SUPPLY CHAIN OPTIMIZATION: SHORT TERM PLANNING AND DISTRIBUTION DECISIONS FOR A PETROCHEMICAL COMPLEX

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Abstract

In this work, a multiperiod MINLP model is proposed for the supply chain optimization of a petrochemical complex. Nonlinear, semi-rigorous models have been included for main plants in the site, allowing the determination of process operating conditions and product properties. Intermediate and final product storage and shipping are considered. Binary variables are associated to intermittent product delivery. The model has been solved for a given scenario and numerical results provide a realistic insight on supply chain management in the petrochemical complex.

Keywords

Petrochemical complex, Supply chain, MINLP optimization, Short term planning.

Introduction

There is an increasing need for the simultaneous planning of production, storage and distribution in most petrochemical complexes to coordinate responses to demands while maximizing profit in the entire supply chain. Decisions have to be taken at different stages of the supply chain yielding economic benefits and improving understanding of the interactions between the plants. Several authors have recently addressed supply chain optimization in continuous processes. Turkay and Grossmann (1996) propose logic-based approaches to solve complex problems. In particular, Turkay et al. (1998) apply these techniques to solve the total site optimization of a petrochemical complex. Bok et al. (2000) propose a bilevel decomposition strategy for the solution of a multiperiod mixed integer linear programming (MILP) model for the supply chain of continuous processes taking into account sales, intermittent deliveries, production shortfalls, delivery delays, inventory profiles and changeovers. More recently, Neiro and Pinto (2003) address supply chain of petroleum refinery complexes as a mixed integer nonlinear programming (MINLP) problem,

including process unit models, storage tanks and pipelines. Jackson and Grossmann (2003) propose Lagrangian decomposition (spatial or temporal) techniques for the solution of a nonlinear programming (NLP) problem that models multisite production planning of production, transportation and sales in a chemical company.

In this work, the supply chain optimization of a petrochemical complex is addressed as a multiperiod model over a short time horizon. Semi-rigorous models are included for main plants in the site, taking into account process operating conditions and product properties, together with intermediate and final product storage and shipping. Intermittent product delivery is represented with binary variables. The objective is the maximization of total profit for the entire site considering operating, shortfall and inventory costs; subject to constraints on mass balances, bounds on product demands, equipment capacities and intermediate and final product storage tanks limitations.

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Petrochemical Complex Description

Figure 1 shows the petrochemical complex model representation. There are two natural gas processing plants, whose main objective is to extract ethane from natural gas to use it as raw material in ethylene plants. Natural Gas Plant I, next to the complex, is fed with natural gas. Residual gas (mainly methane) is recompressed to pipeline pressure; part of it is taken as feed for the ammonia plant and the rest is delivered as sales gas. Pure ethane, propane, butane and gasolines are plant products. Natural Gas Plant II has its cryogenic sector (referred to as Demethanizing Plant) several kilometers away from the conventional separation train (NGL Fractionation Plant). Light gases (methane, nitrogen and carbon dioxide) are separated from the heavy ones (ethane, propanes, butanes and gasolines) and injected to the natural gas pipeline in the demethanizing sector. The rich gas mixture is stored in thermal vessels and pumped to the petrochemical complex where it is fed to containers to damp any pulsation or flow changes that may occur along the pipeline. The feed mixture undergoes a conventional distillation train in the NGL Fractionation Plant to obtain LPG (Liquefied Petroleum Gas: propane, butane and gasoline) and ethane. Ethylene plants process pure ethane. Ethylene is provided as raw material to polyethylene and VCM plants and the rest is exported. Most of the ammonia plant production is fed to the urea plant to produce 3,250 ton/d of urea. Urea, ammonia, polyethylenes and PVC are delivered by ship, train and trucks.



Figure 1. Petrochemical complex

Mathematical Model

Both natural gas plants are based on turboexpansion processes. Linear models have been derived for ethane and carbon dioxide recovery in the cryogenic sector, as function of main operating variables: high-pressure separation tank temperature and demethanizing column top pressure. These correlations have been obtained based on simulations with a plant rigorous model. Product flows are calculated as products between inlet flowrate and recovery, resulting in bilinear equations. For propane, butanes, pentanes and hexane, 100 % recovery is assumed. Residual gas flowrate (methane and nitrogen) is calculated as the difference between feed gas flowrate and the summation over the heavy components flowrates. The stream of liquids to the NGL Fractionation Plant is composed of carbon dioxide, ethane, propane, butanes, pentanes and hexane, which are fed to intermediate containers as a multicomponent mixture.

There are storage tanks for pure propane, butane and gasolines (modelled as pentanes + hexane). The tanks have capacity lower and upper limits.

$$V_j^t = V_j^o + \sum_t f \hat{i}_j^t - \sum_t f k_j^t - \sum_t f v_j^t,$$

 $v = C3, C4, Gasoline, t = 1 \dots SCH$

where V_j^t are the moles of component *j* (in tank *j*) at time period *t* and V_j^0 are the initial moles of component *j* in the tank, f_{ij}^t are the inlet molar flows of component *j* (plant production); $f_{v_j^t}$ are outlet molar flows of component *j* intermittently delivered by ship and $f_{k_j^t}$ are outlet molar flows of component *j* daily delivered by truck.

(1)

Ship delivery for these products is modeled through binary variables (Lee et al., 1996; Schulz et al., 2003):

$$\sum_{t} y f_{v}^{t} = 1, v = C3, C4, Gasoline$$
(2)

$$\sum_{t} y l_{v}^{t} = 1, v = C3, C4, Gasoline$$
(3)

$$\sum_{t} t y f_{v}^{t} = TF_{v}, v = C3, C4, Gasoline$$
(4)

$$\sum_{t} t y l_{v}^{t} = TL_{v}, v = C3, C4, Gasoline$$
(5)

$$TF_{v} - TL_{v} \ge tv_{v}^{min}, \qquad v = C3, C4, Gasoline \qquad (6)$$

$$TF_v - TL_v \le tv_v^{\max}$$
, $v = C3, C4, Gasoline$ (7)

$$xw_{v}^{t} = \sum_{t} yf_{v}^{t} - yl_{v}^{t},$$

$$v = C_{v}^{2} C_{v}^{2} Gasoling t = 1 \quad SCH$$

$$v = C3, C4, Gasoline, t = 1...SCH$$
 (8)

$$fv_v^{\ t} \le fv_v^{\ to} \ xw_v^t, v = C3, C4, Gasoline, t = 1... SCH$$
(9)

$$fv_v^t \ge fv_v^{tL} xw_v^t, v = C3, C4, Gasoline, t = 1 ... SCH$$
 (10)

$$demv_{v} \geq \sum_{t} fv_{v}^{t}, v = C3, C4, Gasoline$$
(11)

$$deltav_{v} = demv_{v} - \sum_{t} fv_{v}^{t}, v = C3, C4, Gasoline$$
(12)

where yf_v^t and yl_v^t are binary variables to denote that ship v starts or completes loading the product. Each ship loads the corresponding product j only once throughout the horizon, Eqs. (2)–(3), and it starts loading at $t = TF_v$ and finishes at $t = TL_v$, Eqs. (4)–(5). Loading time is limited, Eqs (6)-(7); xw_v^t is a continuous variable to denote if ship v is loading its product at time t, Eqs. (8). Eqs. (9)-(10) are operating constraints on product transfer rate fv_v from storage tanks to the ship.

In ethylene plants, semi-rigorous models have been included based on Schulz et al. (2000), as function of main operating variables: For each plant *i*, cracked gas compressor suction pressure $(P_{CGCi}^{\ l})$, hydrocarbon dilution ratio with steam $(Rd_i^{\ l})$, conversion in each furnace *k* (*Conv*_{*i*,*k*}) are among optimization variables. There are nonlinear correlations for ethane recycle stream $(R_{i,j}^{\ l})$, Eqs. (13), furnaces inlet pressure $(Pin_i^{\ l})$, Eqs. (14), individual component furnace production $(Ff_{i,k,j}^{\ l})$, Eqs. (15), plant process streams exiting unit *u* in the separation train $(Ft_{u,i,j}^{\ l}, Fb_{u,i,j}^{\ l})$, Eqs. (16), (17).

$$R_{i,j}^{t} = f(P_{CGC,i}^{t}, Rel_{i}^{t}, Fsep_{i}^{t}), \forall i, j, t$$
(13)

$$Pin_i^t = f(fin_i^t, Rd_i^t, Pout_i^t, Conv_{i,k}^t), \forall i,k,t$$
(14)

$$Ff_{i,k,j}^{t} = f(fin_{i}^{t}, Rd_{i}^{t}, Pin_{i}^{t}, Conv_{i,k}^{t}), \forall i,k,t$$
(15)

$$Ft_{u,i,j}^{t} = f(P_{CGC,i}^{t}, Rel_{i}^{t}, fs_{u,i,j}), \forall i, u, t$$

$$(16)$$

$$Fb_{u,i,j}^{t} = f(P_{CGC,i}^{t}, Rel_{i}^{t}, fs_{u,i,j}), \forall i, u, t$$
(17)

where fin_i^t is total furnaces charge, Rel_i^t and $Fsep_i^t$ are ethylene/ethane ratio and total molar flowrate at the entrance of separation train, $fs_{u,ij}$ is the separation factor in plant *i*, unit *u* for component *j*.

In polyethylene plants, inlet-outlet models have been included, based on information from the literature. For polyethylene storage, an economic penalty is used when inventory levels do not satisfy given storage targets (Jackson and Grossmann, 2003). Also, the sales cannot exceed the daily forecast demand and the difference between the demand and the sales is used as penalty in the objective function for not meeting the demand, (Jackson and Grossmann, 2003). Inlet-outlet models have been included for ammonia, urea, VCM, chlorine and PVC plants. Urea and ammonia are intermittently delivered by ship, which is modelled in an analogous way to LPG. They are also daily delivered by train and truck.

The objective function is profit maximization. Incomes from product sales are considered. Negative terms are: operating costs, tank inventory costs (calculated according to the trapezoidal area), penalties for not satisfying forecast demands, ship capacities and inventory targets.

Numerical Results and Discussion.

The multiperiod MINLP supply chain model for the petrochemical complex has been solved in GAMS (Brooke et al., 1992), with DICOPT++, in three major iterations, selecting CONOPT2 and OSL, as solvers for the NLP and MILP subproblems, respectively. The model has 16373 equations. 18408 continuous variables and 200 binary variables, for a 20 days horizon. Raw material cost and product prices, as well as forecast demands and ship capacities have been taken from the open literature (Hydrocarbon Processing, Internet). Figure 2 shows LPG storage tanks profiles and it can be clearly seen that propane, butane and gasoline ships arrive on days 15, 17 and 19, respectively, and the plant decreases its production during the last days in the time horizon. Figure 3 shows that Ethylene Plant II, mainly fed by this plant, decreases its production during the last days. The model also gives conversion profiles (Fig. 4) for each furnace in the ethylene plants, as it is shown for three furnaces (there are eight in this plant), in Ethylene Plant I. Finally, Fig. 5 shows LLDPE production and inventory level, as compared to an inventory target (360 Ton).



Figure 2. LPG tanks profiles in Natural Gas Plant II



Figure 3. Ethane recycle and total furnaces charge profiles in Ethylene Plant II



Figure 4. Conversion profiles in three furnaces from Ethylene Plant I



Figure 5. LLDPE production and inventory profiles

Conclusions.

Modern petrochemical sites tend to be single integrated facilities to optimize total processing economics for converting natural gas to final industrial products. An optimization approach in which all the processes are highly integrated has proved to be a useful tool to detect operational and economical improvements. The inclusion of further details on plant models and solution techniques for the large scale MINLP model is part of current work.

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References

- Brooke, A., Kendrick, D., Meeraus, A. A. (1992). GAMS- A User's Guide (Release 2.25). *The Scientific Press*. San Francisco, CA.
- Bok J., I.E. Grossmann, S. Park, 2000, Supply Chain Optimisation in Continuous Flexible Process Networks, *Ind.Eng.Chem.Res.*, 39, 1279.
- Jackson J.R., I.E. Grossmann, 2003, Temporal Decomposition Scheme for Nonlinear Multisite Production Planning & Distribution Models, *Ind.Eng.Chem.Res.*, 42, 3045.
- Lee H., J.M. Pinto, I.E. Grossmann and S. Park, 1996, Mixed -Integer Linear Programming Model for Refinery Short
 – Term Scheduling of Crude Oil Unloading with Inventory Management, *Ind.Eng.Chem Res.*, 35, 1630.
- Neiro S.M., Pinto J.M., 2003, Supply Chain Optimization of Petroleum Refinery Complexes, *Found.Comp.-Aided Proc.Oper.*, Eds. I.E. Grossmann and C.M. McDonald,
- Schulz E., S. Diaz, A. Bandoni, 2000, Interaction Between Process Plant Operation and Cracking Furnaces Maintenance Policy in an Ethylene Plant, *Comp. Aided Proc. Engng.*, 8, 487-492.
- Schulz E., S. Diaz, A. Bandoni, 2004, Supply Chain Optimisation in a Petrochemical Complex, *Proceedings of ESCAPE14*,Lisbon, Portugal.
- Quesada I., I.E. Grossmann, 1995, Global Optimization of Bilinear Process Networks with Multicomponent Flows, Comp. Chem. Engng., 19, 12, 1219.
- Turkay M., Asakura, Fujita K., Chi Wai Hui, Natori Y., 1998, Total Site Optimization of a Petrochemical Complex, AIChe Symposium Series, 94, 185-189.