A Mathematical Model for Optimum Petrochemical Multi-Grade Selection, Production, and Sequencing

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A mixed integer programming model is presented for the optimum planning of multi-grade, multi-plant petrochemical production. When producing several grades of a given petrochemical product in the same reactor, the amount of transitional off-spec production depends on the sequencing of different grades. The model determines the optimum mix of petrochemical grades for each plant, the quantity to produce of each selected grade, and the optimum production sequence of different grades. The model incorporates demand, capacity, raw material availability, and sequencing constraints, in order to maximize the total profitability. The model is applied to real-life data of multi-grade polypropylene production of a large local petrochemical company.

1. Introduction

The petrochemical industry is increasingly competitive. During the last few years, the impacts of globalization, World Trade Organization, and growing environmental regulations have put increasing pressures on petrochemical producers around the world. In order to compete globally, petrochemical industries in Saudi Arabia have been looking for ways to maximize both their management effectiveness and manufacturing efficiency. In order to achieve these goals, petrochemical companies have resorted to several modern approaches, aiming to minimize cost and maximize profitability. These include, for example, Enterprise Resource Planning (ERP) systems, Supply Chain Management (SCM), and optimization tools such as linear and integer programming.

In the production of many petrochemicals, it is possible to produce several grades of each product by altering the production conditions, i.e. chemical reaction process variables. For example, temperature, pressure, and feed rates of raw materials and catalyst are manipulated in order to control the density, melt flow rate, and production rate for various grades. Different grades of the same petrochemical product differ from each other in chemical and physical properties and therefore in the industrial or consumer use, which leads to widely varying demand levels. Moreover, such grades vary in their raw material consumption, production cost, and selling price.

When switching from one grade to another, there is a changeover period in the reactor, in which a certain amount of transitional material is produced that does not conform to the specification of either grade. Naturally, the non-conforming "off-spec" material has a much lower sales value than regular grades. The amount of this "off-spec" material depends on the production sequence, i.e., the preceding grade and the following grade. Therefore, it is important to determine the right sequence of producing different grades in order to minimize off-spec production. In this paper, a mixed integer programming model is presented to determine the optimum selection, quantity, and sequence of different grades in multi-grade petrochemical production.

In the following section, relevant literature on multi-grade petrochemical production problem is reviewed. Subsequently, the mixed integer programming model is of this problem presented. This is followed by a case study application of this model in the multi-grade polypropylene production. Finally, conclusions drawn and suggestions for future research are provided.

2. Literature review

Previous approaches to multi-grade petrochemical production are generally fall under two main categories: control theory, and mathematical programming. The literature below is presented in the same order.

Tjoat and Raman (1999) discuss the need to link the enterprise business data system and the process automation/control systems to optimize the enterprise performance. This link will enable the chemical industry to have efficient and flexible production processes in order to effectively implement supply-chain management. Meeting this requirement will put a challenge on the process control technology, and will lead to significant SCM impacts on chemical plant operations. Using robust control theory, Mahadevan et al. (2002) propose tools and heuristics to identify operationally difficult grade transitions in the presence of uncertainty. The relationship between the cost, gain, and time constant of each transition is investigated to determine the effect of process nonlinearities on the scheduling system. This approach is applied to the scheduling of grade transitions in an isothermal methyl methacrylate polymerization reactor.

Feather et al. (2004) present a hybrid approach for the predictive control of polymer grade transition. The controller is represented as mixed integer linear programming model, incorporating both linear switching models and operating heuristics. The approach is tested in a polypropylene reactor system, leading to robust performance under varying production conditions. BenAmora et al. (2004) construct a nonlinear model predictive control (NLMPC) using orthogonal collocation to develop model equations, and use dynamic programming to solve the resulting nonlinear equations. Using an industrial real-time optimization package, they test the algorithm on two simulated polymerization case studies: (i) continuous methyl methacrylate, and (ii) gas-phase polyethylene. Bosgra et al. (2004) develop a closed-loop stochastic predictive control framework for production scheduling of multi-grade chemical processes. The procedure involves a deterministic feed-forward optimization stage and a stochastic feedback stage. In a related work, Tousain and Bosgra (2006) formulate multi-grade production scheduling for a continuous chemical process as a mixed integer linear programming model. By considering grade transition costs and sales orders and opportunities, the model integrates economics of production and company-market interaction. The approach is illustrated on a gas phase HDPE manufacturing plant.

In the above, mathematical programming models were utilized within a control theory framework. These optimization models have also been used independently. Karmarkar and Rajaram (2001) develop a nonlinear mixed-integer programming model of the chemical grade selection, production, and blending problem. Utilizing heuristics and lower bounds, the model minimizes the total cost while meeting quality and demand constraints. Applied on real-life data from a large European chemical producer, the model reduced the annual costs by $5 million (7%).

Alfares and Al-Amer (2002) develop a mixed integer linear programming model for planning the Saudi Arabian petrochemical industry expansion in four product categories: propylene derivatives, ethylene derivatives, synthesis gas derivatives, and aromatic derivatives. Considering production technologies, capacities, production costs, and selling prices, the model recommends products in each category under different scenarios. Joly et al. (2002) present nonlinear and mixed-integer programming models for planning and scheduling problems in petroleum refineries. Three practical refinery applications are presented: (i) inventory management for crude oil, (ii) production, inventory, and distribution for fuel oil and asphalt, and (iii) sequencing for liquefied petroleum gas (LPG).

3. Mixed integer programming model

The following mixed integer linear programming (MILP) model is presented to determine the optimum selection, quantity, and sequence of different grades in multi-grade petrochemical production. In order to maximize total profits, the model is flexible in terms of satisfying the given demands for different grades. If there is excess capacity, the given demand values are taken as lower bounds. However, in the case of insufficient capacity, the model considers these demands as upper bounds in order to preserve feasibility. Off-spec and sequencing constraints are represented using logical binary variables.

- Notations

C_i = production capacity (tons) of plant i per month
D_j = net demand in tons for grade j per month
EP = excess production capacity of all plants
ER_k = excess availability of raw material k
EX = minimum excess capacity $= min(EP, ER_1, , ER_K)$
J_i = set of indices of grades produced in plant i
G_i = set of reactor grade types which can be produced in plant i
g_i = set of indices of grades belonging to reactor grade g which can be produced in plant $i, g \in G_i$
M = a large number (as in the big-M method)
O_{igh} = off-spec production per transition between reactor grades g and h in plant i
P_{ij} = profit per ton of grade j produced in plant i
T_{igh} = profit of off-spec j produced in transition between reactor grades g and h in plant i
r_{ikj} = consumption of raw material k per ton of grade j in plant i
R_k = total availability of raw material k in tons per month
r_{ikgh} = usage of raw material k per transition between reactor grades g and h in plant i

- Decision variables

X_{ij} = tons of grade j produced at plant i

$$Q = \begin{cases} 1, & \text{if there is excess capacity } (EX > 0) \\ 0, & \text{otherwise} \end{cases}$$

$$Y_{ig} = \begin{cases} 1, & \text{if some grades from reactor grade } g \text{ are produced at plant } i \\ 0, & \text{otherwise} \end{cases}$$

$$F_{ig} = \begin{cases} 1, & \text{if some reactor grades } h \text{ higher than grade } g \text{ are produced at plant } i \\ 0, & \text{otherwise} \end{cases}$$

$$F_{ig} = \begin{cases} 1, & \text{if transition is made between reactor grades } g \text{ and } h \text{ at plant } i \\ 0, & \text{otherwise} \end{cases}$$

- Objective function

Maximize total profit of selected regular grades and off-spec produced in all plants:

$$\max \sum_{i=1}^{I} \sum_{j \in J_i} P_{ij} X_{ij} + \sum_{i=1}^{I} \sum_{\substack{g,h \in G_i, \\ h \geq g+1}} T_{igh} Z_{igh} \tag{1}$$

The above objective function is optimized subject to the following constaints:

- Capacity constraints

Total amount produced of regular grades and off-spec in each plant cannot exceed the plant's capacity:

$$\sum_{j\in J_i} X_{ij} + \sum_{\substack{g,h\in G_i,\\ h\geq g+1}} O_{igh} Z_{igh} \leq C_i, \qquad \text{i} = 1,\ldots,\text{I} \tag{2}$$

- Raw material constraints

Total amount consumed of each raw material k cannot exceed its availability:

$$\sum_{i=1}^{I}\left(\sum_{j\in J_i} r_{ikj} X_{ij} + \sum_{\substack{g,h\in G_i,\\ h\geq g+1}} s_{ikgh} Z_{igh}\right) \leq R_k, \qquad \text{k} = 1,\ldots,\text{K} \tag{3}$$

- Demand constraints

If there is no excess capacity ($Q = 0$), then production of each grade should be no more than demand. If excess capacity is available ($Q = 1$), then production of each grade should be no less than demand.

$$\sum_{i=1}^{I} X_{ij} \leq D_j + MQ \qquad \text{j} = 1,\ldots,\text{J} \tag{4}$$

$$\sum_{i=1}^{I} X_{ij} \geq Dj + M(Q-1) \qquad \text{j} = 1,\ldots,\text{J} \tag{5}$$

To calculate the value of minimum excess capacity EX:

$$EP = \sum_{i=1}^{I} C_i - \sum_{j=1}^{J} D_j \tag{6}$$

$$ER_k = R_k - \sum_{i=1}^{I}\sum_{j=1}^{J} r_{ikj} D_j \qquad \text{k} = 1,\ldots,\text{K} \tag{7}$$

$$EX \leq EP \tag{8}$$

$$EX \leq ER_k \qquad \text{k} = 1,\ldots,\text{K} \tag{9}$$

To ensure Q satisfies its definition:

$$EX \leq MQ \tag{10}$$

$$QEX \geq 0 \tag{11}$$

- Sequencing constraints

Transition can be made from reactor grade g only to one higher reactor grade h, given both grades are produced in plant i.

To ensure $Y_{ig} = 1$ only if reactor grade g is produced in plant i:

$$\sum_{j\in g_i} X_{ij} \leq MY_{ig} \qquad \text{i} = 1,\ldots,\text{I}, \ \cup g \in G_i \tag{12}$$

$$F_{ig} \leq \sum_{\substack{h\in G_i,\\ h\geq g+1}} Y_{ih} \qquad \text{i} = 1,\ldots,\text{I}, \ \cup g \in G_i \tag{13}$$

To ensure only one of the higher reactor grades h is chosen as the immediate successor of grade g:

$$Z_{igh} \leq 0.5(Y_{ig} + Y_{ih}) \qquad \text{i} = 1,\ldots,\text{I}, \quad g,h \in G_i,\ h \geq g+1 \tag{14}$$

$$\sum_{\substack{g,h\in G_i,\\ h\geq g+1}} Z_{igh} \geq Y_{ig} + F_{ig} - 1 \qquad \text{i} = 1,\ldots,\text{I}, \quad g,h \in G_i \tag{15}$$

It must be noted that restricting the next reactor grade h to be higher (h g + 1) produces a sequence in increasing order of reactor grades. This restriction reflects the physical realities of multi-grade petrochemical production. In order to minimize off-spec production, change in reactor grades must be as gradual as possible. Therefore, the different grades are sequenced in a cycle of two-phases: one phase with increasing order of reactor grades, and the other in decreasing order (Bosgra et al. 2004). Since the cost structure makes it undesirable to jump grades, the above model gives a gradually-increasing grade sequence for the first phase of the production cycle. This sequence is simply reversed to obtain the decreasing-order sequence for the second phase of the cycle.

- Non-negativity constraints

$$X_{ij} \geq 0 \qquad \mathrm{i} = 1,\ldots,\mathrm{I},\ \mathrm{j} = 1,\ldots,\mathrm{J} \tag{16}$$

4. Case Study

The above model was applied to a real-life data of a large local petrochemical company which has two polypropylene (PP) plants. There are 14 homo-polymer PP grades which can be produced in either plant, and 6 impact PP grades which can be produced only in plant 1. For each grade, monthly demands and total monthly production levels in each plant were recorded for a whole year. Table 1 shows different data relevant to Plant 1, as well as total demand for one sample month. The model was applied to the 12 monthly demand data, to determine the optimum monthly production of each grade. Compared with actual production, the optimum solution improved the annual profit by $4.7 million.

Table 1 PP grades data relevant to plant 1, and total monthly demand

No j	Pelleting Grade	Reactor Grade	Melt flow rate	Batch size (ton)	C3 use rj (ton/ton)	Demand Dj (tons/month)
	Homopolymer					
1	HG1	RG1	3	250	1.04	4750
2	HG2	RG1	3	250	1.04	2750
3	HG3	RG1	3	250	1.04	500
4	HG4	RG6	12	250	1.04	750
5	HG5	RG1	18	235	1.04	2250
6	HG6	RG1	25	235	1.04	3525
7	HG7	RG1	25	235	1.04	3525
8	HG8	RG4	10	250	1.04	1250
9	HG9	RG2	3	250	1.04	6500
10	HG10	RG2	3	250	1.04	379
11	HG11	RG3	8	250	1.04	1250
12	HG12	RG5	11	250	1.04	750
13	HG13	RG2	15	235	1.04	1000
14	HG14	RG1	25	235	1.04	470
	Impact					
15	IG15	RG7	8	250	0.945	5000
16	IG16	RG7	12	250	0.945	4500
17	IG17	RG7	25	235	0.945	500
18	IG18	RG7	7	200	0.945	0
19	IG19	RG7	25	200	0.945	0
20	IG20	RG7	14	200	0.945	0

5. Conclusions and suggestions

In this paper, an MILP model was presented to determine the optimum selection, quantity, and sequence of producing a multi-grade petrochemical product on different plants. The model maximizes total profit subject to production capacity, raw material availability, demand, and sequence-dependent off-spec production. The model uniquely adjusts the role of given demands in light of available capacity, treating them as upper bounds in case of insufficient capacity and as lower bounds in case of excess capacity. The model could be extended by including nonlinear relationships, multiple periods, and linking to inventory control.

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