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RIGOROUS SIMULATION AND MODEL PREDICTIVE CONTROL OF A CRUDE DISTILLATION UNIT

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Abstract: This paper describes the application of a widely-used commercial multivariable predictive controller to a rigorously simulated crude distillation process. After describing the main process and controller features, it is shown how the two simulation and control environments can be interfaced together. A number of simulation results of typical product quality changes and crude switches are presented. The final goal of this paper is to demonstrate how rigorous dynamic simulators can be effectively used to reduce the costs of Advanced Process Control projects by shortening model identification, controller design and commissioning phases.

Keywords: Dynamic simulators, model predictive control, model identification, complex distillation processes.

1. INTRODUCTION

Process industries, such as the petroleum and chemical industries, face very dynamic and unpredictable market conditions, due to world-wide competition, limitation in natural resources, strict national and international regulations. In order to improve the production safety, quality and flexibility, plant automation has become increasingly important and is now recognized as a very effective way to achieve the production goals with satisfaction of safety and quality constraints.

Modern automation control systems for processing plants usually consist of a multi-level hierarchy of control layers. The first layer (starting from the bottom) is usually a distributed control system (DCS) which gathers process measurements, performs simple monitoring and PID-based control of some process variables (such as flow rates, levels, temperatures) to guarantee automatic operation of the plant. The second layer, usually referred to as Advanced Process Control (APC), performs multivariable model-based constrained control to achieve stable unit operation and push the process towards its operational limits for maximum economic benefits. APC regulators typically fall within the class of Model Predictive Control (MPC) algorithms (Morari and Lee, 1999; Mayne *et al.*, 2000; Qin and Badgwell, 2003). On top of APC other layers can be present, such as a Real-Time Optimization (RTO) layer and a Planning and Scheduling layer.

Reduction of costs for application of the second layer is a relevant issue since it would enlarge considerably the range of applicability of APC systems, which at present are mostly limited to capital intensive sectors, such as refinery and petrochemical industries. Qin and Badgwell (2003) reported nearly five thousand MPC applications all over the world, as a snap-shot of the situation in 1999, with a rough increase of about 80% in the subsequent three years. An MPC/APC project typically consists of a number of phases, such as:

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Table 1. TBP of the Zarzaitine crude oil.

Volume %	3.4	12.4	27.5	44.1	56.6	67.5
BP (°C)	20	80	145	225	290	350

(1) A preliminary study comprising selection of manipulated (MV), controlled (CV) and disturbance (DV) variables, check of all instrumentation, and possible re-tuning of regulatory PID controllers.
(2) Plant testing and model identification in which MVs are varied and data of CVs (and DVs) are collected to build a process model, by means of identification techniques.
(3) Controller tuning, simulation and commissioning including selection of MVs and CVs limits and weights, open and closed-loop simulation on the identified plant model and final closed-loop implementation on the plant.

Phase 2 is particularly time-consuming and during plant testing (which may last several weeks) the products may violate some quality specifications. Phase 3 is also time-consuming although most of controller tuning and simulation needs not to be done "on-site".

Rigorous (steady-state and dynamic) simulators, i.e. those based on first-principles/fundamental equations, have become widely-used tools in process analysis, design and control (Yiu *et al.*, 1994; Berber and Coskun, 1996; Luyben and Tyreus, 1998; Huang and Riggs, 2002). In particular dynamic simulators can be useful to simplify Phase 2 and Phase 3 since they "surrogate" the true plant, thus allowing data collection for model identification, controller tuning and simulation. Moreover, it is important to remark that nowadays it is possible to carry out closed-loop model identification using an MPC regulator based on some preliminary model (e.g. one obtained from the data collected using the simulator). This approach can reduce dramatically the required plant testing duration and finally improve the controller performance by means of a more accurate model and more effective tuning.

In the present work, an industrially relevant example of a Crude Distillation Unit is simulated by means of HYSYS™ and controlled by using the commercial MPC algorithm DMCplus™. More details on this study can by found in (Gallinelli, 2005).

2. PROCESS AND CONTROLLER DESCRIPTION

2.1 Crude distillation unit

Crude oil is a mixture of a large number of components (whose exact determination is impossible), ranging from alkanes and iso-alkanes to cycloalkanes and aromatic compounds. Different oils are usually characterized in terms of density, often expressed in API degrees, and in terms of distillation curves, such as True Boiling Point (TBP), Equilibrium Flash Vaporization (EFV) or ASTM curves. In this study a Zarzaitine (Algerian) crude oil is considered, whose TBP data are reported in Table 1.

Crude distillation units (CDU) represent the core plant of any refinery site since most of its products are the starting point for a number of subsequent operations and final products. A typical CDU consists, mainly, of four operations:

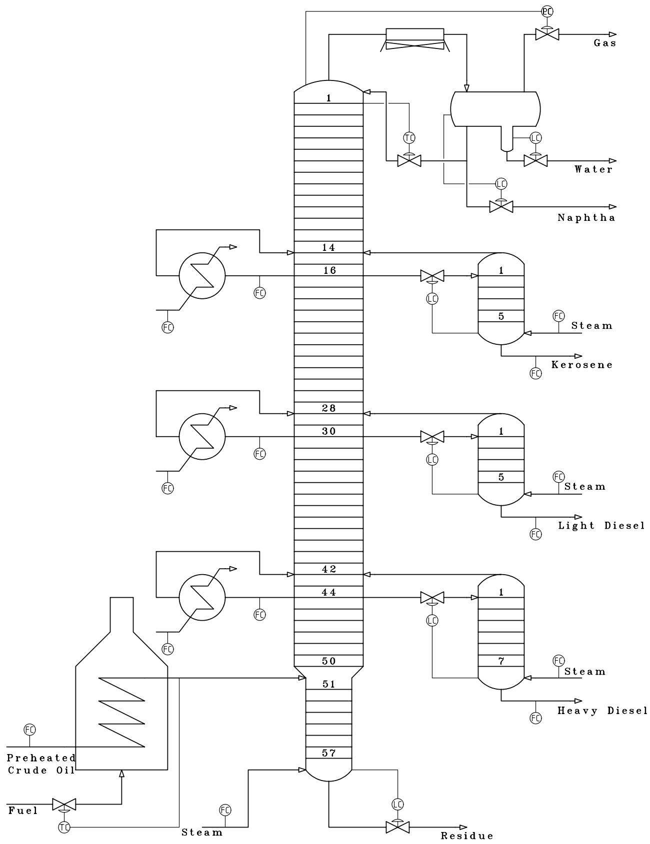

Fig. 1. CDU layout

(1) Desalting and pre-heating: before and after desalting, crude oil is pre-heated at expense of other hot streams available in the plant.
(2) Pre-flash: light components are vaporized in a flash drum to reduce the load at the furnace.
(3) Heating: crude oil is heated at high temperature (350÷390°C) in a furnace.
(4) atmospheric distillation: crude oil is separated into a number of products (such as naphtha, kerosene, light diesel, heavy diesel and a residue) in a complex rectification column featuring side strippers and external coolers (pumparounds).

The CDU layout is depicted in Figure 1, in which only the furnace and the complex distillation column (with strippers and pumparounds) are shown for simplicity of representation. The main column top and bottom pressures are 1.9 atm and 2.8 atm, respectively; the reflux ratio is 1.5. All specifications can be found in (Gallinelli, 2005). Products are themselves mixtures of components and are characterized by given boiling temperature ranges. The boiling temperature ranges of products considered in the present study are reported in Table 2 along with the corresponding expected yield for the chosen crude.

2.2 DMCplus™ algorithm

In order to provide a brief description of the controller algorithm used in this work, it is assumed that a

Table 2. Boiling ranges for CDU products and expected yield.

Product	Boil. Range (°C)	Yield %
Naphtha	35÷150	24.5
Kerosene	150÷240	18.1
Light Diesel	240÷350	21.2
Heavy Diesel	350÷390	7.5
Residue	390÷548	28.7

(stable and proper) convolution model of the process is known. According to this model, the predicted value of the outputs (CVs) at time k given past values of the inputs (MVs) is:

$$\hat{y}_k = \sum_{i=1}^{k} S_i \Delta u_{k-i} \tag{1}$$

in which $\hat{y}_k \in \mathbb{R}^p$ is the predicted output vector at time k, $\Delta u_{k-i} \in \mathbb{R}^m$ is the input variation vector at time $k-i$ and $S_i \in \mathbb{R}^{p\times m}$ is the $i-$th matrix of step response coefficients from each input/output pair. Given the output measurement y_k, a correction term is then computed as:

$$d_k = y_k - \hat{y}_k \tag{2}$$

This term, which is meant to lump different sources of plant/model mismatch (such as disturbances, nonlinearities, noise), is used to guarantee offset-free control (Pannocchia and Rawlings, 2003). Other more general and effective correction terms can be considered (Muske and Badgwell, 2002; Pannocchia and Rawlings, 2003; Pannocchia and Brambilla, 2005).

The DMCplus™ controller, as well as most MPC algorithms, is based on two optimization modules (executed at each sampling time):

- A steady-state target optimizer, which computes optimal targets for inputs and outputs.
- A dynamic optimizer, which computes optimal trajectories for inputs and outputs from their current value towards the computed targets in a fixed-length time window (horizon).

The steady-state optimizer solves a linear program (LP) in the form:

$$\min_{\Delta\bar{u}_k} c^T \Delta\bar{u}_k \tag{3a}$$

subject to

$$u_{\min} \le \bar{u}_{k-1} + \Delta\bar{u}_k \le u_{\max} \tag{3b}$$
$$-\Delta\bar{u}_{\max} \le \Delta\bar{u}_k \le \Delta\bar{u}_{\max} \tag{3c}$$
$$y_{\min} \le G(\bar{u}_{k-1} + \Delta\bar{u}_k) + d_k \le y_{\max} \tag{3d}$$

in which $u_{\min}$ ($u_{\max}$) and $y_{\min}$ ($y_{\max}$) are vectors which contain the minimum (maximum) value for inputs and outputs, $\bar{u}_{k-1}$ is the previous input target vector, $\Delta\bar{u}_k$ is the input target variation vector, $\Delta\bar{u}_{\max}$ is maximum target variation vector, $G \in \mathbb{R}^{p\times m}$ is the model gain matrix and c is a vector of steady-state "costs". Solution of (3) yields the following input and output optimal targets:

$$\bar{u}_k = \bar{u}_{k-1} + \Delta\bar{u}_k, \quad \bar{y}_k = G(\bar{u}_{k-1} + \Delta\bar{u}_k) + d_k \tag{4}$$

It is clear that when it is desirable to maximize (minimize) an input, the corresponding cost should be chosen negative (positive). Possible infeasibility outcomes of (3), due to the output constraints (3d), are handled by iteratively softening output constraints (starting from low priority variables) and penalizing the corresponding variation in the objective function.

Given the optimal targets, the dynamic optimizer computes an optimal sequence of future input variations by solving the following quadratic program (QP):

$$\min_{\Delta u_k,\ldots,\Delta u_{k+N-1}} \sum_{j=k}^{k+N-1} \Delta u_j^T R \Delta u_j + \sum_{j=k+1}^{k+P} \left\{ e_j^T Q e_j + {\eta_j^u}^T Q^u \eta_j^u + {\eta_j^l}^T Q^l \eta_j^l \right\} \tag{5a}$$

subject to

$$e_j = \bar{y}_k - \hat{y}_{j|k} = \bar{y}_k - \left(\sum_{i=1}^{j} S_i \Delta u_{j-i} + d_k \right) \tag{5b}$$
$$u_{\min} \le u_{k-1} + \sum_{i=k}^{j} \Delta u_i \le u_{\max} \tag{5c}$$
$$-\Delta\bar{u}_{\max} \le \Delta u_j \le \Delta\bar{u}_{\max} \tag{5d}$$
$$y_{\min} - \eta_j^i \le \hat{y}_{j|k} \le y_{\max} + \eta_j^s \tag{5e}$$
$$\eta_j^i \ge 0, \quad \eta_j^s \ge 0 \tag{5f}$$

where: N and P are positive integers referred to as control and prediction horizon, respectively; R, Q, Q^u and Q^l are diagonal matrices with positive entries; u_{k-1} is the previous input vector; e_j is the vector of errors between target and future predicted outputs at time j; $\Delta u_{\max}$ is the maximum input variation vector; η_j^u and η_j^l are non-negative vectors which represent (possible) violations of upper and lower output constraints, respectively. It is important to remark that due to the output soft-constraint approach adopted, problem (5) is always feasible. Moreover, due to patent restrictions, DMCplus™ solves (5) in a suboptimal fashion. Given the "optimal" input sequence only the first "move" is implemented, i.e.

$$u_k = u_{k-1} + \Delta u_k \tag{6}$$

and both modules are re-executed at the next sampling time.

3. SIMULATION AND CONTROL ENVIRONMENT

In this section a description of the process simulation model built using HYSYS™ (version 3.2) and of the commercial controller DMCplus™ (version 6.0) used in this work is given.

3.1 Process simulation model

As remarked, crude oil exact composition is unknown; however this piece of information is necessary to simulate a crude distillation process. It is, therefore, common practice to represent the crude oil as a mixture of true components (light ends) and a number of pseudo-components. In the present work, seven light components (ranging from methane to n-pentane) and fifty pseudo-components are used.

After defined the crude composition and flow rate, the next step is to build a steady-state flow-sheet. Since the main interest of this work is to focus on the column dynamics and control, a number of "sensible" simplifications are made. First of all, the pre-heat train is simulated as a single heat exchanger; then, each pumparound is considered as a simple heat exchanger in which the hot fluid (column draw) flow rate and the exchanger duty are specified; finally, the cooling system is simulated as a single air cooler with a plant equivalent holdup.

Once a steady-state flow-sheet is defined, a number of steps are necessary to obtain a dynamic simulation model in HYSYS™.

(1) Design and sizing (holdup definition) of each equipment. In particular sieve trays are used throughout the column except for the draw stages where partial chimney trays are chosen.
(2) Specification of pressure and/or flow rate for a number of streams.
(3) Specification of the pressure profiles in each equipment.
(4) Addition of regulatory control loops (flow-rate, level, pressure and temperature controllers) to guarantee automatic operation of the column.

In the present work a further degree of simulation rigor is achieved by considering the static height of each equipment. With regards of the regulatory control loops, shown in Figure 1, PI controllers are used and tuned using IMC-like rules (Skogestad, 2003). It should be remarked that, although not shown, all level, temperature and pressure controllers are actually implemented in cascade on the corresponding flow-rate controllers.

3.2 DMCplus™ controller

In order to implement a predictive controller using the DMCplus™ software a list of manipulated and controlled variables is defined. In particular:

- 17 manipulated variables are considered: these variables are the setpoints of temperature, pressure and (non-cascaded) flow-rate controllers.
- 23 controlled variables are selected: these variables are the ASTM-D86 95% of the four main products (Naphtha, Kerosene, Light Diesel, Heavy Diesel) and the opening percent of all control valves.

Once the controller structure is defined, it is necessary to generate simulation data that can be used for the identification of the dynamic model matrix. This is done by imposing a series of setpoint changes to all the manipulated variables and observing their effect on the controlled variables. The size, direction and duration of the setpoint changes must be chosen so that significant changes are induced in the controlled variables and that all the typical operating conditions of the unit are explored. The sequence of moves can be pre-programmed and then the simulation can run unattended and the results are continuously collected and archived inside the HYSYS™ environment.

The data can then be exported from HYSYS™ and imported in DMCplus™ Model, the identification tool for DMCplus™ controllers. The next step is of course the analysis of the simulation data and the identification of the dynamic model: this can be done exactly as if the data were coming from a non-simulated step-test on a real process unit.

The identified model is then loaded in DMCplus™ Build to prepare the controller configuration file which will then be used by the on-line control engine. The tuning of a DMCplus™ controller is usually performed with the aid of its associated closed-loop simulation tool, Simulate. These simulations are based on the linear model that has been obtained during the model identification, and even if it is possible to introduce some extent of plant/model mismatch, it will always be difficult to closely reproduce the behavior of the controller once it will be applied to a real plant or, as in this case, to a rigorous dynamic simulation.

3.3 Simulator and controller interfacing

The interfacing of the dynamic simulation with the controller is performed with the use of the DMCplus™ block which is available in the HYSYS™ control libraries, together with PID or ratio controllers. This block is connected to the PID controllers which are manipulated variables in a simple master/slave cascade arrangement and is capable of reading the values of the controlled variables even if they are calculated values such as the ASTM qualities of selected streams.

When the HYSYS™ simulation is started with this block in place, the integrator runs until the time specified as the controller execution cycle (1 minute for the current application) has elapsed and pauses the simulation; it then passes the current values of manipulated, controlled and feed-forward variables (if present) to the DMCplus™ online control engine and waits for it to execute and return the new values for the manipulated variables. These values are applied in the HYSYS™ environment and the simulation is then started again for the time corresponding to one controller execution cycle.

4. SIMULATION RESULTS

A number of different closed-loop simulation studies were conducted to test the controller effectiveness in different situations, and to verify the flexibility of the proposed simulation and controller environment (Gallinelli, 2005). In this section some significant examples are presented.

Figure 2 shows the closed-loop results obtained for variations of the products' ASTM-D86 95% limits. In

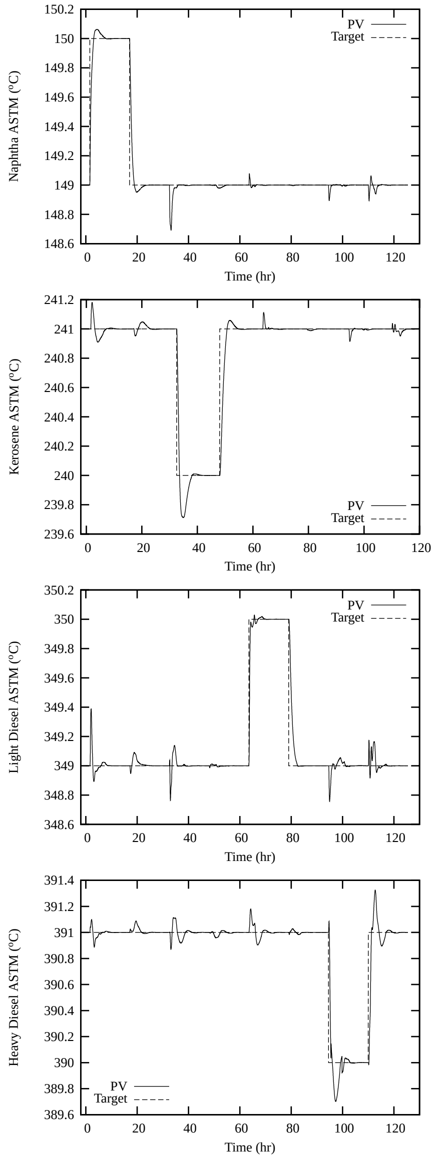

Fig. 2. Closed-loop results for variations of the products' ASTM-D86 95% limits: time behavior of products' ASTM-D86 95%.

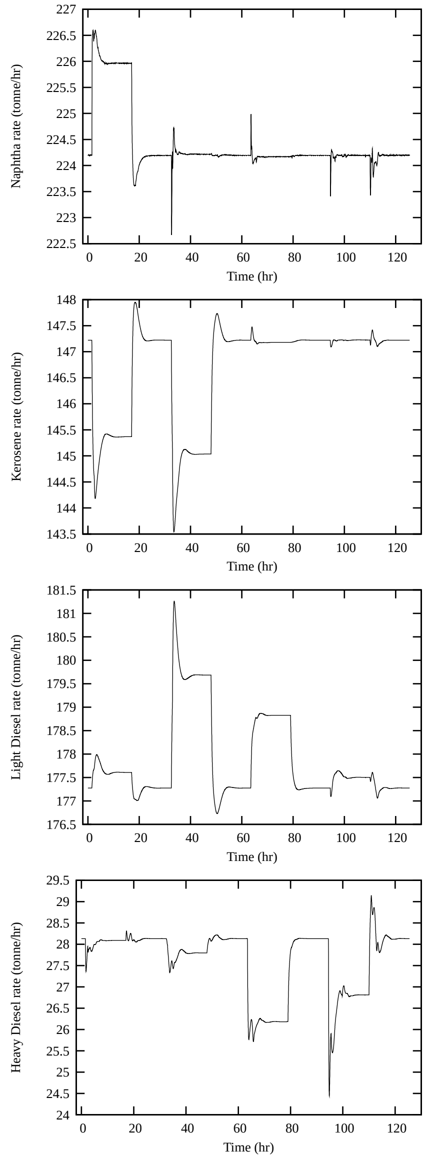

Fig. 3. Closed-loop results for variations of the products' ASTM-D86 95% limits: time behavior of products' flow rates.

each plot the time behavior of the "measured" controlled variables (ASTM-D86 95%) and of the corresponding steady-state targets calculated by the controller are reported. In Figure 3, instead, the corresponding time behavior of the flow rate of each product is reported.

A typical disturbance that occurs in refinery plants is associated to the crude switching. Starting from the original Zarzaitine crude oil, a new crude obtained by mixing the Zarzaitine oil with an Arabian Heavy one is fed to the CDU. For this case, closed-loop results of the products' ASTM-D86 95% are reported in Figure 4, while the corresponding product flow rates are reported in Figure 5.

5. CONCLUSIONS

In this paper, the design and study of a rigorous simulation model of crude distillation unit controlled by a commercial multivariable predictive controller has been presented. A crude distillation unit has been simulated using HYSYS™ with a very high degree of accuracy (equipment design and sizing, pressure profiles, static heads, etc.). This rigorous dynamic model has been interfaced with a commercial controller, DMCplus™, whose (linear) process model was derived from data collected on the simulated plant. Closed-loop results of common setpoint changes and disturbance rejections showed the effectiveness of the implemented control algorithm.

The main contribution of this work is to emphasize the potential advantages of using rigorous simulators on complex processes of industrial relevance. In particular rigorous simulators can be effectively used to generate data for preliminary model identification and controller tuning. This "initial" controller can be implemented on the actual plant to carry out closed-loop identification tests from which the final process

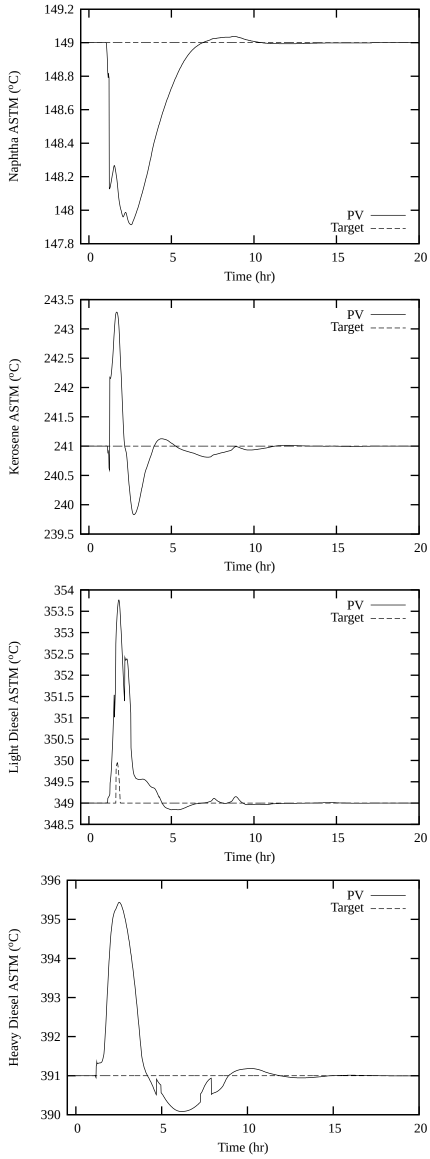

Fig. 4. Closed-loop results for crude switch: time behavior of products' ASTM-D86 95%.

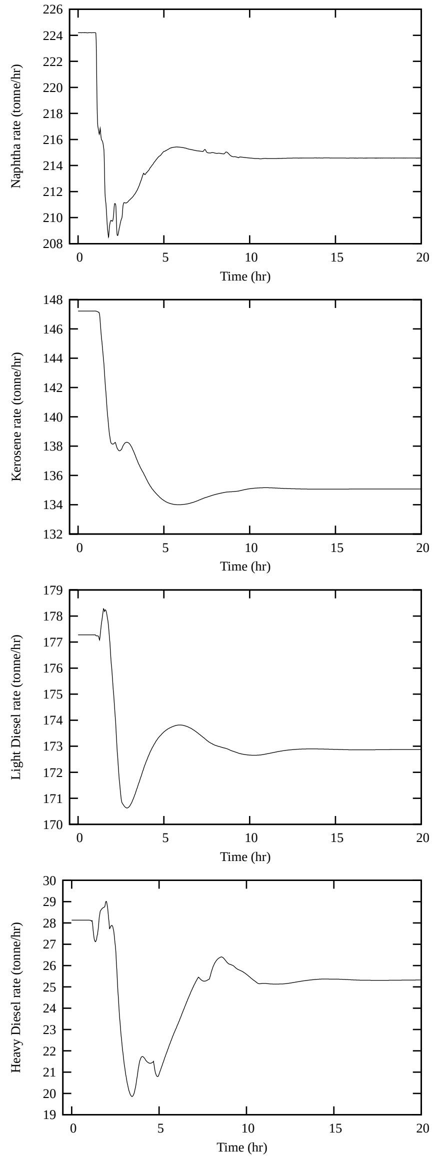

Fig. 5. Closed-loop results for crude switch: time behavior of products' flow rates.

model can be identified and the predictive controller implemented. Simulators can also be used to carry out closed-loop simulations, useful to refine the controller tuning (selection of costs, equal concern errors, limits, etc.) and effectively compare different predictive control algorithms. Therefore, the methodology illustrated in the present paper can potentially lead to reduction of costs for MPC applications, with consequent enlargement of the range of applicability of APC systems.

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