U. Supply Chain Optimization in Continuous Flexible Process Networks

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Abstract – A multiperiod optimization model is proposed for addressing the supply chain optimization in continuous flexible process networks. The main feature of this study is that detailed operational decisions are considered over a short time horizon ranging from one week to one month. For given flexible process networks where dedicated and flexible processes coexist, we take into account the supply chain for sales, intermittent deliveries, production shortfalls, delivery delays, inventory profiles, and job changeovers. The proposed optimization model requires efficient solution strategies to reduce the computational expense. We describe a bilevel decomposition algorithm that involves a relaxed problem (RP) and a subproblem (SP) for the original supply chain problem. Decisions for purchasing raw materials are made in the (RP) problem in which the changeover constraints are relaxed, yielding an upper bound to the profit. In the (SP) subproblem, fixing the delivery predicted in (RP), the supply chain optimization is performed with job changeovers, yielding a lower bound. As will be shown in the examples, the algorithm achieves significant reduction in CPU time for the larger problems.

Introduction

As discussed by Shah[1], a number of papers have been published on the long term planning of process networks and batch plants over a long-range horizon[2-10]. These papers consider the choice of capacity expansion, start-up/shut-down policy for existing processes, and allocation of resources over a specified time horizon in order to maximize the net present value of the projects. For midterm production planning problems, Wilkinson et al.[11] and McDonald and Karimi[12] presented deterministic models for semicontinuous processes. The consideration of uncertainties in prices of materials and demands for the final products has been addressed in several recent papers[6-9,13,14].

In this paper the time interval of concern in the short-term planning of continuous flexible process networks is generally between one week and one month. Decisions to be determined include: (1) process operating modes for each time period, (2) sales and purchases for each time period, and (3) profiles for production and inventory. Often we also need to take into consideration job changeovers that incur corresponding costs. Furthermore, deliveries for sales or purchases can be intermittent with limited transportation availability. In the case when the demand for the final customers cannot be satisfied, we also need to account for the shortfalls or delay for the demand.

In order to effectively solve multiperiod optimization problems for short-term planning of continuous processes, a number of solution strategies have been proposed that rely on decomposition and reformulation. Benders decomposition [6,9,13,15] and bilevel decomposition[10,16,17] are two major approaches that have been applied to multiperiod optimization problems. Benders decomposition algorithm divides a problem into a subproblem and a master problem. The master problem is derived from a dual representation of the original problem. The subproblem involves the solution for fixed variables that are determined from the master problem. The bilevel decomposition is different from Benders decomposition in that the master problem is given by a special purpose aggregation of the original problem which generally tends to predict tighter upper bounds. Sahinidis and Grossmann[3,4] proposed a reformulation that is based on disaggregating variables for producing a tighter linear programming relaxation, which in turn reduces the number of nodes that need to be examined in the branch and bound tree.

As for the classification of chemical process networks, they can be characterized as consisting of dedicated processes or flexible processes. While dedicated processes operate with only one production scheme at all times and are usually used for the manufacturing of high-volume chemicals, flexible processes can manufacture different products at different times and are frequently used for the manufacturing of low-volume chemicals. Examples of flexible processes are paper mills that produce several types of paper of different weight or color, and refineries that process different types of crude oils. Sahinidis et al.[2] proposed a multiperiod model for networks with dedicated processes. Later, Sahinidis and Grossmann[3] proposed a planning model for process networks where flexible and dedicated processes can be interconnected. The flexible processes they considered were for producing different products from different raw materials. Norton and Grossmann[5] extended the model of Sahinidis and Grossmann[3] so that process flexibility is expanded to processes producing the same product with different raw materials, or different products with the same raw material.

This paper presents a multiperiod planning model for continuous process networks with dedicated and flexible plants operating over a short-term horizon that is aimed at addressing the supply chain optimization in these systems. A multiperiod MILP model is proposed that extends the model by Norton and Grossmann[5] by incorporating inventory profile, changeover costs, intermittent supplies, and production shortfalls. The model also considers transportation costs for deliveries when the network of processes is located in multiple sites. Due to the limitations in computational time with the LP-based branch and bound method, we describe a bilevel decomposition model that enhances computational efficiency. Several numerical examples are presented.

Problem Statement

A process network consists of a set of processes that are interconnected in a finite number of ways. The processes that can be either dedicated or flexible, involve a set of chemicals (raw materials, intermediates, and products) over a given time horizon. The raw materials and products are purchased or sold respectively in a set of markets, or else are intermediates for other processes. The process flexibility is expressed in terms of a set of production schemes that determine output materials from input materials as illustrated in Fig. 1.

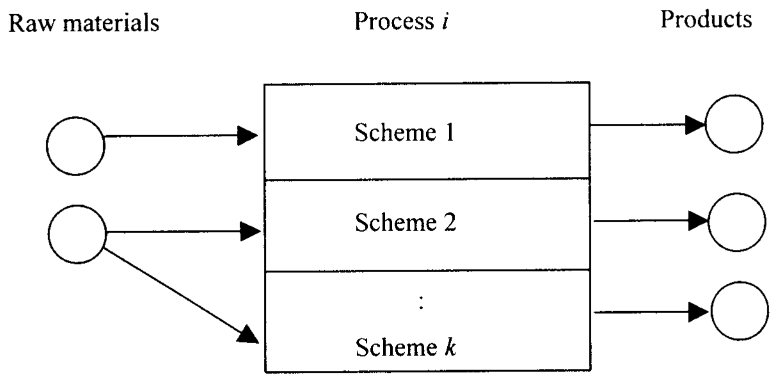


Fig. 1. Flexible processes with alternative production schemes

For all processes and schemes, we assume that material balances for raw materials and byproducts are expressed in terms of a linear unit ratio to the production of the main product for that scheme. It is also assumed that all the processes have fixed capacities, and that they might be located in multiple sites as shown in Fig. 2.The products and production schemes for each process in Fig. 2 are as follows. Raw materials are purchased from two marketplaces L1 and L2, and final products or intermediates that are specified as nodes are sold in two markets, L3 and L4. There are two production sites C1 and C2. First, we describe the site C1.

Process I1 is a dedicated continuous process producing chemical J3 from chemicals J1 and J6. Process I2 is a flexible continuous process with two production schemes. Scheme K1 for process I2 produces chemical J3 from chemical J1, while scheme K2 produces chemical J4 from chemicals J1 and J6. Process I4 is a flexible continuous process with two production schemes that demonstrates feedstock flexibility. Scheme

K1 for process I4 produces chemical J5 and byproduct J6 from chemical J3 while scheme K2 produces the same product and byproduct from chemical J4. Flexible process I3 has four production schemes and shows flexibiltiy with respect to both of product and feedstock. Scheme K1 for process I3 produces J3 from J1, while scheme K2 produces J4 from J1. Alternatively, scheme K3 produces J3 from J2, and scheme K4 produces J4 from J2. Chemical J1 is a raw material that is purchased from markets L1 and L2 and used in processes I1, I2, and I3. Chemical J2 is also a raw material used in process I3. Chemical J3 is a product of process I1, I2, or I3 and is either sold or used in process I4. Chemical J4 is produced by process I2 or I3, or can be purchased, and is used in process I4. Chemical J5 is a product of process I4 which is sold, and chemical J6 which can be bought from markets is a byproduct of process I4 which is recycled and used in process I1 or I2. Site C2 is similar to C1 but process I1 does not exist and process I3 has three production schemes K1, K2, and K3. One more difference is that site C2 has no recycle stream for chemical J6, which is not produced from process I4 at site C2.

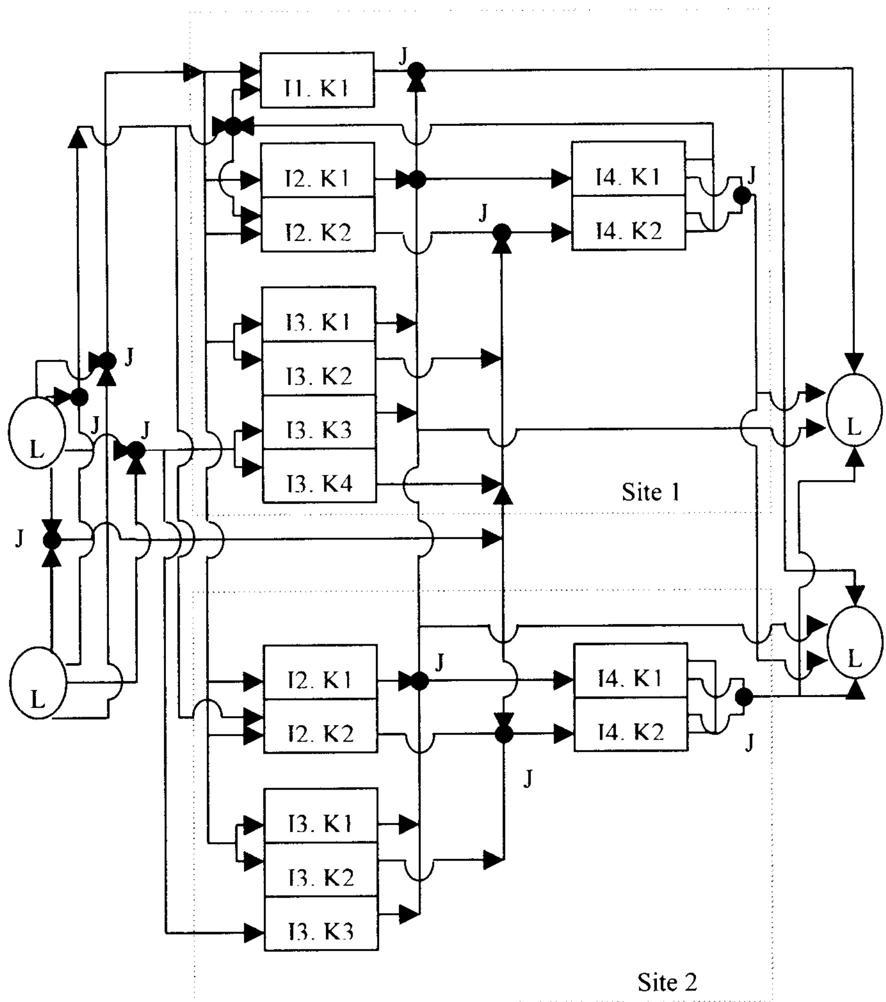


Fig. 2. Network diagram for multiple process sites.

The objective function to be maximized is the operating profit of the network over a short-term planning horizon consisting of a set of time periods during which prices and demands of chemicals and costs of operating and inventory can vary. The operating costs for each process and production scheme are assumed to be proportional to the flow of the main product. We also assume that the length of each time period is one day, and that each plant can only operate in one mode each day. Finally, we also assume that the effect of changeovers is only reflected through the cost since the actual changeover times are assumed to be negligible.

The short-term planning model (STPM) is expressed as a multiperiod mixed integer linear programming (MILP) problem. The indices, sets, parameters, and variables defined in the model are as follows:

Indices

c = site

d = delivery mode

i = process

j = chemical

k = production scheme

l = market

t = time period

Sets

C = set of sites

D = set of delivery modes

I = set of processes

I_j = set of processes that consume chemical j

J = set of chemicals

J_{ik} = set of chemicals involved in production scheme k of process i

JM_{ik} = set of main products for production scheme k of process i

K = set of production schemes

K_i = set of production schemes for process i

L = set of markets

O_j = set of processes that produce chemical j

T = set of time periods

Parameters

a^L_{jlt}, a^U_{jlt} = lower and upper bound for the amount of chemical j purchased from market l during time period t

d^L_{jlt}, d^U_{jlt} = lower and upper bound for the amount of chemical j sold from market l during time period t

Q_{ic} = capacity for process i at site c

V^U_{jct} = upper bound for the inventory amount of chemical j at site c during time t

W^U_{ijkc} = upper bound for the amount of chemical j produced from production scheme k of process i at site c

δ_{ikct} = unit operating cost for production scheme k for process i at site c during time t

ϕ_{jct} = cost for transporation of chemical j to site c during time t

τ_c = minimum time interval that an intermittent delivery can be made for site c

φ_{jlt} = price of purchase of chemical j in market l during time t

γ_{jlt} = price of sales of chemical j in market l during time t

ρ_{ijkc} = relative maximum production rate of main product j, for production scheme k in continuous flexible process i at site c

μ_{ijkc} = material balance coefficient for chemical j for production scheme k of process i at site c

θ_{jlt} = penalty cost for shortfall of chemical j in market l during time period t

ω_{jlct} = transportation cost of chemical j from market l to site c during time period t

ξ_{jc} = inventory cost for chemical j at site c

$\zeta_{ikk'c}$ = changeover cost for changing from production scheme k to k' in process i at site c

Variables

F_{jct} = amount of chemical j shipped to site c during time period t

NPV = net present value for the process

P_{jlct} = amount of chemical j purchased from market l for site c during time period t

S_{jlct} = amount of chemical j made from site c and sold at market l during time period t

SF_{jlt} = amount of shortfall of chemical j in market l during time period t

V_{jct} = amount of inventory of chemical j at site c during time period t

W_{ijkct} = amount of chemical j produced from scheme k of process i at site c during time period t

Y_{ikct} = 0-1 variable that denotes whether process i at site c operates with scheme k during time period t

YP_{dlct} =0-1 variable that denotes whether delivery type d is available in delivering from market l to site c during time period t

$Z_{ikk'ct}$ = 0-1 variable that denotes whether process i at site c operates with scheme k during the time period t and operates with scheme k' during the following time period t+1

In order to address detailed operations in the supply chain in the proposed model, we extend it to cover the detailed level of scheduling. Each time period is one-day long and the discrete or intermittent delivery of raw materials is taken into account.

Penalties for product shortfalls, as well as costs for product changeovers are also considered in the proposed model.

In the short-term planning model, the operating profit is given by

OP:

Maximize Profit =

$$\sum_{j\in J}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\gamma_{jlt}S_{jlct}-\sum_{j\in J}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\varphi_{jlt}P_{jlct}-\sum_{i\in I}\sum_{j\in JM_{ik}}\sum_{k\in K_i}\sum_{c\in C}\sum_{t\in T}\delta_{ikc}W_{ijkct}-\sum_{j\in J}\sum_{c\in C}\sum_{t\in T}\xi_{jc}V_{jct}$$
$$-\sum_{i\in I}\sum_{k\in K_i}\sum_{k'\in K_i}\sum_{c\in C}\sum_{t\in T}\zeta_{ikk'c}Z_{ikk'ct}-\sum_{j\in J}\sum_{l\in L}\sum_{t\in T}\theta_{jlt}SF_{jlt}-\sum_{d\in D}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\omega_{dlct}YP_{dlct}-\sum_{j\in J}\sum_{c\in C}\sum_{t\in T}\phi_{jct}F_{jct}$$

(1)

where each term accounts for income from sales, purchase cost, operating cost, inventory cost, product changeover cost, shortfall cost, delivery cost, and transportation cost between sites, respectively.

All chemical flows associated with scheme k in process i other than the main product are given by the mass balance coefficients. The following equation relates the input to the output of processes:

$$W_{ijkct}=\mu_{ijkc}W_{ij'kct}$$

$$i\in I,\ j\in J_{ik}\setminus j',\ j'\in JM_{ik},\ k\in K_i,\ c\in C,\ t\in T \qquad (2)$$

Equation (3) specifies the limitation on production. Only when production scheme k is allowed for process i ($Y_{ikct}=1$), can the production amount be up to the daily production rate, otherwise it is set to zero.

$$W_{ijkct}\le\rho_{ijck}Q_{ic}Y_{ikct}$$

$$i\in I,\ j\in JM_{ik},\ k\in K_i,\ c\in C,\ t\in T \qquad (3)$$

where $\rho_{ijk}Q_i$ represents the daily production rate.

In general, when the process changes production schemes, changeover costs are involved. In order to take this into account, we introduce a 0-1 variable: $Z_{ikk'ct}$ denoting the production changeovers. That is, $Z_{ikk'ct}$ should take the value of 1 if and only if process i operates with scheme k during time horizon t ($Y_{ikct}=1$), and it operates with scheme k' during the following time horizon t+1 ($Y_{ik'c,t+1}=1$). This logical condition can be represented by the following proposition:

$$Y_{ikct} \wedge Y_{ik'c,t+1} \Leftrightarrow Z_{ikk'ct}$$

$$i \in I, k \in K_i, k' \in K_i, c \in C, t \in T \qquad (4)$$

We can derive the following inequalities to represent the above condition as Raman and Grossmann[18] presented:

$$Y_{ikct} + Y_{ik'c,t+1} - 1 \le Z_{ikk'ct}$$

$$i \in I, k \in K_i, k' \in K_i, c \in C, t \in T \qquad (5)$$

$$Y_{ikct} \ge Z_{ikk'ct}$$

$$i \in I, k \in K_i, k' \in K_i, c \in C, t \in T \qquad (6)$$

$$Y_{ik'c,t+1} \ge Z_{ikk'ct}$$

$$i \in I, k \in K_i, k' \in K_i, c \in C, t \in T \qquad (7)$$

Equations (6) and (7) can easily be shown to be redundant since the objective function involves $Z_{ikk'ct}$, which will tend it to be zero. Furthermore, we do not have to treat $Z_{ikk'ct}$ as a 0-1 variable if we give it an upper bound, i. e. $Z_{ikk'ct} \le 1$.

The condition that each continuous process should be operated with exactly one production scheme during a time period (one day) can be imposed as shown in the equation:

$$\sum_{k \in K_i} Y_{ikct} = 1$$

$$i \in I, c \in C, t \in T \qquad (8)$$

Equation (9) corresponds to the mass balance of chemical *j* in the network:

$$V_{jc,t-1} + \sum_{i \in O_j} \sum_{k \in K_i} W_{ijkct} + \sum_{l \in L} P_{jlct} + F_{jct} = V_{jct} + \sum_{l \in L} S_{jlct} + \sum_{i \in I_j} \sum_{k \in K_i} W_{ijkct} + \sum_{c' \in C - \{c\}} F_{jc't}$$

$$j \in J, c \in C, t \in T \qquad (9)$$

In contrast with the common assumption of continuous delivery of raw materials[5,9], we consider that the purchase delivery can be intermittent as a discrete event that is specified by the inequality:

$$P_{jlct} \le \sum_{d \in D} YP_{dlct} P^U_{jlct}$$

$$j \in J, l \in L, c \in C, t \in T \qquad (10)$$

The purchase of a chemical can take place only when YP_{dlct} is 1. The limitation of delivery availability over the planning horizon is considered by assuming that only one delivery of the various raw materials can be made with each delivery type from each market during a specifed time interval τ_c as given by the inequalities:

$$\sum_{t'=t}^{t+\tau_c} YP_{dlct'} \le 1$$

$$d \in D, l \in L, t \in T, c \in C \qquad (11)$$

Equation (12) forces the sum of raw materials delivered to the processes not to be greater than the available amount during the time period:

$$\sum_{c \in C} P_{jlct} \le a^U_{jlt}$$

$$j \in J, l \in L, t \in T \qquad (12)$$

In general, the demand is assumed to be flexible in the sense that it is given by a range of values having a hard upper bound (see equation (13)) and a soft lower bound (see equation (14)) as Birewar and Grossmann[19] presented. The lower bounds are given by fixed orders booked by the sales department. Production shortfalls with respect to the lower bounds stand for loss of potential sales which is penalized in the objective function, equation (1).

$$\sum_{c \in C} S_{jlct} \le d_{jlt}^U$$

$$j \in J, l \in L, t \in T \qquad (13)$$

$$SF_{jlt} \ge SF_{jl,t-1} + d_{jlt}^L - \sum_{c \in C} S_{jlct}$$

$$j \in J, l \in L, t \in T \qquad (14)$$

$$SF_{jlt} \ge 0$$

$$j \in J, l \in L, t \in T \qquad (15)$$

Note that the shortfalls of the previous time period $SF_{jl,t-1}$ are considered in the current time period, as indicated in equation (14).

Finally, equations (16) and (17) represent the upper or lower bounds for each variable.

$$V_{jct} \le V_{jct}^U$$

$$j \in J, c \in C, t \in T \qquad (16)$$

$$F_{jct}, P_{jlct}, S_{jlct}, V_{jct}, W_{ijkct}, Z_{ikk'ct} \ge 0,$$

$$Y_{ikct}, YP_{dlct} \in \{0,1\} \qquad (17)$$

Example 1

In this section, the example problem in Fig. 2 is solved to illustrate the performance of the model in three cases: (1) No intermittent deliveries without product changeovers, (2) intermittent deliveries without changeovers, (3) intermittent deliveries with changeovers. It is obvious that case 3 is the most rigorous and reflects the real nature most properly. Cases 2 and 3 can be obtained by relaxing the discrete nature of case 3. In the case of intermittent deliveries, we assume that the minimum time interval between successive deliveries, τ_c, is 2 days regardless of the chemicals or the sites. The data for this example are shown in Appendix 1.

The problem is modeled using the GAMS[20] modeling language, and solved in the full space using the CPLEX solver[21] on a HP 9000/7000. The optimization results for example 1 are as follows. In case 1, no 0-1 variable is needed since there are no intermittent deliveries, nor any changeovers. The more rigorous the model (cases 2 or 3), the larger the number of 0-1 variables that is required. This in turn results in more computation time for the optimization as shown in Table 1.

Table 1. Computational statistics for example 1

*Case	0-1 variables	Constraints	Continuous variables	CPU[sec]	Nodes	Relaxed Solution	MILP solution
1	-	837	1072	1.0	-	2398.4	-
2	28	837	1044	2.4	12	2398.4	2392.9
3	252	1605	1642	24.5	347	2398.4	2362.2

*1. No intermittent deliveries and without changeovers

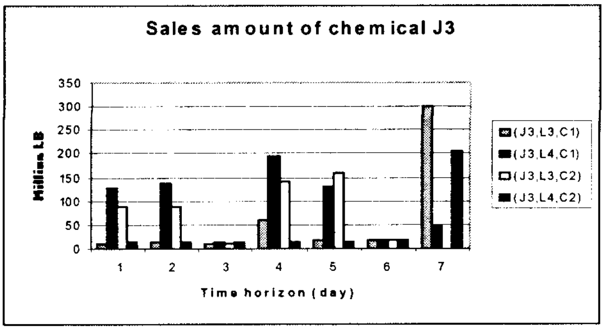
2. Intermittent deliveries and without changeovers

3. Intermittent deliveries and with changeovers

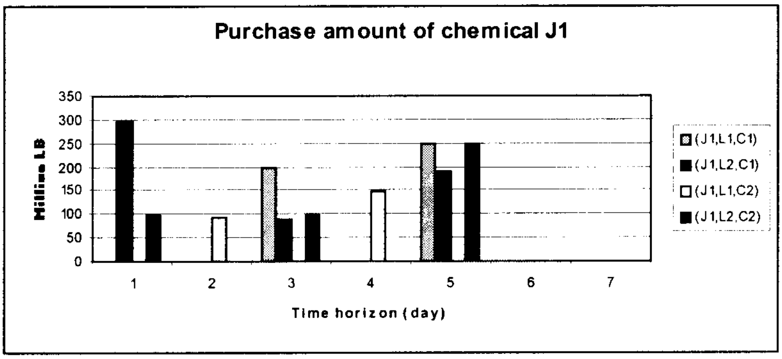
Figures 3 to 5 show the optimization results for case 3 that considers the intermittent deliveries and changeovers. Fig. 3(a) illustrates the sales of chemical J3 from each site (C1 and C2, respectively) to each market (L3 and L4, respectively). For given demand data (See in Tables A.7 and A.8), sales results can be obtained over 7 time periods. Fig. 3 (b) shows the delivery of chemical J1, which by constraint 11 should take place every two days from a given market to a given site.

Fig. 4(a) shows production profiles for chemicals from a flexible process I3 in sites C1 and C2, respectively. We can observe that process I3 in both sites C1 and C2 operate at the maximum capacity rate (See Table A.1). From process I3 at site C1, chemicals J3 and J4 are produced by alternating the production schemes while only chemical J3 is produced from process I3 at site C2. Fig. 4(b) shows the production profile of chemical J5 in process I4 at sites C1 and C2 over the horizon.

Fig. 5 shows the transportation of chemicals from site C1 to C2. Chemical J6 produced from process I4 in site C1 is transported to C2, and used in order to produce chemical J4 from process I2 with scheme K2 in site C2. Chemical J4 which is surplus in site C1 is also transported to site C2 at time periods, 5 to 7. In Fig. 6, the inventory of chemicals J3 and J4 at each site and shortfall amount of chemicals J3 and J5 are illustrated. Fig. 6(b) shows that more profit can be made at an enhanced production rate at the first time period.

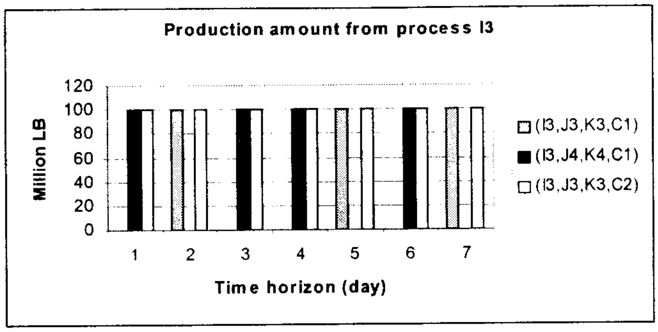


(a)



(b)

Fig. 3. Optimization results for sales and purchases in example 1.



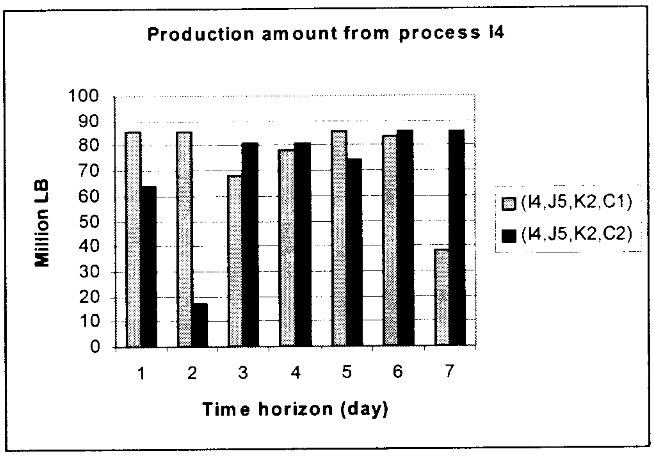


Fig. 4. Optimization results for production amount in example 1.

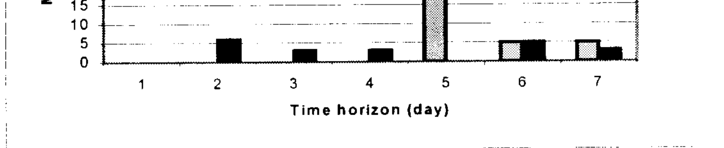
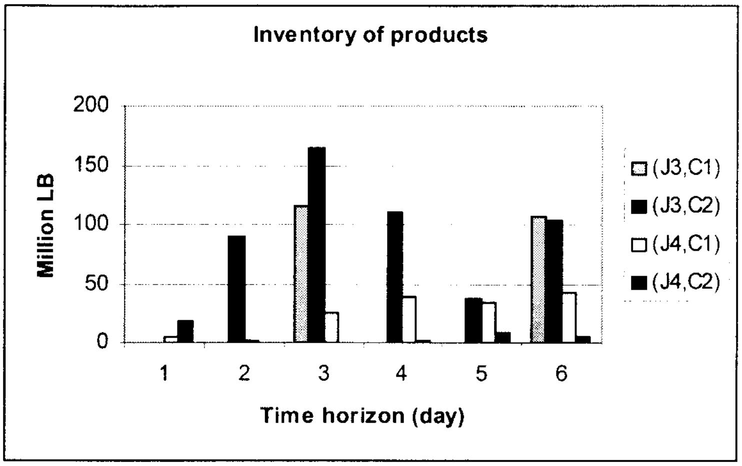
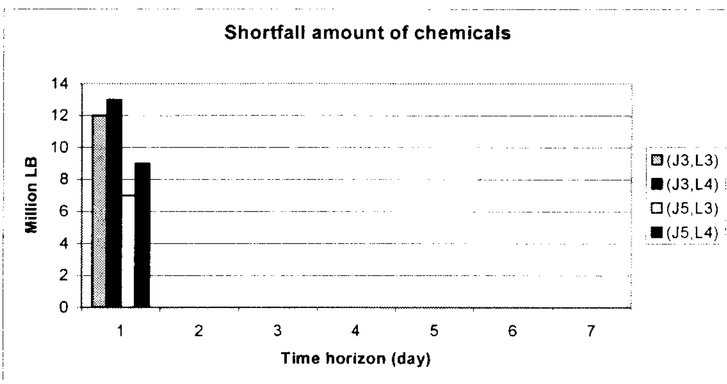


Fig. 5. Optimization results for transportation of chemicals between sites in example



(a)



(b)

Fig. 6 Inventory of chemicals J3 and J4 and the amount of production shortfalls.

Solution method

In order to solve larger process networks that involve longer time horizons (e.g. up to 30 days), it is clear that we require a special solution method, as otherwise the LP-based branch and bound method becomes expensive, or simply unable to solve these problems.

One important aspect in the solution is the potential source of degeneracy in the model, that is mainly due to the fact that binary variables denoting the assignment of production scheme to each process during a time horizon are not present in the objective function. Adding the following term to the objective function can help somewhat to expedite the search,

$$\varepsilon \sum_{i \in I} \sum_{k \in K_i} \sum_{c \in C} \sum_{t \in T} Y_{ikct} \qquad (18)$$

where ε is a parameter with a very small value (e.g. it is of the order of 0.001).

Another way of expediting the branch and bound enumeration is specifying a priority for the binary variables according to their contribution to the objective function. In addition, nonzero tolerance for the relative optimality criterion can be used to reduce the computation time for large problems. While the above schemes can help to reduce the computational time, they may not be enough to effectively tackle large problems. Therefore, we consider a bilevel decomposition algorithm that is inspired by the work of Iyer and Grossmann[10] (see Fig. 7).

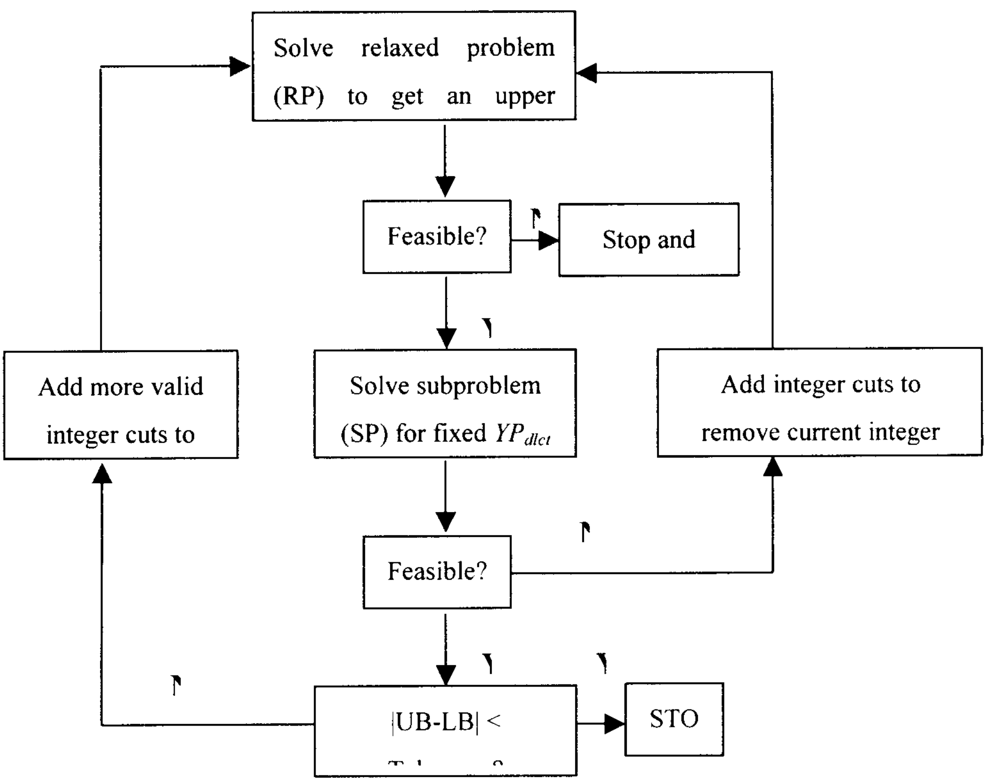


Fig. 7. Flowchart for the bilevel decomposition algorithm.

The bilevel decomposition algorithm solves first a relaxed problem (RP), which provides an upper bound to the profit. The relaxed problem does not consider production changeovers since it aggregates equations (3) and (8), and it only contains 0-1 variable YP_{dlct} associated with the intermittent deliveries. In the subproblem (SP), the supply chain is optimized for fixed flows of the delivery of raw materials as given by the values of variables $YP_{dlct}=1$ that were determined by (RP). Hence, the subproblem yields a lower bound to the profit. The main advantage of the bilevel decomposition algorithm is that the relaxed problem and subproblem have fewer 0-1 variables than the original problem. The relaxed problem is updated at each iteration by adding the integer cuts described in Iyer and Grossmann[10] (see Appendix B). Convergence is achieved when the lower and upper bound lie within a specified tolerance.

The relaxed problem is given as follows:

RP:

Maximize Profit =

$$\sum_{j\in J}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\gamma_{jlt}S_{jlct}-\sum_{j\in J}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\varphi_{jlt}P_{jlct}-\sum_{i\in I}\sum_{j\in JM_{ik}}\sum_{k\in K_i}\sum_{c\in C}\sum_{t\in T}\delta_{ikct}W_{ijkct}-\sum_{j\in J}\sum_{c\in C}\sum_{t\in T}\xi_{jc}V_{jct}$$
$$-\sum_{j\in J}\sum_{l\in L}\sum_{t\in T}\theta_{jlt}SF_{jlt}-\sum_{d\in D}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\omega_{dlct}YP_{dlct}-\sum_{j\in J}\sum_{c\in C}\sum_{t\in T}\phi_{jct}F_{jct}$$

(19)

subject to

$$\sum_{k\in K_i}\frac{W_{ijkct}}{\rho_{ijk}Q_{ic}}\leq 1$$

$$i\in I,\ j\in JM_{ik},\ k\in K_i,\ c\in C,\ t\in T \qquad (20)$$

Constraints (2) and (9)-(17).

Equation (20) is used as a relaxed constraint instead of equations (3) and (8), and is derived by dividing equation (3) by $\rho_{ijck} Q_{ic}$ and then summing it over k.

The subproblem is defined as follows.

SP:

Maximize Profit =

$$\sum_{j\in J}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\gamma_{jlt}S_{jlct}-\sum_{j\in J}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\varphi_{jlt}P_{jlct}-\sum_{i\in J}\sum_{j\in JM_k}\sum_{k\in K_i}\sum_{c\in C}\sum_{t\in T}\delta_{ikc}W_{ijkct}-\sum_{j\in J}\sum_{c\in C}\sum_{t\in T}\xi_{jc}V_{jct}$$
$$-\sum_{i\in J}\sum_{k\in K_i}\sum_{k'\in K_i}\sum_{c\in C}\sum_{t\in T}\zeta_{ikk'c}Z_{ikk'ct}-\sum_{j\in J}\sum_{l\in L}\sum_{t\in T}\theta_{jlt}SF_{jlt}-\sum_{d\in D}\sum_{l\in L}\sum_{c\in C}\sum_{t\in T}\omega_{dlct}YP^{p}_{dlct}-\sum_{j\in J}\sum_{c\in C}\sum_{t\in T}\phi_{jct}F_{jct}$$

(21)

subject to

$$P_{jlct} \le \sum_{d\in D} YP^{p}_{dlct} P^{U}_{jlct}$$

$$j\in J, l\in L,\ c\in C, t\in T \qquad (22)$$

Constraints (2), (3), (5), (8), (9), and (13)-(17)

Note that in (SP) YP^{p}_{dlct} is treated as a fixed value that is given by (RP) in the pth iteration. Hence, the purchase amount is constrained by equation (22).

Bilevel Decomposition Algorithm

For the relaxed problem and subproblem as defined above, the steps of the bilevel decomposition algorithm are presented below.

1. Set iteration count p = 0, upper bound UB = ∞, and lower bound LB = $-\infty$.
2. Set p= p+1. Solve (RP) to determine $\overline{YP}^{p}_{dlct}$, and an upper bound UB for the

proft. Define

$$M_p = \{(d,l,c,t) \mid \overline{YP}^p_{dlct} = 1\} \qquad (23)$$

$$N_p = \{(d,l,c,t) \mid \overline{YP}^p_{dlct} = 0\} \qquad (24)$$

3. For fixed $YP^p_{dlct} = \overline{YP}^p_{dlct}$, solve (SP) to obtain a lower bound LB^p. Set $LB = \max_p \{LB^p\}$.

(a) If (SP) is infeasible, add the following integer cut to (RP).

$$\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} \le |M_p| - 1 \qquad (25)$$

Go to step 2.

(b) If (SP) is feasible, then add the following integer cuts to (RP) (see Appendix B).

$$P_{jlct} \ge \overline{P}^p_{jlct}\Big[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p| - 1)\Big]$$

$$\forall j,l,c,t \qquad (26)$$

$$W_{ijkct} \ge \overline{W}^p_{ijkct}\Big[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p| - 1)\Big]$$

$$\forall i,j,k,c,t \qquad (27)$$

$$V_{jct} \ge \overline{V}^p_{jct}\Big[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p| - 1)\Big]$$

$$\forall j,c,t \qquad (28)$$

$$SF_{jlt} \ge \overline{SF}^p_{jlt}\Big[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p| - 1)\Big]$$

$$\forall j,l,t \qquad (29)$$

$$F_{jct} \ge \overline{F}^p_{jct}\Big[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p| - 1)\Big]$$

$$\forall j,c,t \qquad (30)$$

Also add the integer cuts (31) and (32) to (RP) in order to preclude supersets and subsets of M_P, respectively[10].

$$\sum_{(d',l',c',t')\in M_p} YP_{d'l'c't'} + YP_{dlct} \le |M_p|$$

$$\forall d,l,c,t \in N_p \qquad (31)$$

$$\sum_{(d',l',c',t')\in N_p} YP_{d'l'c't'} + YP_{dlct} \ge 1$$

$$\forall d,l,c,t \in N_p \qquad (32)$$

4. If (UB-LB) is less than a given tolerance, stop. The solution corresponding to LB is the optimal solution. Else, go to step 2.

Example 2

In order to show the efficiency of the bilevel decomposition algorithm, we expand the time horizon for the same process network given in Fig. 2 to 14, 21, and 30 days, respectively. Both intermittent deliveries and chageovers are considered. Table 2 shows the computational statistics for each problem. Note that the CPU times for the bilevel decomposition correspond to the sum of the times required by the (RP) and (SP) subproblems. The optimality criteria for each problem solved with the standard full space method is also shown with the MILP solutions.

Table 2. Comparison of computation results using bilevel decomposition algorithm

*Problem		0-1 Var	Constraints	Conti Var	CPU [sec]	Major Itera	Nodes	Relaxed Solution	MILP solution
.1		108	613	646	6.1		265	973.03	953.9 (0.00)
1.2	RP	12	321	364	8.1	2	-	-	953.86
	SP	96	605	646					
2.1		252	1605	1642	24.5		347	2398.4	2362.2 (0.01)
2.2	RP	28	753	848	35.4	3	-	-	2362.1
	SP	224	1581	1642					
3.1		504	3327	3385	775.5		7120	4519.3	4417.7 (0.01)
3.2	RP	56	1501	1605					

	SP	448	3289	3385	229.4				
4.1		756	5073	5128	2763.1		23562	6698.1	6376.6 (0.05)
4.2	RP	84	2257	2542	1841.4	6	-	-	6383.7
	SP	672	4997	5128					
5.1		1080	7305	7369	8925.3		65432	9378.1	9047.6 (0.04)
5.2	RP	120	3229	3631	3798.6	6	-	-	9056.7
	SP	960	7553	8329					

* 1.1. Standard full space solution for a small problem with 3 time period

1.2. Bilevel decomposition for a small problem with 3 time period

2.1. Standard full space solution for the example 1 revisited (7 periods)

2.2. Bilevel decomposition for the example 1 revisited (7 periods)

3.1. Standard full space solution for a problem with 14 periods

3.2. Bilevel decomposition for a problem with 14 periods

4.1. Standard full space solution for a problem with 21 periods

4.2. Bilevel decomposition for a problem with 21 periods

5.1. Standard full space solution for a large problem with a month time horizon consisting of 30 periods

5.2. Bilevel decomposition for a large problem with a month time horizon consisting of 30 periods

Problem 1 with only three time periods is also included to study the computational performance of the bilevel decomposition applying to from a small problem to a large problem. For Problem 1, it takes 8.1 seconds of CPU time, which is longer than for the standard full space method, 6.1 seconds. However, the bilevel decomposition algorithm shows much better performance as the problem size becomes larger. In Problem 3 the bilevel decomposition algorithm finds the solution in 229.4 seconds CPU time compared to 775.5 seconds with the standard full space method. The optimality criterion of Problem 3 with the standard full space method is 0.01. Finally, in Problem 5, a 30 period problem, the bilevel decomposition requires 3798.6 seconds versus the 8925.3 seconds of the full space, which ended with a suboptimal solution due to the 4% tolerance. As these problems show, we can conclude that the bilevel decomposition is an effective algorithm for large-size problems. Fig. 8 shows the comparison of computational performance between the bilevel decomposition and the standard full space method with respect to problem size.

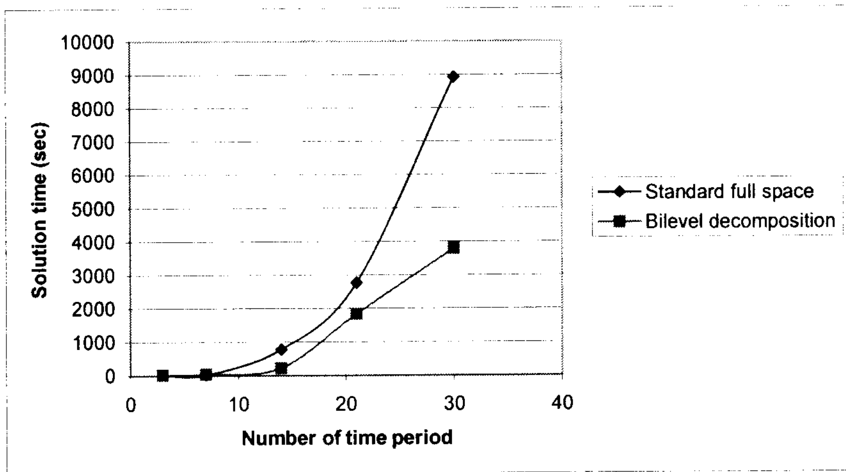
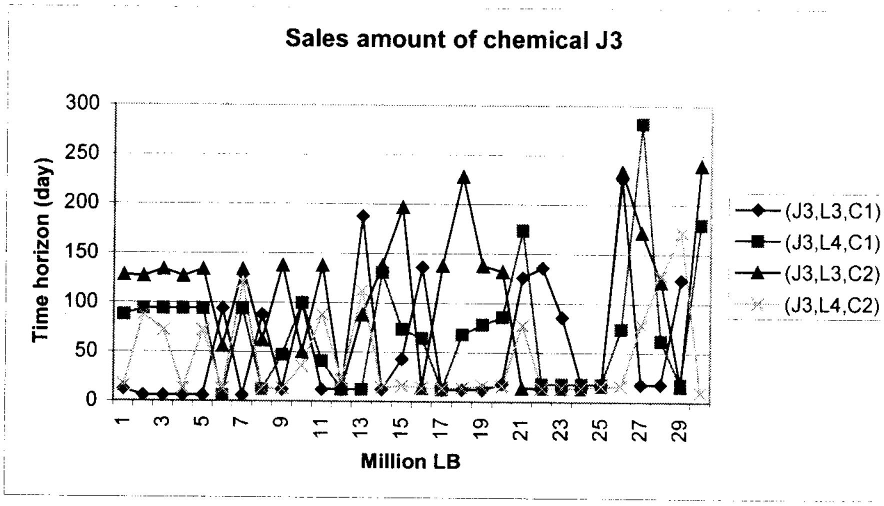
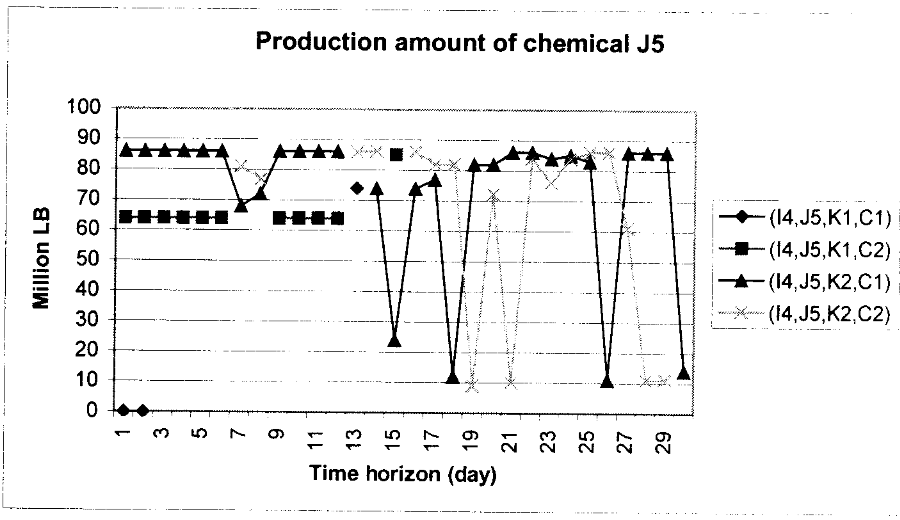


Fig. 8. Comparison of CPU times between two methods

Figures 9 and 10 illustrate the optimization results for Problem 5 with 30 time periods. Fig. 9 shows profiles for sales amount of chemical J3 and production of chemical J5, respectively. From sites C1 and C2, we illustrate the amount of sales in markets L3 and L4 at each time period (Fig. 9(a)). In Fig. 9 (b), production of chemical J5 with schemes K1 and K2 in each site is shown. Fig. 10 shows the optimal inventories for chemicals J1 and J2 in each site, and shortfalls for chemical J3 and J5, respectively. Over a month or 30 time periods, we observe that production shortfall takes place only at the first time period (Fig. 10(b)).

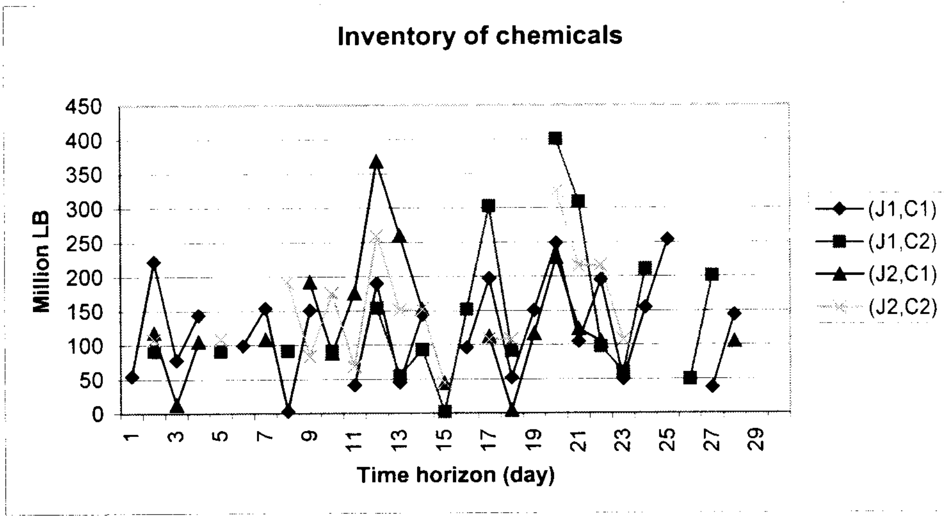


(a)

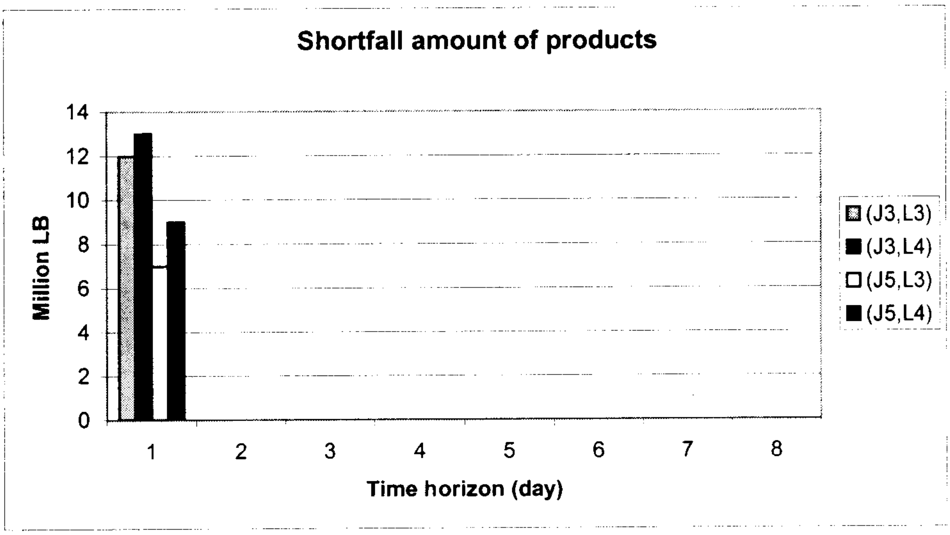


(b)

Fig. 9. Sales amount of chemical J3 and production amount of chemical J5.



(a)



(b)

Fig. 10. Inventory trends and production shortfalls.

Example 3

We consider an extension of the chemical process network consisting of 38 processes, 28 chemicals, and 2 markets presented by Iyer and Grossmann[10]. While the original problem[10] was a long term planning problem arising from a real industry, in this example a short term planning with decisions at a detailed level are considered based on their data. We take into account inventory profiles, production shortfalls, and intermittent deliveries for the network diagram shown in Fig. 11. The time horizons that were considered are for 7, 14, 21, and 30 days. Table 3 shows the computational statistics for the bilevel decomposition in each instance, and Fig. 12 shows the comparison of CPU times with the full space branch and bound. As the problem size becomes larger, the bilevel decomposition algorithm clearly shows better performance.

Table 3. Computation results using bilevel decomposition algorithm

Problem		0-1 var	Constraints	Continu var	CPU [sec]	Major Iterations	LP relaxed solution	MILP solution
7	RP	7	1329	8821	88.9	2	8290.2	8278.4
	SP	14	1615	8821				
14	RP	14	2717	17641	225.8	3	16771.1	16402.2
	SP	28	3290	17641				
21	RP	21	4075	26461	861.7	4	25311.3	25284.6
	SP	42	4935	26461				
30	RP	30	5821	37801	1754.4	5	36011.4	35325.4
	SP	60	7050	37801				

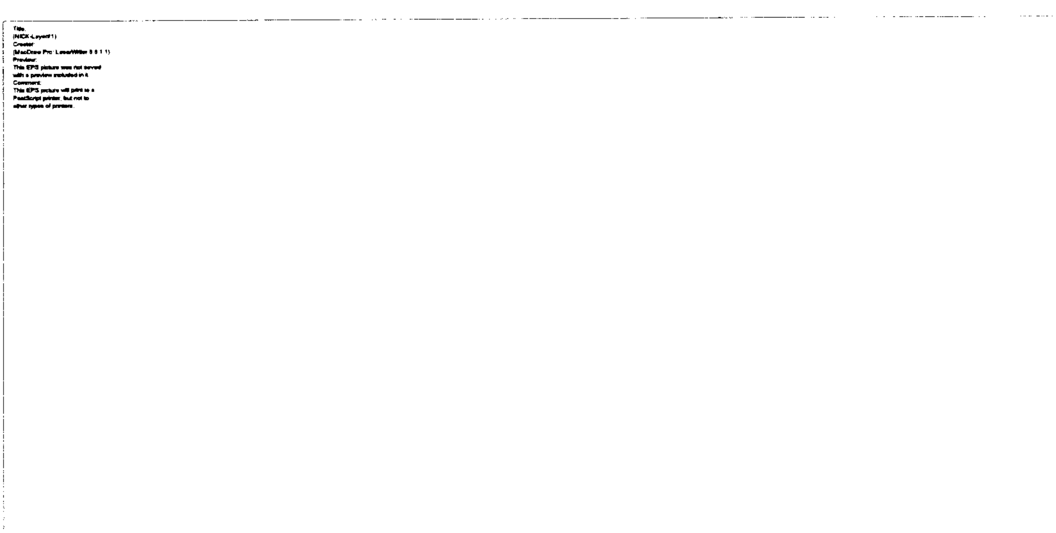


Fig. 11. Diagram for process network in Example 3.

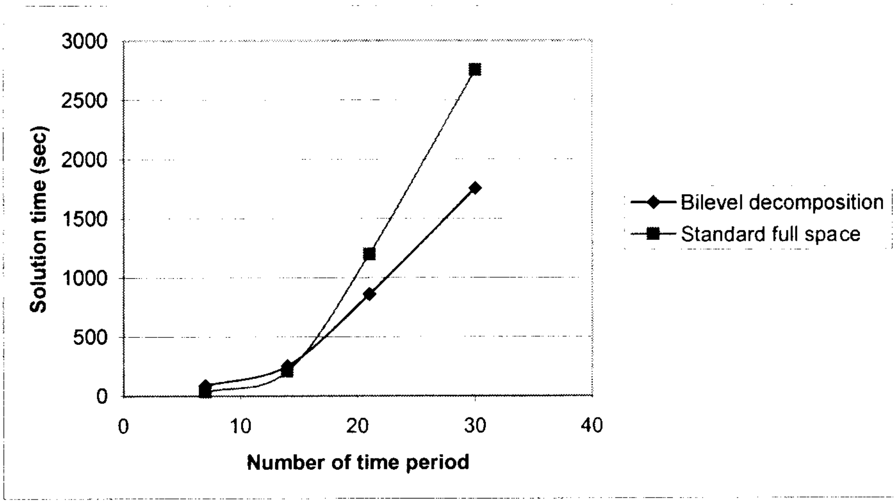


Fig. 12. Solution times for example 3.

Conclusions

We have presented an MILP model for maximizing profit in supply chains arising in multisite continuous flexible process networks. Short term operation was considered for these problems (1 week or 1 month), as well as one-day periods of operation, such as product changeovers, inventory profiles, intermittent deliveries, transportation between sites, and production shortfalls. A large number of 0-1 variables is necessary for representing the changeovers and the intermittent deliveries, making the model computationally very expensive. To circumvent this problem, a bilevel decomposition algorithm has been proposed that reduces a large original problem into a smaller relaxed problem (RP) and a smaller subproblem (SP). (RP) yields an upper bound to the profit, while (SP) yields a lower bound solution for the original problem. For several large problems, it was found that the solution time of the bilevel decomposition algorithm is significantly smaller than that of the full space model with LP branch and bound methods.

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Appendix A.

The following tables are given data for example 1.

Table A.1. Production capacity of each process (million lb)

Site	I1	Capacity of each process I2	I3	I4
C1	50	90	100	86
C2		90	100	86

Table A.2. Prices of raw materials ($/lb) at time period *t*

Market	Chemical	Time period (day)						
		1	2	3	4	5	6	7
L1	J1	0.75	0.75	0.75	0.75	0.75	0.90	0.90
L1	J2	0.50	0.50	0.50	0.75	0.75	0.90	0.90
L1	J4	2.00	2.00	2.00	2.00	2.00	2.00	2.00
L1	J6	0.25	0.25	0.25	0.25	0.25	0.25	0.25
L2	J1	0.75	0.75	0.75	0.75	0.75	0.90	0.90
L2	J2	0.50	0.50	0.50	0.75	0.75	0.90	0.90
L2	J4	2.00	2.00	2.00	2.00	2.00	2.00	2.00
L2	J6	0.25	0.25	0.25	0.25	0.25	0.25	0.25

Table A.3. Prices of products ($/lb) at time period *t*

Market	Chemical	Time period (day)						
		1	2	3	4	5	6	7
L3	J3	1.50	1.50	1.50	1.55	1.55	1.55	1.70
L3	J5	2.00	2.00	2.00	2.00	2.00	2.00	2.00
L4	J3	1.50	1.50	1.50	1.55	1.55	1.55	1.70
L4	J5	2.00	2.00	2.00	2.00	2.00	2.00	2.00

Table A.4. Operating cost coefficients ($/lb) in site C1 at time period *t*

Process	Scheme	Time period (day)						
		1	2	3	4	5	6	7
I1	K1	0.10	0.10	0.10	0.10	0.10	0.10	0.10
I2	K1	0.10	0.10	0.10	0.10	0.10	0.10	0.10
I2	K2	0.10	0.10	0.10	0.10	0.10	0.10	0.10
I3	K1	0.10	0.10	0.10	0.10	0.10	0.10	0.10
I3	K2	0.10	0.10	0.10	0.10	0.10	0.10	0.10

I3	K3	0.10	0.10	0.10	0.10	0.10	0.10	0.10
I3	K4	0.10	0.10	0.10	0.10	0.10	0.10	0.10
I4	K1	0.10	0.10	0.10	0.10	0.10	0.10	0.10
I4	K2	0.10	0.10	0.10	0.10	0.10	0.10	0.10

Operating cost data of site C2 is same as those of site C1.

Table A.5. Mass balance coefficients in site C1

		Chemical					
Process	Scheme	J1	J2	J3	J4	J5	J6
I1	K1	1.05		-1.00			1.03
I2	K1	1.02		-1.00			
I2	K2	1.10			-1.00		0.09
I3	K1	1.10		-1.00			
I3	K2	1.20			-1.00		
I3	K3		1.08	-1.00			
I3	K4		1.05		-1.00		
I4	K1			1.20		-1.00	-1.00
I4	K2				1.10	-1.00	-0.05

In Table A.5, mass balance coefficients are represented as + values and - values with respect to input and output, respectively. The chemicals with −1 value of mass balance coefficient corroespond to main products for each scheme in processes. The data of site C2 is same as those of site C1.

Table A.6. Upper bound for raw material availability (million lb) at time period *t*

Market	Chemical	Time period (day)						
		1	2	3	4	5	6	7
L1	J1	200	200	200	250	250	250	250
L1	J2	200	200	200	220	220	220	220
L1	J4	200	200	200	230	230	230	230
L1	J6	10	5	10	10	10	10	10
L2	J1	300	300	300	250	250	250	250
L2	J2	300	300	300	220	220	220	220
L2	J4	250	250	250	230	230	230	230
L2	J6	10	5	10	10	10	10	10

Table A.7. Upper bound for product demand (million lb) at time period t

Market	Chemical	Time period (day)						
		1	2	3	4	5	6	7
L3	J3	100	100	200	200	200	300	300
L3	J5	75	75	75	80	80	85	90
L4	J3	150	150	210	210	250	250	250
L4	J5	75	75	75	80	80	85	90

Table A.8. Lower bound for product demand (million lb) at time period t

Market	Chemical	Time period (day)						
		1	2	3	4	5	6	7
L3	J3	6	6	12	12	12	18	18
L3	J5	3.5	3.5	4.5	4	4	4.5	5
L4	J3	6.5	6.5	13	13	14	14	16
L4	J5	4.5	4.5	4.5	5	5	5.5	6

Table A.9. Changeover cost in processes ($E04/number of setup)

(Process, Scheme)	Scheme			
	K1	K2	K3	K4
(P1, K1)				
(P2, K1)		10		
(P2, K2)	12			
(P3, K1)		14	15	16
(P3, K2)	14		20	18
(P3, K3)	17	23		17
(P3, K4)	12	14	16	
(P4, K1)		17		
(P4, K2)	14			

Table A.10. Inventory cost for each chemical ($/lb)

Site	Chemical					
	J1	J2	J3	J4	J5	J6
C1	0.02	0.03	0.025	0.05	0.4	0.55
C2	0.02	0.03	0.025	0.05	0.4	0.55

Table A.11. Upper bound of inventory for each chemical (million lb)

Site	Chemical					
	J1	J2	J3	J4	J5	J6
C1	560	680	270	275	250	265
C2	560	680	270	275	250	265

Appendix B.

Property 1. The following constraints based on Iyer and Grossmann[10] are valid integer cuts for the p+1 th relaxed problem (RP).

$$P_{jlct} \geq \overline{P}^{p}_{jlct}\left[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p|-1)\right]$$

$$\forall j,l,c,t \qquad \text{(B1)}$$

$$W_{ijkct} \geq \overline{W}^{p}_{ijkct}\left[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p|-1)\right]$$

$$\forall i,j,k,c,t \qquad \text{(B2)}$$

$$V_{jct} \geq \overline{V}^{p}_{jct}\left[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p|-1)\right]$$

$$\forall j,c,t \qquad \text{(B3)}$$

$$SF_{jlt} \geq \overline{SF}^{p}_{jlt}\left[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p|-1)\right]$$

$$\forall j,l,t \qquad \text{(B4)}$$

$$F_{jct} \geq \overline{F}^{p}_{jct}\left[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (|M_p|-1)\right]$$

$$\forall j,c,t \qquad \text{(B5)}$$

where $M_p = \{(d,l,c,t) \mid \overline{YP}^{p}_{dlct} = 1\}$ (B6)

$$N_p = \{(d,l,c,t) \mid \overline{YP}^{p}_{dlct} = 0\} \qquad \text{(B7)}$$

Proof: The proof for this property is analogous to that of Iyer and Grossmann[10]. Let

P_{jlct}, W_{ijkct}, V_{jct}, SF_{jlt}, and F_{jct} be X for simplicity. Then we can represent all inequalities as the following representative constraint.

$$X \geq \overline{X}^{p}\left[\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} - (\left|M_p\right| - 1)\right] \qquad \text{(B8)}$$

For given $\overline{YP}^{p}_{dlct}$, the solution to the subproblem gives an optimal $\overline{X}^{p}$ that is the optimal value for the original problem when the corresponding deliveries are made ($\overline{YP}^{p}_{dlct}=1$). For the selected value $\overline{YP}^{p}_{dlct}$, the right-hand side for $\overline{X}^{p}$ is multiplied by a positive number or 1. Therefore, the inequality $X \geq \overline{X}^{p}$ is enforced through the above equation. Clearly, these inequalities are valid cuts since the objective function has X with negative coefficients. Note that for any other choice of $\overline{YP}^{p}_{dlct}$, $X \geq 0$ dominates equation, since $\sum_{(d,l,c,t)\in M_p} YP_{dlct} - \sum_{(d,l,c,t)\in N_p} YP_{dlct} \leq \left|M_p\right| - 1$. (B9) □