Supply Chain Optimisation in a Petrochemical Complex
Erica P. Schulz, M. Soledad Diaz* and J. Alberto Bandoni
Planta Piloto de Ingeniería Química – PLAPIQUI (UNS- CONICET)
Camino La Carrindanga Km 7, 8000 Bahia Blanca, Argentina

Abstract
This paper addresses the supply chain optimisation of a petrochemical complex as a multiperiod model over a short time horizon. In order to coordinate responses to demands while maximising profit, simultaneous planning of production and each plant production distribution has been undertaken. The model is optimised along a short-term planning horizon spanning multiple periods and supports the decision-making process of supply, production, intermediate and final product storage and distribution. Intermittent deliveries and demand satisfaction have been considered. Nonconvexities arise from blending and storage of multicomponent streams. The resulting nonconvex large scale mixed integer nonlinear model has been solved with GAMS using as initial point a linear model where bilinerities have been reformulated into linear equations.

Keywords: supply chain, petrochemical complex, optimisation, production planning.

1. Introduction
Production planning is a valuable tool to help inventory level management in order to decrease production costs and satisfy demand requirements. Optimisation of the supply chain reveals the advantages of corporate planning with respect to multiple one-site plant production planning. All members that directly or indirectly participate in the work to satisfy a customer demand should be taken into account and the importance of physical distribution and integrated logistics should be emphasised. Recently, several authors have solved the supply chain optimisation of process networks, refineries and polymer plants (Bok et al., 2000; Neiro and Pinto, 2003; Jackson et al., 2003) as mathematical programming models.

In this work, the objective is to develop a short-term planning production model that includes feedstock procurement, product delivery, inventory management and decisions such as individual production levels for each product as well as operating conditions for each plant in a petrochemical complex. The system (Schulz et al., 2003) 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. Linear mathematical models have been derived for the NGL, ethylene and polyethylene plants, based on rigorous existing models tuned with actual plant data. Simplified models take into account variations in production with key plant operating variables, such as temperature and pressure in separation units.

* Author to whom correspondence should be addressed: sdiaz@plapiqui.edu.ar
Available yield data for chemical transformations and utilities consumption have been used to model the rest of the petrochemical complex.

Figure 1 shows the petrochemical complex model representation. The demethanization plant is fed with 36 MMm$^3$/d of natural gas. Light gases (residual gas: 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 charged into containers to equalize the charge, i.e. to damp any pulsation or flow changes that may
occur anywhere along the pipeline. The feed mixture undergoes a distillation process to obtain LPG (Liquefied Petroleum Gas: propane, butane and gasoline) and ethane to be used in ethylene production.

The ethane extraction plant next to the petrochemical complex is fed with 24 Mm$^3$/d of natural gas. Residual gas is recompressed to pipeline pressure; part of it is taken as feed for the ammonia plant and the rest is delivered as sales gas. The ethylene plants process 480,000 ton/y of pure ethane; ethylene is consumed in the three polyethylene plants, the VCM plant and the rest is exported by ship. The ammonia plant produces 120,600 kmol/d of ammonia and most of them are fed to the urea plant to produce 3,250 ton/d of urea. In these processes, 1.28 Mm$^3$/d of natural gas are used as raw material and 689,000 Nm$^3$/d, as fuel.

3. Mathematical Model

The objective function is the maximisation of the total profit, defined as the difference between the sales revenue and the total operating cost for the entire site during the given time horizon.

The molar balance equations for each container at each discrete time interval is calculated as the initial moles plus the summation of inflows subtracted by the summation of outflows up to each time interval (Lee et al., 1996). The material balance equations for the multicomponent streams in the splitters are nonconvex equations that involve bilinear terms for the total flows and component compositions. These bilinear terms impose the condition that the ratios of flows between components be the same for the different streams. In both natural gas plants, ethane and carbon dioxide recovery is a linear function of high-pressure separation tank temperature and top pressure in demethanizing column:

$$\eta_j^t = aT_t + bP_t + c \quad \forall t; j = CO_2, C_2H_6$$  \hspace{1cm} (1)

Product flows ($F_{s_j^t}$) are calculated as products between inlet flowrate ($F_{e_j^t}$) and recovery ($\eta_j^t$), also resulting in bilinear equations:

$$F_{s_j^t} = F_{e_j^t} \cdot \eta_j^t \quad \forall t; j = CO_2, C_2H_6$$  \hspace{1cm} (2)

All the tanks have a minimum security inventory level. Tank inventory costs for the rich gas mixture, propane, butane, gasoline, urea, ammonia and ethylene are calculated according to the trapezoidal area, as illustrated in Fig. 2.

<table>
<thead>
<tr>
<th>Table 1. Arrival days of ships</th>
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<tbody>
<tr>
<td><strong>Product</strong></td>
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<tr>
<td>Propane</td>
</tr>
<tr>
<td>Butane</td>
</tr>
<tr>
<td>Gasoline</td>
</tr>
<tr>
<td>Ammonia</td>
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<tr>
<td>Urea</td>
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An economic penalty is used when the inventory levels of polyethylenes do not meet the given storage targets (Jackson et al., 2003).
\[ C_{poly}^t = C_{poly}^0 + \sum_{t} FIM_{poly}^t - \sum_{t} FM_{poly}^t \quad \forall t, \forall poly \] (3)

\( C_{poly}^t \) is the inventory of polyethylene (poly = HDPE, LDPE, LLDPE) in the current period \( t \), \( C_{poly}^0 \) is the initial inventory, \( FIM_{poly}^t \) is the final production of product \( poly \) in period \( t \) and \( FM_{poly}^t \) corresponds to sales of polyethylene \( poly \) in period \( t \) (Eqn. 3). For polyethylene storage, an economic penalty is used when inventory levels do not satisfy given storage targets (Jackson et al., 2003). The sales cannot exceed the daily forecast demand (\( dem_{poly}^t \)) and the difference between the demand and the sales (\( delta_{poly}^t \)) is used as penalty (\( delta_{poly}^t \) times product price) in the objective function for not meeting the demand, Eqns. (4-5)

\[ dem_{poly}^t \geq FM_{poly}^kt \quad \forall t, \forall poly \] (4)

\[ delta_{poly}^t = dem_{poly}^t - FM_{poly}^kt \quad \forall t, \forall poly \] (5)

There are storage tanks for propane, butane, gasolines, ammonia and urea. These products are intermittently delivered by ship \( (F_v^t) \), Eqn. (6). Each product is stored in a different tank \( v \). The tanks have capacity lower and upper limits. Ship delivery for these products was modelled as it is shown in Eqns. (7-14) (Lee et al., 1996).

\[ V_v^t = V_v^0 + \sum_{t} F_i^t - \sum_{t} F_i^t, \quad \forall v, \forall t \] (6)

\[ \sum_{t} XF_v^t = 1 \quad \forall v \] (7)

\[ \sum_{t} XL_v^t = 1 \quad \forall v \] (8)

\[ \sum_{t} XF_v^t = TF_v \quad \forall v \] (9)

\[ \sum_{t} XL_v^t = TL_v \quad \forall v \] (10)

\[ TF_v - TL_v \geq tv_v^{min} \quad \forall v \] (11)

\[ TF_v - TL_v \leq tv_v^{max} \quad \forall v \] (12)

\[ XWV_v^t = \sum_{m=1}^{t} XF_v^t - XL_v^t \quad \forall v, \forall t \] (13)

\[ F_v^t \leq F_v^{MU} XWV_v^t \quad \forall v, \forall t \] (14)

\[ F_v^t \geq F_v^{MD} XWV_v^t \quad \forall v, \forall t \] (15)

\[ dem_v \geq \sum_{t} F_v^t \quad \forall v \] (16)

\[ delta_v = dem_v - \sum_{t} F_v^t \quad \forall v \] (17)

\( XF_v^t \) and \( XL_v^t \) are binary variables to denote if ship \( v \) starts or completes loading the product. Each ship loads the corresponding product only once throughout the horizon,
Eqns. (7-8), and it starts loading at $t = TF_v$ (Table 1) and finishes at $t = TL_v$, Eqns. (9-10). Loading time is limited, Eqns. 11-12. $XW_v t$ is a continuous variable to denote if ship $v$ is loading its product at time $t$. Eqns. (14-15) are operating constraints on product transfer rate $F_v^i$ ($F_v^{il} \leq F_v^i \leq F_v^{iu}$) from the storage tanks to the ship. Total product sales during the horizon cannot exceed the forecast demand. Eqns. (16-17) monitor the customer satisfaction.

As the nonconvex large scale MINLP model requires a good initial point, a reformulation – linearization technique has been applied to obtain a valid linear model (Quesada and Grossmann, 1995). The linear model has 13,376 equations, 6,207 continuous variables, and 200 binary variables while the nonlinear model comprises 6,956 equations, 6,207 continuous variables and 200 binary variables. The multiperiod MILP and MINLP problems have been coded in GAMS 2.25 modelling environment and solved with OSL and DICOPT++ (CONOPT2 and OSL), respectively. The problems have been solved in a 1GHz Pentium III PC, with 256 Mbytes of RAM. The MILP demanded 749.781 CPUs and the MINLP 1061.879 CPUs. The MINLP solution has required three major iterations.

4. Numerical Results

Figures 1 to 3 show the sales of polyethylene and the difference between the sales and the forecast demand (demand satisfaction) in tons for a horizon of 20 days. Figures 4 to 6 show the inventory and the penalty for not meeting the storage target of the polyethylenes in tons. The HDPE Plant has higher penalties but lower differences between sales and demands since it is more profitable. Figures 7 and 8 show inventory levels in kmol of propane, butane and gasoline in the NGL Fractionation Plant. Propane and butanes forecast demands were satisfied but the difference between the demand and the sales in the case of gasoline was 43,681 kmol since gasoline is cheaper than propane and butane and its production is less profitable. The model also provides optimal operating conditions for main units in the gas plant (high pressure separator temperature and demethanizing column top pressure) to achieve production levels required along the considered time horizon.

5. Conclusions

A realistic multiperiod model has been presented for optimal short-term production planning in a petrochemical complex as an MINLP problem. A typical scenario has been considered, but the model is able to address different conditions, such as daily demand profiles, storage conditions, etc. A valid linearization technique was applied to obtain a valid initial point for the MINLP problem. The determination of main process operating conditions for a few plants of the entire complex has also been obtained. The inclusion of more detailed process models for the ethylene plant and the exploration of solution methods that can cope with the resulting large-scale MINLP is part of current work.

References

Schulz E., Diaz S. and A. Bandoni, 2003, Total Site Scheduling in a Petrochemical Complex, Chemical Engineering Transactions, Eds. S. Pierucci, 3, 1221.

Figure 1 LDPE demand satisfaction sales in tons
Figure 2 LLDPE demand satisfaction sales in tons
Figure 3 HDPE demand satisfaction sales in tons
Figure 4 HDPE inventory penalty
Figure 5 LDPE inventory penalty
Figure 6 LLDPE inventory penalty
Figure 7 Propane inventory in the NGL Fractionation Plant in kmol
Figure 8 Butane inventory in the NGL Fractionation Plant in kmol