_2) \\ \Delta y(t_3) \\ \vdots \\ \Delta y(t_n) \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix} \Delta u(t_0) \tag{7}$$

Demonstration of Dynamic Matrix Control

DMC control behavior has been presented within figure 7. With the noise and digital filter turned off, the DMC controller acquires an accurate model of the system. The DMC settings are input horizon = 10 and the output horizon = 4 and the time interval is 5. The controller is then placed into the automatic mode and the set point is changed from 50 to 40. The controller calculates an adjustment for 1 time interval (5 seconds) that will bring the controlled variable to the new set point and then moves the manipulated variable to the new equilibrium value, all before the controlled variable starts to react. The result (figure 7) is an impressive demonstration of DMC's capabilities.

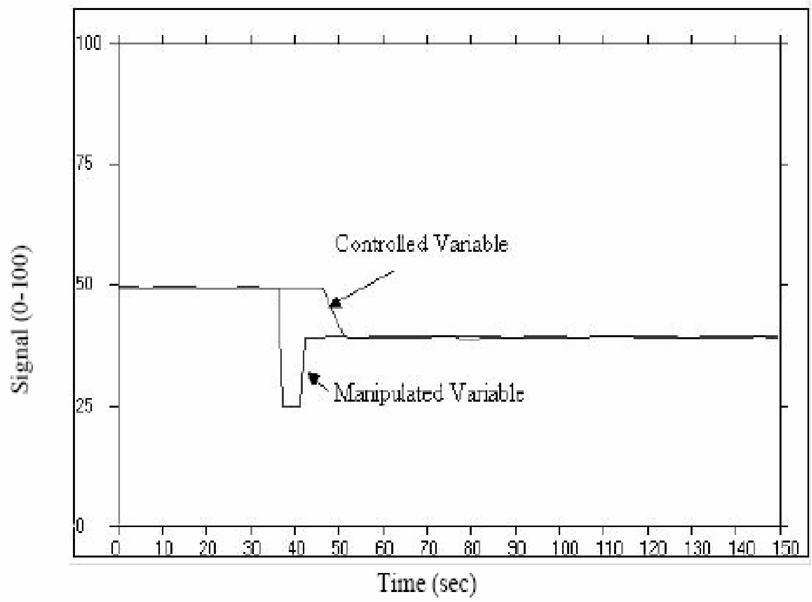

Fig.7. Demonstration of DMC control

Analysis of plant historical data showed that the top quality specification was never exceeded whereas the bottom quality was somewhat erratic. It was therefore decided to stagger the implementation of advanced controls into 2 stages. The first stage was to implement a simplified MISO strategy in the DCS in which bottom quality only is controlled by minor reflux, with feed rate and atmospheric temperature providing feedforward compensation. The second stage was the full DMCplus implementation with 3 manipulated, 3 feedforward and 3 controlled variables.

Process data may be imported from the historian database into DMCplus in order to validate the dynamic model created. Predicted output data, as generated by the prediction facility in

DMCplus, could have been compared to actual output data. As observed within figure 8 for each prediction was obtained a reasonable response [8,9].
Finally, a DMCplus controller was built and connection to the Honeywell TPS DCS system could have been established. The DMCplus web interface is shown in Figure 8.

Due to the extensive simulation effort both in HYSYS and DMCplus simulate, and the fact that the underlying HYSYS model of the propylene/propane splitter provided a sound basis on which to build the controller, next to no additional tuning of the controller was necessary during commissioning. Figure 14 shows the top and bottom quality trends before and after implementation of the controller.

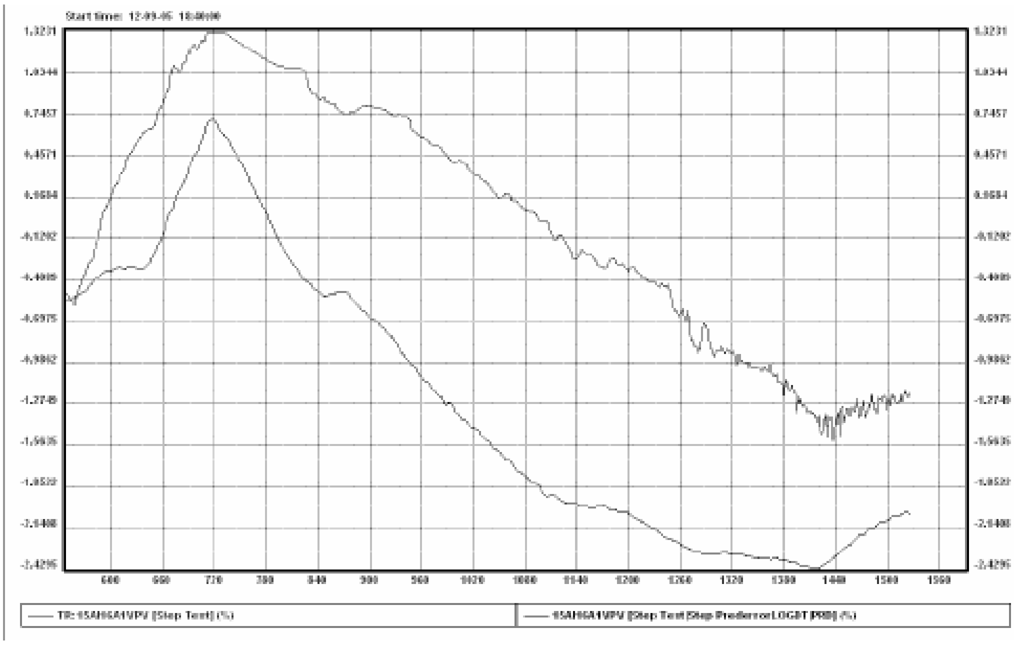

Fig. 8. Predicted and obtained impurities within bottom product (top graph dynamic simulation prediction, bottom graph real process value after DMC model implementation)

The controller was turned off for a period of about a week due to upsets in the FCC unit which is upstream of the propylene/propane splitter. As shown, control of top and bottom quality is resumed immediately the controller is placed on line again.

Conclusions

A design procedure for advanced process controllers utilizing first principles steady state and dynamic models as an alternative to empirical models identified from plant tests has been presented.

The APC strategy was illustrated on the challenging control problem posed by the propylene/propane splitter for which it was argued that a classical plant step test was not feasible.

The procedure is based on the premise that a realistic dynamic simulation of the process and every variable that participates in the control scheme can be developed, like most of the distillation units with long settling times. Unfortunately this is not always the case, like in reactor units where the modeling efforts are more time consuming than plant step testing.

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Simularea în regim dinamic - etapă preliminară implementării tehnologiei APC

Rezumat

Articolul prezintă succesiunea de etape specifice privind implementarea metodologiei de control specifice coloanei de separe propan/propilenă aferentă instalației fracționare gaze din secția Cracare Catalitică. Lucrarea abordează succesiv etapele specifice privind introducerea tehnologiei APC pentru coloana de fracționare care face obiectul studiului. La baza dezvoltării modelului de conducere avansată APC a stat modelarea în regim staționar şi ulterior în regim dinamic folosind simulatorul Hysys.