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# AN MILP PROCESS OPTIMIZATION MODEL FOR A PETROCHEMICAL COMPLEX

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**Abstract.** *This paper develops a multiperiod mixed integer nonlinear programming (MINLP) model for planning the production and operation of a real world petrochemical complex. Solving the MINLP model directly results in inconsistency in solution quality and time. Therefore, a reformulation and linearization technique is first applied to the bilinear terms of the model to obtain an mixed integer linear programming (MILP) formulation which is the initial point to solve the NLP obtained by the reformulation of the MINLP. The model is solved with GAMS 2.25 using OSL and CONOPT2. Two case scenarios are shown to illustrate the scope of this model.*

## INTRODUCTION

Production planning in a petrochemical complex is a large-scale problem. There are several plants operating under multiple sets of conditions to produce a diverse array of intermediate and finished products. Savings can often be realized by introducing more efficient means of planning the operation and production of different plants at a site. Key issues include operating conditions of individual processes, intermediate product handling and finished product storage.

The studied petrochemical complex comprises two natural gas liquids (NGL) processing plants, two ethylene plants, a caustic soda and chlorine plant, a VCM plant, a PVC plant, three polyethylene plants (LDPE, HDPE, LLDPE), an ammonia and an urea plant (Figure 1). Both NGL plants have two process trains, each of which is equipped with a turboexpander, but one of them has its cryogenic separation sector many kilometres away from the petrochemical site.

Linear mathematical models have been derived for the NGL, ethylene and polyethylene plants, based on rigorous existing models tuned with actual plant data[1 2]. Simplified models take into account variations in production with key plant operating variables, such as temperature and pressure in separation units. Available yield data for chemical transformations and utilities consumption have been used to model the rest of the petrochemical complex[3,]

The natural gas separator plant is fed with 36 $MMm^3$/d of natural gas. Light gases (methane, nitrogen and carbon dioxide) are separated from the heavy gases (ethane, propanes, butanes and gasolines) and compressed to be injected in the natural gas pipeline. The rich gas mixture (5 $MMm^3$/d of heavy gases) is stored in thermal vessels and pumped along a 600-km pipeline to the petrochemical complex where it is loaded into containers to equalize the charge, that is to say, to damp any pulsation or flow changes that may occur anywhere along the pipeline. The feed mixture undergoes a distillation process which allows to obtain LPG (Liquefied Petroleum Gas: propane, butane and gasoline) and ethane to be used in the ethylene production[4]

The natural gas processing plant is fed with 24 $MMm^3$/d of natural gas prior compression. Part of the residual gas feeds the ammonia plant and the rest is recompressed to pipeline pressure and delivered as sales gas. 480,000 ton/y of pure ethane is sent to the ethylene plants. If both ethylene plants are shut down, the ethane is rejected to the methane pipeline.

The ammonia plant produces 120 600 kmol/d of ammonia and 107 300 kmol/d are fed to the urea plant to produce 3 250 ton/d of urea. In these processes, 1.28MM $Nm^3$/d of natural gas are used as raw material and 689 000 $Nm^3$/d as fuel. The ethylene plant I produces 275,000 ton/y of 99.9% pure ethylene[5] and the ethylene plant II, which is more efficient, 425,000 ton/y. This ethylene is used to feed three polyethylene plants, a VCM plant and the

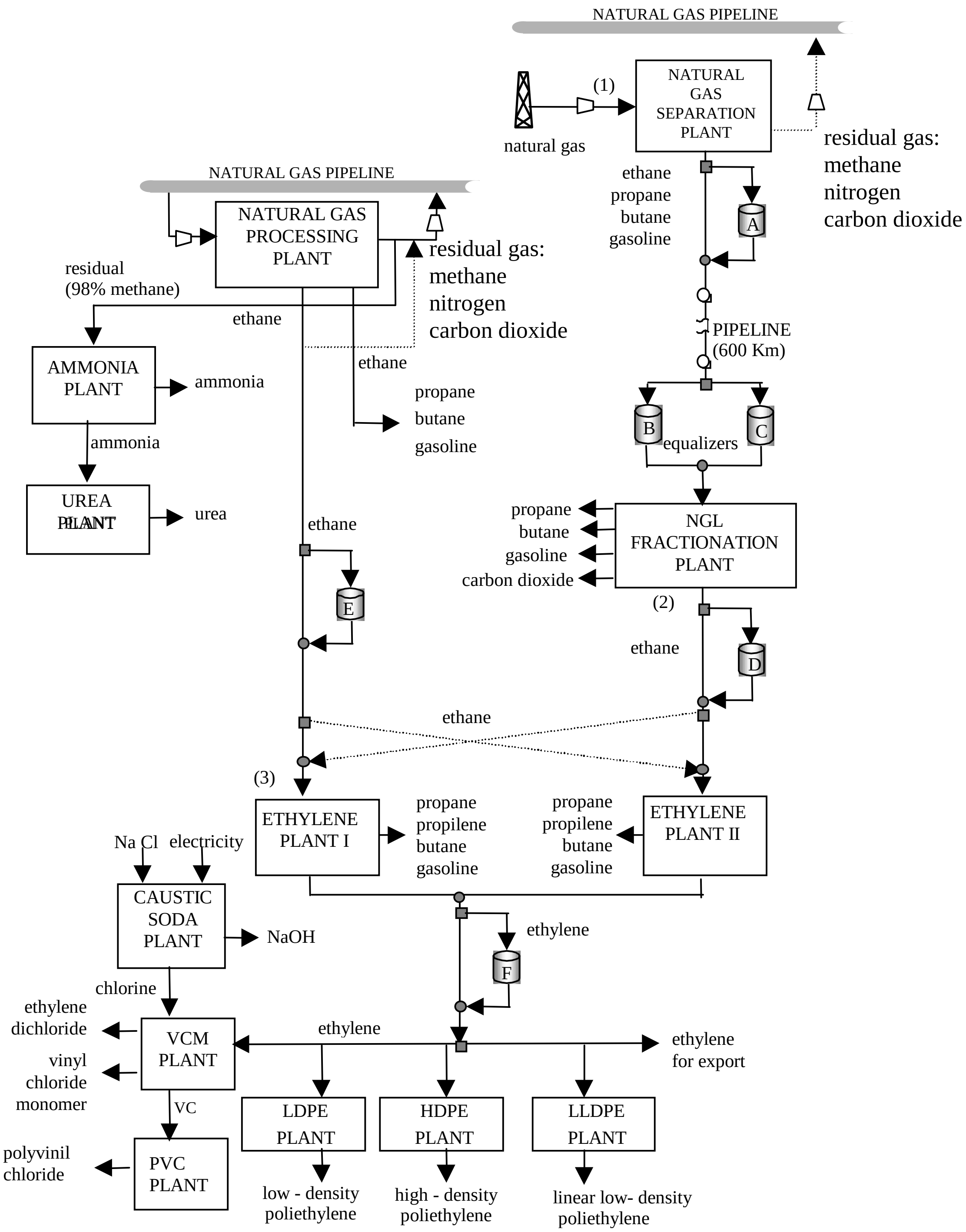


Figure 1: Total site model representation

rest is exported.

## GENERAL MATHEMATICAL MODEL

The model integrates all the plants to form a multiperiod optimization model of the entire site whose generalized form is shown below:

$$\max \quad \sum_{t}^{SCH} f\left(x_t, x_{t-1}, y, \theta,\right)$$

$$\text{subject to} \quad g(x_t, x_{t-1}, y, \theta) \le 0 \quad t=1...SCH$$
$$h(x_t, x_{t-1}, y, \theta) = 0 \quad t=1...SCH$$
$$x^L_t \le x_t \le x^U_t$$
$$y \in [0,1]$$

t is the time variable which has been uniformly discretized. SCH is the length of the time horizon, x are the continuos variables, y are the binary variables and θ are parameters. Note that the coupling of the time periods occurs through the inventory variables $x_{t-1}$.

The objective function is the maximization of the total profit for the entire site during the given time horizon; binary variables are used to include economic penalties for plant shutdowns due to start up costs. The constraints are the mass and energy balances, bounds on product demands, equipment capacities and intermediate product storage tanks limitations.

The pipeline is modelled as a time delay. Logical relationships are used to model the constraint that storage tanks cannot be charged and discharged simultaneously, except the equalizers[6].

### Reformulation – linearization technique

The bilinear terms F $x_j^t$ appear in material balance equations for the multicomponent streams in the splitters to impose the condition that the ratios of flows between components be the same for the different streams. A reformulation and linearization technique[7] is applied considering the upper and lower bounds of the variables involved in these terms:

$$\begin{gathered} x_j^{tL} \le x_j^t \le x_j^{tU} \\ F^{tL} \le F^t \le F^{tU} \end{gathered} \tag{1}$$

These bound can be expressed as follows:

$$\begin{gathered} g_1 = F^t - F^{tL} \ge 0 \\ g_1 = F^{tU} - F^t \ge 0 \end{gathered} \tag{2}$$

$$\begin{gathered} g_2 = x_j^{tU} - x_j^t \ge 0 \\ g_2 = x_j^t - x_j^{tL} \ge 0 \end{gathered} \tag{3}$$

The following nonlinear constraint is clearly valid since it is satisfied if the constraints (2) and (3) are satisfied.

$$g_1 \; g_2 \ge 0 \tag{4}$$

Replacing (2) and (3) in (4) for the four possible combinations of $g_1$ and $g_2$, the following linear bounding constraints can be generated for the bilinear terms:

$$\begin{aligned}
F^t\, x_j^t &\geq F^{tL}\, x_j^t + F^t\, x_j^{tL} - F^{tL}\, x_j^{tL} \\
F^t\, x_j^t &\geq F^{tU}\, x_j^t + F^t\, x_j^{tU} - F^{tU}\, x_j^{tU} \\
F^t\, x_j^t &\geq F^{tU}\, x_j^t + F^t\, x_j^{tL} - F^{tU}\, x_j^{tL} \\
F^t\, x_j^t &\geq F^{tL}\, x_j^t + F^t\, x_j^{tU} - F^{tL}\, x_j^{tU}
\end{aligned} \tag{5}$$

It has been shown[8], that equations (5) correspond to the convex and concave envelopes of the bilinear terms over the given bounds.

### Storage tanks

The moles of component j for time period t is given by the initial moles plus the summation of inflows substracted by the summation of outflows up to each time interval where $V_j^t$ are the moles of component j at the time period t and $V_j^0$ are the initial moles of j, SCH is the time horizon length, $f_j^{im}$ and $f_j^{km}$ are the inlet and outlet molar flows of component j respectively.

$$V_j^t = V_j^o + \sum_{m=1}^{t} f_j^{im} - \sum_{m=1}^{t} f_j^{km}, \qquad \forall i, t = 1 \ldots SCH \tag{6}$$

### Plant shutdown

Given $TP_p$, the shutdown day of plant p, and $t^{min}_p$ and $t^{max}_p$, the minimum and maximum shutdown duration, the following equations force a plant to shut down only once throughout the scheduling horizon [9].

$$\begin{aligned}
\sum_{t=1}^{SCH} XA_p{}^t &= 1 \\
\sum_{t=1}^{SCH} XP_p{}^t &= 1
\end{aligned} \tag{7}$$

$XP_p^t$ and $XA_p^t$ are binary variables to denote if the plant shuts down or starts working respectively. The plant shuts down and starts working only once throughout the scheduling horizon. SCH is the time horizon length.

$$\begin{aligned}
\sum_{t=1}^{SCH} t\; XA_p{}^t &= TA_p \\
\sum_{t=1}^{SCH} t\; XP_p{}^t &= TP_p
\end{aligned} \tag{8}$$

$TP_p$ is the day when the plant shuts down and $TA_p$ when it starts working.

$$TA_p - TP_p \geq t^{\min}{}_p$$
$$TA_p - TP_p \leq t^{\max}{}_p \qquad (9)$$

The duration of the shutdown is bounded: between $t^{min}{}_p$ and $t^{max}{}_p$ days.

$$XW^t{}_p = \sum_{m=1}^{t} XP^t{}_p - XA^t{}_p \qquad (10)$$

$XW_p^t$ is a continuous auxiliary variable which is forced to be 1 between TP and TA and 0 during the rest of the horizon.

$$Y^t{}_p = 1 - XW^t{}_p \qquad (11)$$

$Y_p^t$ is a binary variable which is null while the plant is shutdown.

$$F^{tL}{}_p \leq F^t{}_p \leq F^{tU}{}_p$$
$$F^t{}_p \leq F^{tU}{}_p \, Y_p^t \qquad (12)$$
$$F^t{}_p \geq F^{tL}{}_p \, Y_p^t$$

Big M constraints are used to nullify the flow rates when the plant p is shutdown.

**MINLP solution**

The MINLP problem is solved as an equivalent NLP using as an initial point the solution of the MILP that is solved with OSL solver. This equivalent NLP is obtained modelling binary variables as continuous (YC) and adding the following constraints to ensure integer values:

$$YC(1 - YC) \leq 0$$
$$0 \leq YC \leq 1 \qquad (13)$$

The resulting NLP is solved with GAMS 2.25 using CONOPT2 solver.

## NUMERICAL RESULTS

Two site operation scenarios are studied. The optimal inventory profiles and the optimal operation levels of the plants are obtained.

Case 1 corresponds to a site operation without forcing any plant to shut down. In the Case 2 the Fractionation Plant is forced to shutdown on the tenth day. In both cases, plants are allowed to shut down if necessary.

**Case1: No forced shutdown**

Figures 2 to 4 show the optimal inventory profile and Figure 5 and 6 show the natural gas processed in the Natural Gas Separator and the ethane processed in Ethylene Plant for the MILP of Case1. Figures 7 to 11 show the same variables´ profiles for the MINLP

**MILP**

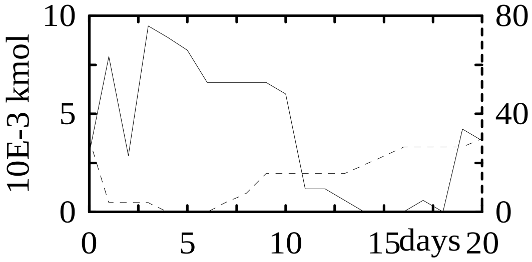


Figure 2 Tank A and D (dash line and right axis)

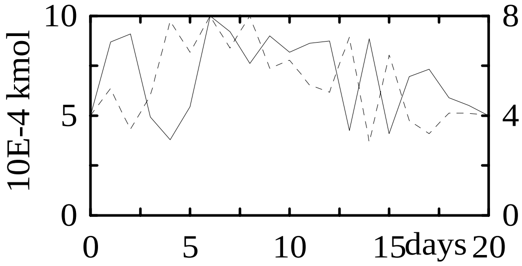


Figure 3 Tank B and C (dash line and right axis)

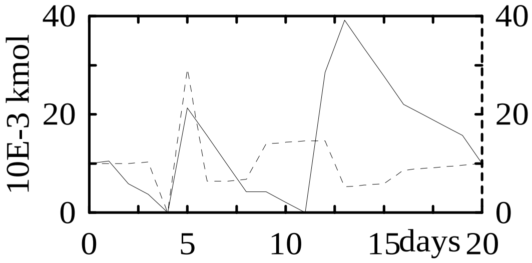


Figure 4 Tank E and F (dash line and right axis)

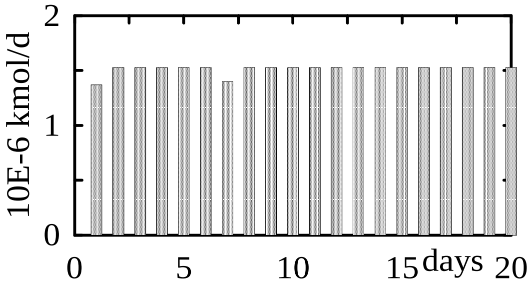


Figure 5 Natural gas processed in the Natural Gas Separator (1)

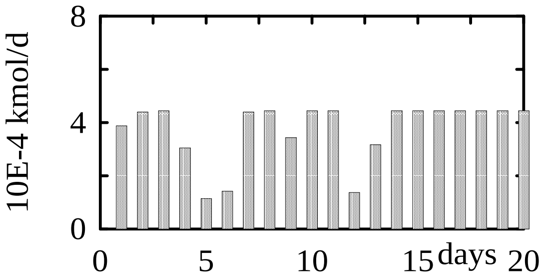


Figure 6 Ethane processed in Ethylene Plant (3)

**MINLP**

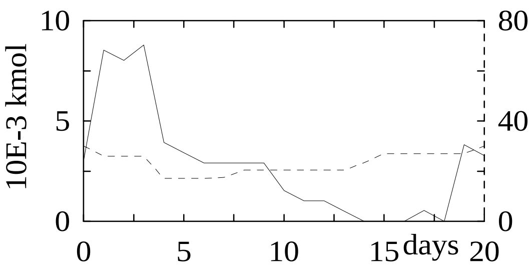


Figure 7 Tank A and D (dash line and right axis)

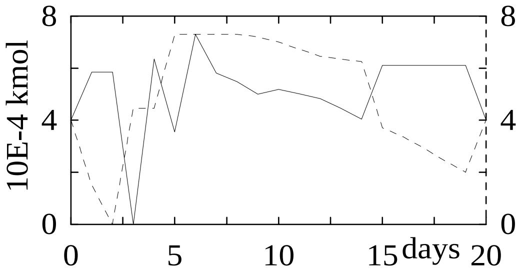


Figure 8 Tank B and C (dash line and right axis

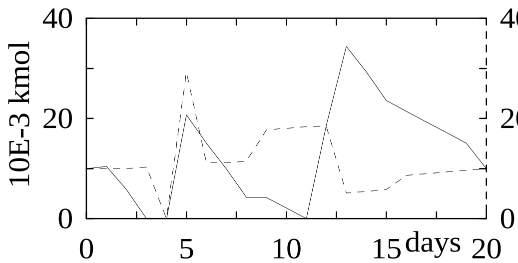


Figure 9 Tank E and F (dash line and right axis)

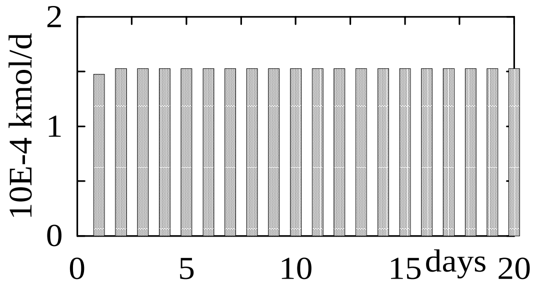


Figure 10 Natural gas processed in the Natural Gas Separator (1)

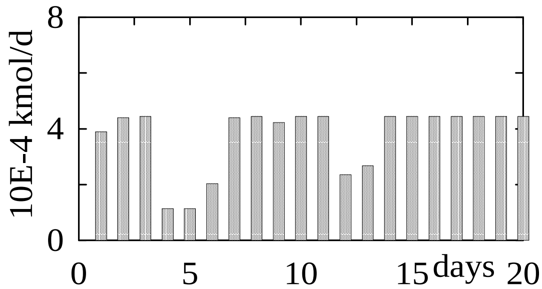


Figure 11Ethane processed in Ethylene Plant (3)

**Case2: Forced shutdown**

Figures 12 to 14 show the optimal inventory profile and Figure 15 and 17 show the natural gas processed in the high-pressure separator, the ethane separated in the NGL fractionator and the ethane processed in ethylene plant for the MILP of Case2. Figures 18 to 23 show the same variables profiles for the MINLP of the same case.

In both cases, the most efficient ethylene plant (II), the natural gas processing plant and the VCM plant, which is the one that renders higher profits among the end product plants, operate at their maximum capacities.

Table 1 shows number of continuous and binary variables and CPU time for the reported cases.

**MILP**

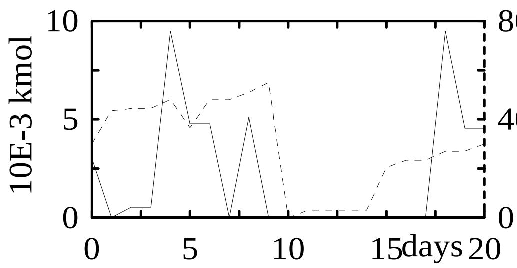


Figure 12 Tank A and D (dash line and right axis)

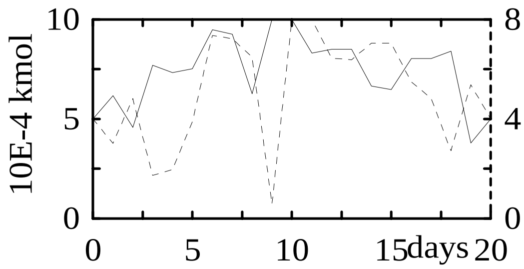


Figure 13 Tank B and C (dash line and right axis)

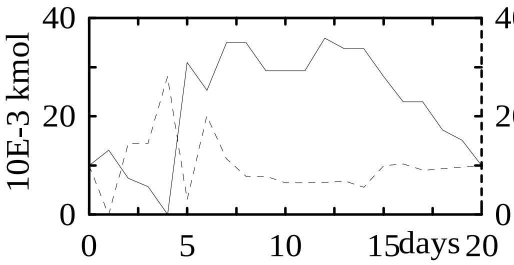


Figure 14 Tank E and F (dash line and right axis)

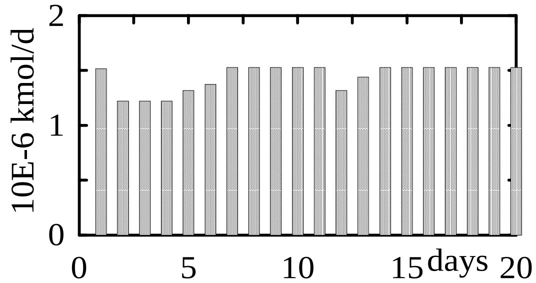


Figure 15 Natural gas processed in the Natural Gas Separator (1)

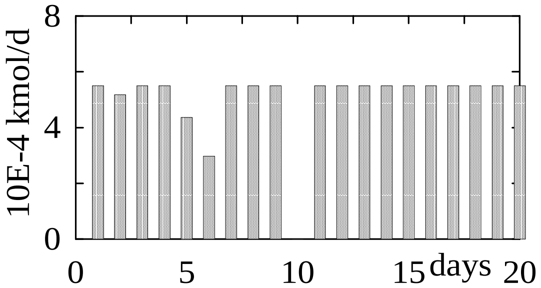


Figure 16 Ethane separated in the NGL Fractionator (2)

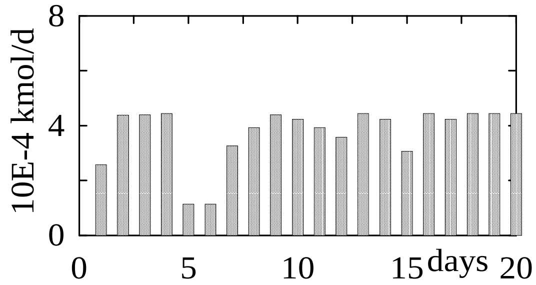


Figure 17 Ethane processed in Ethylene Plant (3)

**MINLP**

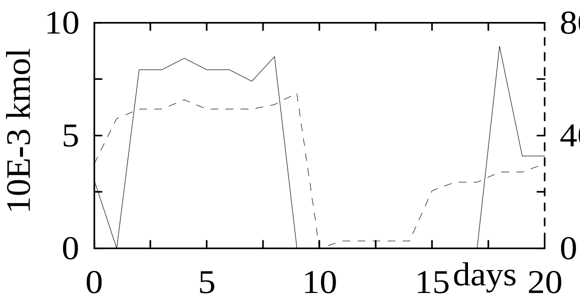


Figure 18 Tank A and D (dash line and right axis)

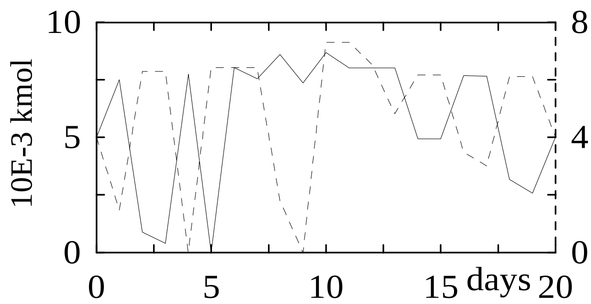


Figure 19 Tank B and C (dash line and right axis)

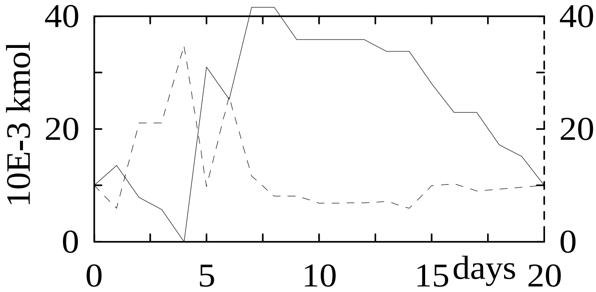

Figure 20 Tank E and F (dash line and right axis)

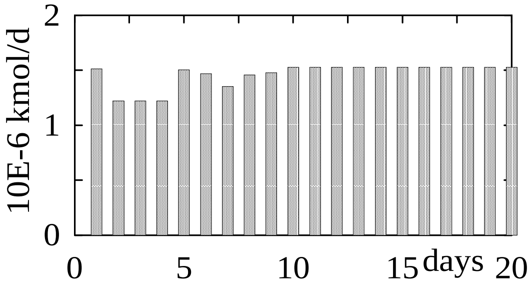

Figure 21 Natural gas processed in the Natural Gas Separator (1)

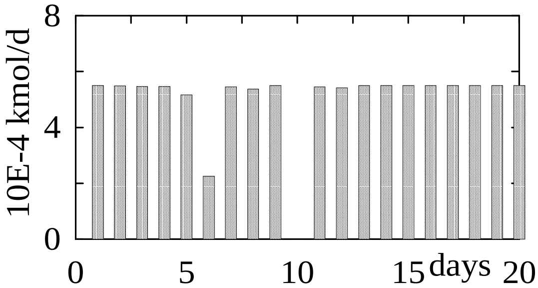

Figure 22 Ethane separated in the NGL Fractionator (2)

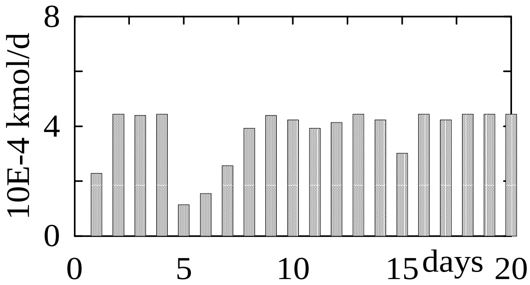

Figure 23 Ethane processed in Ethylene Plant (3)

In order to have all plants working the first six days of the horizon, the flow rates at the end of the pipeline for the first six days (residence time in the pipeline = 6 days) have to be fixed arbitrarily due to the time delay introduced by the pipeline.

A lower bound on the final mass of the tanks is used to avoid that the tanks be empty at the end of the horizon since the production cost of the intermediate products would not be recovered if they were not sold during the horizon.

These modelling recourses explain the fluctuating behaviour of the inventory levels and flowrate profiles during the first part of the studied horizon. A longer time horizon would show that operating profiles tend to a steady state, as can be observed in the last days in the figures.

Table 1: Problem size.

| | CASE 1 | | CASE 2 | |
|---|---|---|---|---|
| | LINEAL | NO LINEAL | LINEAL | NO LINEAL |
| EQUALITIES | 3960 | 6280 | 3966 | 6286 |
| INEQUALITIES | 11242 | 4250 | 11244 | 4252 |
| CONTINUOUS VARIABLES | 5997 | 5997 | 6058 | 6058 |
| BINARY VARIABLES | 400 | 0 | 400 | 0 |
| CPU Time | 489 | 243 | 23725 | 830 |

Table 1 shows that in Case 2 (forced shutdown) only six equalities (equations 7,8,10 and

11) and two inequalities (equations 9) are added to the model, but the model complexity increases noticeably as it is shown by the required CPU time.

## CONCLUSIONS

A solution method for a large scale MINLP problem with bilinearities is presented. A reformulation and linearization technique is applied to obtain an MILP that is used as the initial point of an equivalent NLP obtained by reformulation of the MINLP. The problems are solved with GAMS, using OSL solver for the lineal problems and CONOPT2 solver for the NLP.

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