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Optimal planning strategy for the supply chains of light aromatic compounds in petrochemical industries

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Abstract

The scope of this research is concerned with the supply chain of light aromatic compounds, i.e., benzene, toluene, *o*-xylene and *p*-xylene, in the petrochemical industries. The proper production scheme of these compounds over a specified time horizon can be configured by selecting throughput, operating conditions and technology options for each unit in the chain, by maintaining the desired inventory level for each process material, by purchasing enough feedstock, and by delivering appropriate amounts of products to the customers. A mixed-integer linear program (MILP) has been developed in this work to synthesize the best multi-period planning strategy under the constraints of given supplies and demands. By solving the proposed model, not only the appropriate inventory level of every process material and the optimal throughput and operation mode of each production unit can be determined, but also the purchase opportunities of intermediate oils can be clearly identified.

Keywords: Light aromatic compounds; Supply chain; MILP

1. Introduction

A typical supply chain of any commodity product involves the production facilities of suppliers, the storage and distribution networks, and the customers. Two tightly integrated components can be identified in a supply-chain management (SCM) scheme: (1) the production planning and inventory control policies, and (2) the distribution logistics. Naturally, the objective of every SCM strategy is to maximize the overall value generated and this value is strongly correlated with profitability. The scope of present study is concerned with the supply chains of light aromatic compounds, i.e., benzene, toluene, *o*-xylene and *p*-xylene (BTX), in the petrochemical industries. To put the significance of the present research in perspective, the general framework of various petroleum processes is sketched in Fig. 1. It should be noted that a large number of related works have already been published in recent literatures. Lee, Pinto, Grossmann, and Park (1996) proposed a short-term scheduling policy for crude supply in a single refinery. Iyer, Grossmann, Vasantharajan, and Cullick (1998) developed a multi-period mixed-integer linear program (MILP) for the planning and scheduling of an offshore oil-field infrastructure. Zhang and Zhu (2000) presented a novel decomposition strategy to tackle a large-scale refinery optimization problem. Julka, Srinivasan, and Karimi (2002), Julka, Karimi, and Srinivasan (2002) presented a decision support system for managing the crude-oil flows in a refinery. Gothe-Lundgren, Lundren, and Persson (2002) studied a production planning and scheduling problem in an oil refinery company. Jia and Ierapetritou (2003) concentrate on the short-term scheduling of refinery operations. Más and Pinto (2003) and Magalhães and Shah (2003) proposed a detailed MILP formulation for the optimal scheduling of an oil supply chain, which includes tankers, piers, storage tanks, substations and refineries. Neiro and Pinto (2004) presented a comprehensive framework for modelling the front end of a petroleum supply chain. Basically, the production units included in this supply chain can be found in typical refineries, e.g., atmospheric distillation columns, vacuum dis-

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Abbreviations: AD, atmospheric distillation unit; D, distributor; DS, domestic supplier; DC, domestic customer; ET, extraction unit; IEF, import and export facility; IM, isomar unit; M, mixer; OS, overseas supplier; OC, overseas customer; PR, parex unit; PDT, product distribution terminal; RF, reforming unit; TT, tatory unit; XF, xylene fractionation unit; bz, benzene; isomarf, feed of isomar unit; mx, mixed xylenes; ox, *ortho*-xylene; parexf, feed of parex unit; px, *para*-xylene; tl, toluene

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Nomenclature

Indices

k	operation mode
p	product
s, s'	feedstock
tp	time period
u	unit

Sets

$\mathbf{C}$	the set of all customers of the final products and/or intermediates
$\mathbf{C}_{\mathrm{BTX}}$	the sets of domestic customers for the final products of supply chain
$\mathbf{C}_{\mathrm{mxyl}}$	the sets of domestic customers for mixed xylenes
$\mathbf{C}_{\mathrm{ovs}}$	the sets of overseas customers for the intermediate and final products of BTX supply chains
$\mathbf{F}_u$	the set of all allowable feeds of unit u
$\mathbf{F}_{v'}$	the set of materials consumed by customer v'
$\mathbf{K}_{u,s}$	the set of all operation modes of unit u for processing feedstock s
$\mathbf{M}_u$	the set of all process materials in unit u
$\mathbf{P}_u$	the set of all products (and by-products) of unit u
$\mathbf{P}_v$	the set of raw materials produced by supplier v
$\mathbf{S}$	the set of all suppliers of the raw materials and/or intermediates
$\mathbf{S}_{\mathrm{BTX}}$	the set of domestic suppliers of the final products of supply chain
$\mathbf{S}_{\mathrm{litnap}}$	the set of overseas suppliers of light naphtha
$\mathbf{S}_{\mathrm{mxyl}}$	the set of overseas suppliers of mixed xylenes
$\mathbf{S}^{\mathrm{I}}_{\mathrm{litnap}}$	the set of suppliers of light naphtha inside the refineries
$\mathbf{S}^{\mathrm{I}}_{\mathrm{pyrgas}}$	the set of suppliers of pyrolysis gasolines inside the refineries
$\mathbf{TP}$	the set of all planning periods
$\mathbf{U}$	the set of all processing units
$\mathbf{UA}$	the set of all reformers, isomar units and tatory units
$\mathbf{UA}'$	the set of all reformers and isomar units
$\mathbf{UB}$	the set of all aromatics extraction units, xylene fractionation units and parex units
$\mathbf{UD}$	the set of all export facilities and product distribution terminals
$\mathbf{UT}$	the set of all import facilities and product distribution terminals
$\mathbf{U}_{\mathrm{tatory}}$	the set of tatory units
$\mathbf{UI}_{u,s}$	the set of all source units (or suppliers) of feedstock s received by unit u
$\mathbf{UO}_{u,p}$	the set of all sink units (or customers) of the product p generated in unit u

Continuous variables

$\mathrm{bdq}_{v',m,p}$	the backlog amount of material m delivered to customer v' in period tp
$\mathrm{cb}_{\mathrm{tp}}$	the total backlog cost in period tp
$\mathrm{cd}_{\mathrm{tp}}$	the total cost of promotion discount in period tp
$\mathrm{ci}_{\mathrm{tp}}$	the total inventory cost in period tp
$\mathrm{co}_{\mathrm{tp}}$	the total operation cost in period tp
$\mathrm{cr}_{\mathrm{tp}}$	the total cost of raw materials in period tp
$\mathrm{ct}_{\mathrm{tp}}$	the total transportation cost in period tp
$\mathrm{pf}_{\mathrm{tp}}$	the net profit in period tp
$q_{u,u',p,\mathrm{tp}}$	the accumulated amount of product p transported from unit u to u' during interval tp
$q_{u',u,s,\mathrm{tp}}$	the accumulated amount of feedstock s transported from unit u' to u during interval tp
$q_{v,v',m,\mathrm{tp}}$	the accumulated delivering amount of material m from unit v to unit v' during interval tp
$\mathrm{qf}_{u,s,\mathrm{tp}}$	the total amount of consumed feedstock s of unit u in period tp
$\mathrm{qp}_{u,p,\mathrm{tp}}$	the total amount of produced product p of unit u in period tp
$\mathrm{qti}_{u,s,\mathrm{tp}}$	the accumulated amount of feedstock s delivered to the buffer tank in unit u during period tp
$\mathrm{qto}_{u,p,\mathrm{tp}}$	the accumulated amount of product p withdrawn from the buffer tank in unit u during period tp
$\mathrm{sdq}_{v',m,p}$	the surplus amount of material m delivered to customer v' in period tp
$\mathrm{rs}_{\mathrm{tp}}$	the total revenue secured from various product sales in period tp
$\mathrm{vin}_{u,m,\mathrm{tp}}$	the inventory of material m in unit u at the end of planning period tp

Binary variables

$\mathrm{fi}_{u,s,k,\mathrm{tp}}$	the binary indicator used to denote if operation mode k of unit u is chosen during period tp to process feedstock s
$l_{u,\mathrm{tp}}$	the binary indicator used to denote if unit u is activated during period tp
$n^{\mathrm{b}}_{v',m,\mathrm{tp}}$	the binary indicator used to denote if there is a backlog of material m delivered to customer v' in period tp
$n^{\mathrm{s}}_{v',m,\mathrm{tp}}$	the binary indicator used to denote if there is a surplus of material m delivered to customer v' in period tp

Parameters

$\mathrm{CBL}_{v',m,\mathrm{tp}}$	the backlog penalty per unit of product m not delivered to customer v' during time period tp
$\mathrm{CBTX}_{v,m,\mathrm{tp}}$	the unit cost for purchasing final product m from supplier v during time period tp
$\mathrm{CIN}_{u,m,\mathrm{tp}}$	the inventory cost per unit of process material m in unit u during period tp
$\mathrm{CLN}_{v,m,\mathrm{tp}}$	the unit cost for purchasing light naphtha m from supplier v during period tp
$\mathrm{CLN}^{\mathrm{I}}_{v,m,tp}$	the unit cost for producing light naphtha m in unit v during period tp
$\mathrm{CMX}_{v,m,\mathrm{tp}}$	the unit cost for purchasing mixed xylene m from supplier v during period tp
$\mathrm{CPD}_{v',m,\mathrm{tp}}$	the promotion discount per unit of product m offered to customer v' during time period tp

$CPG^{I}_{v,m,p}$	the unit cost for producing pyrolysis gasoline m in unit v during period tp
$CVA_{u,k,s,\mathrm{tp}}$	the variable operating cost of reaction unit u for processing feedstock s under operation mode k during period tp
$CVB_{u,\mathrm{tp}}$	the variable operating cost of separation unit u during period tp
$CTP_{v,v',m,\mathrm{tp}}$	the unit transportation cost for moving material m from unit v to unit v'during period tp
$CXA_{u,\mathrm{tp}}$	the fixed operating cost of unit u in **UA** during period tp
$CXB_{u,\mathrm{tp}}$	the fixed operating cost of unit u in **UB** during period tp
$FC_{u,s,p}$	the recovery ratio of product p in feedstock s of unit u
$INV^{L}_{u,m}$	the lower bound of the inventory of material m in unit u
$INV^{U}_{u,m}$	the upper bound of the inventory of material m in unit u
$Q^{L}_{v,v',m}$	the lower limit of the transportation capacity for delivering material m from unit v to unit v'
$Q^{U}_{v,v',m}$	the upper limit of the transportation capacity for delivering material m from unit v to unit v'
$QBTX^{L}_{v,m,\mathrm{tp}}$	the lower bound of the available amount of final product m from supplier v during period tp
$QBTX^{U}_{v,m,\mathrm{tp}}$	the upper bound of the available amount of final product m from supplier v during period tp
$QFA^{L}_{u,s,k}$	the minimum allowable throughput of reaction unit u for feedstock s under operation mode k
$QFA^{U}_{u,s,k}$	the maximum allowable throughput of reaction unit u for feedstock s under operation mode k
QFB^{L}_{u}	the minimum allowable throughput of separation unit u
QFB^{U}_{u}	the maximum allowable throughput of separation unit u
QFT^{L}_{u}	the minimum allowable throughput of totary unit u
QFT^{U}_{u}	the maximum allowable throughput of totary unit u
$QLN^{I}_{v,m,\mathrm{tp}}$	the amount of light naphtha m produced in unit v during period tp
$QLN^{L}_{v,m,\mathrm{tp}}$	the lower bounds of the available amount of light naphtha m from supplier v during period tp
$QLN^{U}_{v,m,\mathrm{tp}}$	the upper bound of the available amount of light naphtha m from supplier v during period tp
$QOS^{L}_{v',m,\mathrm{tp}}$	the acceptable minimum amount of intermediate or final product m delivered to customer v' in period tp
$QOS^{U}_{v',m,\mathrm{tp}}$	the acceptable maximum amounts of intermediate or final product m delivered to customer v' in period tp
$QPG^{I}_{v,m,\mathrm{tp}}$	the amount of pyrolysis gasoline m produced in unit v during period tp
$QPT^{L}_{v',m,\mathrm{tp}}$	the lower bound of the amount of product m delivered to customer v' in period tp
$QPT^{T}_{v',m,\mathrm{tp}}$	the *target value* of the amount of product m delivered to customer v' in period tp
$QPT^{U}_{v',m,\mathrm{tp}}$	the upper bound of the amount of product m delivered to customer v' in period tp
$QXI^{L}_{v,m,\mathrm{tp}}$	the lower bound of the available amount of mixed xylenes m from supplier v during period tp
$QXI^{U}_{v,m,\mathrm{tp}}$	the upper bound of the available amount of mixed xylenes m from supplier v during period tp
$QXO^{L}_{v',m,\mathrm{tp}}$	the acceptable minimum amount of material m delivered to customer v' in period tp
$QXO^{U}_{v',m,\mathrm{tp}}$	the acceptable maximum amount of material m delivered to customer v' in period tp
$RT_{u,s,k}$	the flow ratio between feedstock s and a reference feed of totary unit u under operation mode k
$SP_{v',m,\mathrm{tp}}$	the selling price of intermediate or final product m sold to customer v' during period tp
$SQP_{v',m}$	the target value of the total amount of material m delivered to customer v' over the planning horizon
$YD_{u,s,k,p}$	the reaction yield of product p from feedstock s under operation mode k of unit u

tillation units, fluidized-bed catalytic cracking units, propane deasphalting units and hydrotreating units, etc. The consumed raw materials are crude oils shipped from overseas suppliers and the products are: liquefied petroleum gas, diesel, gasoline, petrochemical naphtha and fuel oil.

It should be pointed out that, in addition to the aforementioned processing systems, the production scheme of benzene, toluene and xylenes can also be considered as an essential and independent element of the overall petrochemical supply chain. This is due to the facts that (1) only two possible sources of raw materials can be consumed by the BTX supply chain and they are the by-products of upstream processes, (2) the main products of this supply chain can be sold on international and/or domestic markets for profit, and (3) most units in this supply chain *do not* interact with external processes. More specifically, the light aromatic compounds are produced from either reformate or pyrolysis gasoline in the petrochemical processes (Franck & Stadelhofer, 1988; Speight & Ozum, 2002). The reformate is generated with light naphtha in the reforming unit and the light naphtha is usually treated as a by-product in the atmospheric distillation units. Similarly, since naphtha cracking is used mainly to produce ethylene, propylene and butadiene, the pyrolysis gasoline created in this process is regarded as a by-product, too. Notice also that, other than the main products mentioned above, several marketable chemicals, e.g., C_3/C_4, LPG, gasoline, C_9-aromatics and C_{10}-aromatics, etc., are produced in small quantities by the BTX supply chain. Their revenues can be easily accounted for in the proposed model if necessary. Finally,

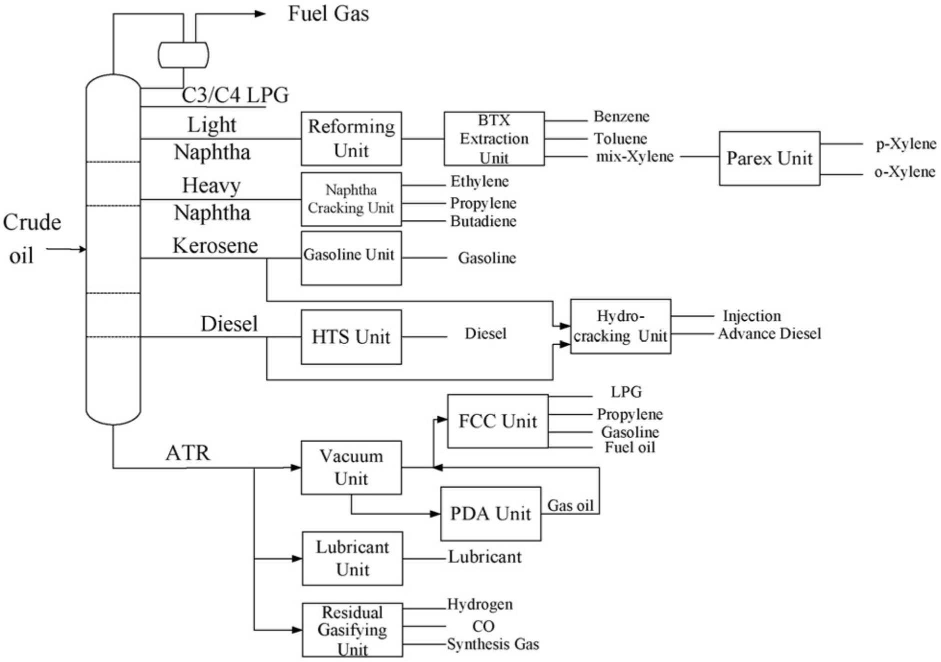

Fig. 1. The simplified flow diagram of a typical refinery.

it should be noted that the detailed descriptions of all related processing units and the overall supply-chain structure will be provided later in this paper for illustration convenience.

Although the production planning and scheduling problems of a *single* aromatic plant have been studied previously, e.g., Ho and Yu (2002), the characteristics of an overall BTX supply network has never been analyzed before. An existing aromatic supply-chain usually consists of a large collection of strategically located production units and storage and transport facilities. For the task of supply-chain planning, the time frames considered by different companies may vary from a quarter to 1 year (Chopra & Meindl, 2004). In the present paper, the short-term forecast of BTX demands is assumed to be quite reliable and, therefore, the uncertainly issues are not addressed for the sake of brevity. Given the predicted demands and supplies, a proper production scheme should be configured in every planning period (e.g., 1 month) over a specified time horizon (e.g., 3 months) by selecting throughput, operating conditions and technology options for each unit, by maintaining the desired inventory level for each process material, by purchasing enough raw materials, and by delivering appropriate amounts of products to the customers. Since there are numerous decisions involved in this planning process and they have to be made on the basis of overall profit, it may not be feasible to optimize each unit individually. This is because the optimal solution for one unit may render other units in the supply-chain inefficient or even inoperable. A mixed-integer linear programming (MILP) model is thus developed in this work to identify the best short-term multi-period SCM policies for the light aromatic compounds. By solving this model, not only the appropriate inventory level of every process material and the optimal throughput and operation mode of each production unit can be determined for each planning period, but also the purchase opportunities of intermediate oils can be clearly identified. The feasibility and benefits of the proposed mathematical programming model are demonstrated with the realistic case studies reported at the end of this paper.

2. Basic processing units

For illustration purpose, a typical single-train supply chain of the light aromatics is presented in Fig. 2. Descriptions of the basic processing units in this chain are presented in the sequel.

2.1. Import and export facilities

Some of the raw materials and intermediates of the supply chain are assumed to be supplied by foreign sources and, in certain cases, the intermediates and/or final products may also be sold to overseas customers. In particular, the crude and other intermediate oils (e.g. light naphtha and mixed xylenes) are usually imported by tankers to terminals equipped with jetties and storage tanks. These terminals can also be utilized to facilitate exportation. A pipeline network is available for connecting the jetties to the crude storage tanks that are present both at the port and at the refinery. Fig. 3 outlines these distribution elements of an oil company.

2.2. Atmospheric distillation unit

In the refinery, the crude oil is separated in an atmospheric distillation unit into several products, i.e., light compounds with three and four carbon atoms (i.e., C_3s and C_4s), light naphtha, heavy naphtha, kerosene, diesel and residual oil (see Fig. 1).

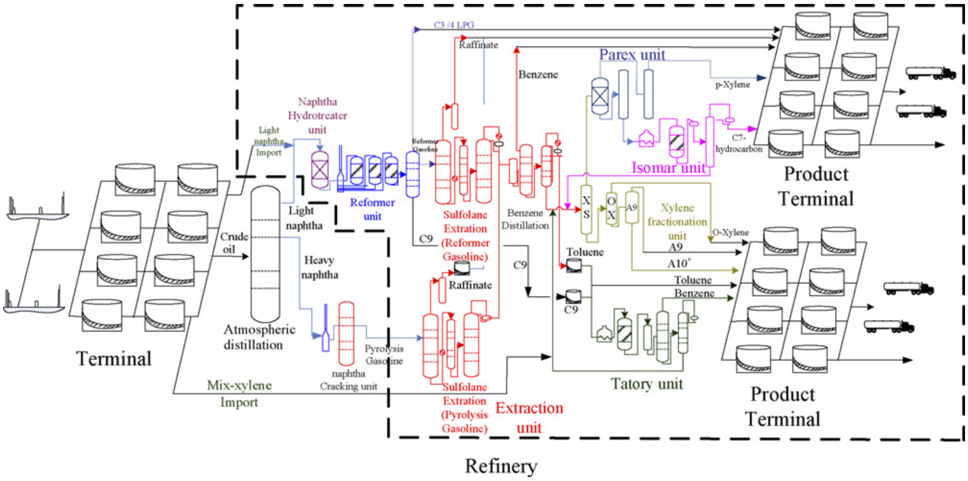

Fig. 2. A typical single-train BTX supply chain.

Notice that the light naphtha is then fed to the reforming unit and the heavy naphtha is usually consumed by the naphtha cracker. The raw materials of the BTX supply chain, i.e., the reformate and pyrolysis gasoline, are produced from these two units, respectively. The other products of the atmospheric distillation unit are sent to various buffer tanks for further processing.

2.3. Naphtha cracker

This process is concerned with steam cracking of hydrocarbons to produce ethylene, propylene, butadiene and other unsaturated compounds with higher molecular weights. When the hydrocarbon chains are heated to around 800 °C, the C–C and C–H bonds can be broken and, consequently, unstable radicals are generated. These radicals can react further to produce unsaturated molecules. In addition, diolefins can cyclize with other olefins to yield aromatics. As a result, various different aromatic components may appear in the pyrolysis gasoline. The pyrolysis gasoline must be treated in a hydrogenation process to remove the olefins, diolefins and sulfur contents. In areas such as Europe and Japan, the pyrolysis gasoline is the most abundant source of aromatics. However, it should also be noted that production planning of the naphtha cracking unit is usually governed by the ethylene demand and, thus, the pyrolysis gasoline should be considered only as a by-product of ethylene. As a result, the naphtha crakers are not included in the BTX supply chain in this study. The pyrolysis gasoline is treated simply as a raw material supplied by the naphtha craker(s).

2.4. Reforming unit (hydroytreater and platforming unit)

In the BTX supply chain, the hydroytreater and platformer unit should be considered as an integrated unit. The sulfur content in the light naphtha is reduced with a hydroytreater. This step is necessary for preparing the feed to comply with the operational constraints of catalytic reformer and for achieving the target product purity. After hydrotreating, the light naphtha is then converted in the reformers to produce the reformer gasoline and also light compounds with three and four carbon atoms. The reformer gasoline is the main BTX source in countries where ethylene production is based on natural gas. Generally speaking, the main purpose of this operation is to convert paraffin into aromatics and/or branched alkanes so as to enhance octane rating. A wide spectrum of reactions take place here, e.g., hydrogenation

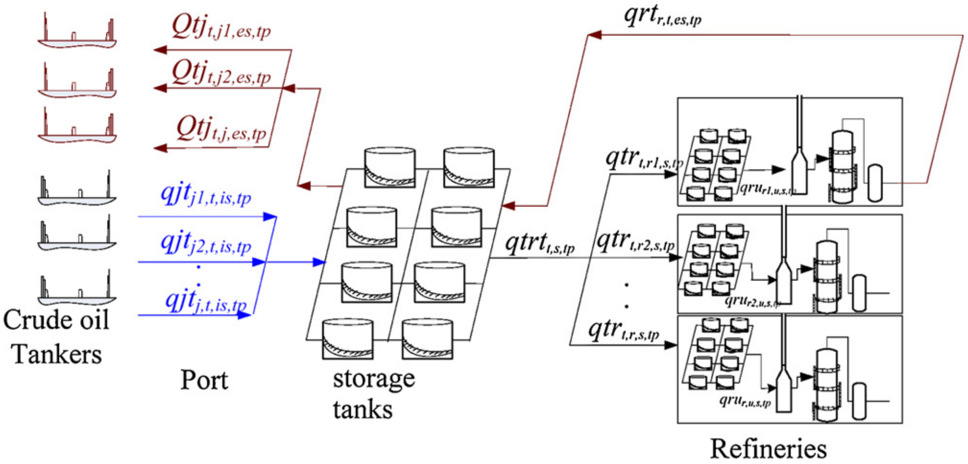

Fig. 3. The general framework of import/export facilities.

of cycloalkanes to form aromatics, isomerization of n-alkanes to form branched alkanes, and ring extension and dehydrogenation of alkylclopentanes to form benzene derivatives, etc.

2.5. *Aromatics extraction units*

This liquid–liquid extraction operation is used to produce the aromatics fraction, i.e., benzene, toluene, C_8- and C_9-aromatics, from a broad boiling range of hydrocarbons. The reformer gasoline and pyrolysis gasoline should be fed to two distinct extraction units separately. Due to the differences in solubilities of aromatics and non-aromatics in polar solvents (i.e., sulfolane), these compounds can be differentiated easily in the extraction units. After extraction, the raffinate (which consists of the non-aromatics) can be blended in gasoline, and the extracted substances (which include the aromatics) are fed to fractionation columns for further separation. Two of the final products, i.e., benzene and toluene, can be obtained from the purified aromatic mixture by simple distillation owing to the fact that their boiling points are well below those of the others. The separation of xylene isomers from the bottom product is more problematic since they form a close-boiling mixture. This stream is sent to the xylene fractionation unit.

2.6. *Xylene fractionation unit*

Since the boiling point of *o*-xylene is 5 °C higher than that of *m*-xylene, these two components are treated as the heavy and light keys, respectively, in the xylene fractionation column (XS). The overhead product of XS is a mixture of *o*-xylene, *p*-xylene, ethylbenzene and *m*-xylene. On the other hand, *o*-xylene (about 28% of feed) and the high-boiling aromatics, i.e., C_9- and C_{10}-aromatics, are obtained at the bottom. The high-boiling aromatics in the bottom product of XS are removed from *o*-xylene in the *o*-xylene column (OX). The C_9-aromatics and C_{10}-aromatics are separated in the distillation column A_9. The former is used as an ingredient of gasoline, while the latter can be mixed in fuel oil.

2.7. *Parex unit*

Since the close-boiling *p*-xylene and *m*-xylene cannot be separated effectively by distillation, the purification of the overhead product of xylene fractionation column (XS) is achieved by selective adsorption in the parex unit. The high-purity *p*-xylene can be produced in this unit with solid adsorbents and suitable liquids. A synthetic zeolite is used as the adsorption agent. The mixture from overhead of column XS, in liquid form, passes through a series of adsorption chambers filled with adsorbent-containing molecular sieves. The liquid flow is controlled with rotating valves. The liquid *p*-xylene is attached on the active surface of the adsorption agents, while other compounds pass through unaffected. The adsorbed *p*-xylene is later desorbed with toluene or *p*-diethylbenzene. The mixture of *p*-xylene and desorbant can be easily separated by further distillation.

2.8. *Isomar unit*

The demand for *p*-xylene is mainly caused by the need to produce terephthalic acid for fibers and, on the other hand, the demand for *o*-xylene arises if there is a need to produce phthalic anhydride for plasticizers. The market of *m*-xylene for the production of isophthalic acid is much smaller than that of *p*-xylene or *o*-xylene. Therefore, *m*-xylene and ethylbenzene from the parex unit are isomerized to form *o*- and *p*-xylene in the xylene isomeric unit. Isomerization is achieved in a catalytic reaction process. The by-products of isomeric unit are light components, i.e., C_7 hydrocarbons, and can be removed from xylenes by distillation. The C_7 hydrocarbon can be either used as the feed to the stabilizer column in reforming unit or as an ingredient of gasoline. The resulting *o*- and *p*-xylenes are recycled back to the xylene fractionation unit.

2.9. *Tatory unit*

Since the benzene content in reformer gasoline is relatively low, the toluene and C_9-aromatics produced in the supply chain may have to be converted again to benzene to meet the market demand. The required methyl-group transfer reactions take place in gas phase in a tatory unit. The two inputs, i.e., toluene and C_9-aromatics, are fed with a fixed ratio. Other than a small amount of light components, the main products of this unit are benzene and xylenes. The reactions occur on a zeolite catalyst, and the yield of benzene and xylene is around 95%. After the catalytic reaction step, benzene, toluene, xylenes, C_9-aromatics and C_{10}-aromatics are separated in a distillation train similar to that in the extraction unit. Toluene and C_9-aromatics are recycled back to the surge tanks, and the xylenes are fed to the xylene fractionation unit.

2.10. *Storage and transportation facilities*

In a typical petrochemical complex, the final products are shipped out to meet the demands of domestic market from a collection of storage and transportation terminals similar to those used for the raw materials. Each terminal is equipped with its own infrastructure including the discharge, storage and pumping equipments. The products are then delivered to the customers via pipelines and/or trucks. There are of course additional storage facilities for the intermediates within the supply chain. In this study, it is assumed that these buffer tanks may be installed for storing the inputs and/or outputs temporarily in every production unit.

3. Basic process models

The various processing units in the BTX supply chain can be classified into three general types. They are referred to in this paper as the reaction processes, the separation processes and the storage processes. Detailed descriptions of the mathematical models of these processes are given as follows.

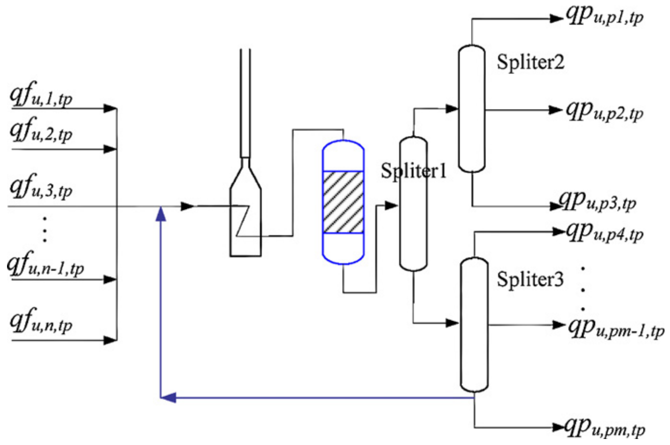

Fig. 4. The generalized reaction process.

3.1. Reaction processes

The reforming units, the isomar units and the tatory units are considered as the reaction processes in this work. As mentioned before, the naphtha crakers are treated as the suppliers of pyrolysis gasoline and, thus, excluded from the BTX supply chain. A sketch of the generalized process flow diagram is provided in Fig. 4. Notice also that a separation system is included for the purpose of removing products and by-products from the un-reacted raw materials. It is assumed that, after the catalytic reaction(s), the reactants can always be recovered and then recycled *completely* with this system. To simplify the mathematical program, only the overall mass balances of the entire reaction process are considered in this study. It should be noted that the reaction yields of every product (or by-product), are assumed to be dependent upon the feedstock compositions and operation modes. However, all of them are regarded as available parameters. The generalized material balance of the reaction processes can be written as

$$\mathrm{qp}_{u,p,\mathrm{tp}} = \sum_{s\in\mathbf{F}_u} \mathrm{qf}_{u,s,\mathrm{tp}} \cdot \left(\sum_{k\in\mathbf{K}_{u,s}} \mathrm{fi}_{u,s,k,\mathrm{tp}} \cdot \mathrm{YD}_{u,s,k,p} \right) \quad \forall u\in\mathbf{UA},\ \forall p\in\mathbf{P}_u,\ \forall \mathrm{tp}\in\mathbf{TP} \tag{1}$$

where **UA** is the union of the sets of all reformers, isomar units and tatory units, i.e., $\mathbf{UA}=\mathbf{U}_{\mathrm{ref}}\cup\mathbf{U}_{\mathrm{isomar}}\cup\mathbf{U}_{\mathrm{tatory}}$, $\mathbf{F}_u$ the set of all allowable feeds of unit u, $\mathbf{P}_u$ the set of all products (and by-products) of unit u, **TP** the set of all planning periods, $\mathbf{K}_{u,s}$ the set of all operation modes of unit u for processing feedstock s, $\mathrm{qf}_{u,s,\mathrm{tp}}$ and $qp_{u,p,\mathrm{tp}}$ denote the process variables representing, respectively, the total amounts of consumed feedstock s and produced product p of unit u in period tp, $\mathrm{fi}_{u,s,k,\mathrm{tp}}$ the binary variable reflecting whether or not operation mode k of unit u is chosen during period tp to process feedstock s and $\mathrm{YD}_{u,s,k,p}$ is a given parameter representing the reaction yield of product p from feedstock s with operation mode k of unit u. To simplify the model formulation, let us next introduce a new variable:

$$\mathrm{qfi}_{u,s,k,\mathrm{tp}} = \mathrm{fi}_{u,s,k,\mathrm{tp}} \cdot \mathrm{qf}_{u,s,\mathrm{tp}} \tag{2}$$

Thus, the generalized material balance in Eq. (1) can be written in a *linear* form as

$$\mathrm{qp}_{u,p,\mathrm{tp}} = \sum_{s\in\mathbf{F}_u}\sum_{k\in\mathbf{K}_{u,s}} \mathrm{qfi}_{u,s,k,\mathrm{tp}} \cdot \mathrm{YD}_{u,s,k,p} \quad \forall u\in\mathbf{UA},\ \forall p\in\mathbf{P}_u,\ \forall \mathrm{tp}\in\mathbf{TP} \tag{3}$$

It should be noted that at least one reforming and one isomar unit must be included to ensure the operability of BTX supply chain. Thus, the following logic constraints are imposed in the proposed model:

$$1 \le \sum_{u\in\mathbf{U}_{\mathrm{ref}}} l_{u,\mathrm{tp}}, \qquad 1 \le \sum_{u\in\mathbf{U}_{\mathrm{isomar}}} l_{u,\mathrm{tp}} \tag{4}$$

where $\mathrm{tp}\in\mathbf{TP}$; $l_{u,\mathrm{tp}}\in\{0,1\}$. It is assumed in this study that only one input is allowed to be processed in a reformer or isomar unit and, obviously, only one operation mode can be adopted in each unit. This feature is stipulated with the following constraints:

$$\sum_{s\in\mathbf{F}_u}\sum_{k\in\mathbf{K}_{u,s}} \mathrm{fi}_{u,k,s,\mathrm{tp}} = l_{u,\mathrm{tp}} \quad \forall u\in\mathbf{UA}',\ \forall \mathrm{tp}\in\mathbf{TP} \tag{5}$$

where $\mathbf{UA}'=\mathbf{U}_{\mathrm{ref}}\cup\mathbf{U}_{\mathrm{isomer}}$. Since the capacities of these processing units are finite, the upper and lower bounds of the throughputs must also be imposed in the model, i.e.,

$$\mathrm{QFA}^{\mathrm{L}}_{u,s,k} \cdot \mathrm{fi}_{u,s,k,\mathrm{tp}} \le \mathrm{qfi}_{u,s,k,\mathrm{tp}} \le \mathrm{QFA}^{\mathrm{U}}_{u,s,k} \cdot \mathrm{fi}_{u,s,k,\mathrm{tp}} \quad \forall u\in\mathbf{UA}',\ \forall s\in\mathbf{F}_u,\ k\in\mathbf{K}_{u,s},\ \forall \mathrm{tp}\in\mathbf{TP} \tag{6}$$

where $\mathrm{QFA}^{\mathrm{U}}_{u,s,k}$ and $\mathrm{QFA}^{\mathrm{L}}_{u,s,k}$ denote, respectively, the maximum and minimum allowable throughputs of reaction unit u for feedstock s under operation mode k.

On the other hand, the use of a tatory unit in a BTX supply chain should be dependent upon the market prices of the final products and the raw material costs. In addition, more than one feedstock is allowed to be processed in this unit. Consequently,

$$\sum_{k\in\mathbf{K}_{u,s}} \mathrm{fi}_{u,s,k,\mathrm{tp}} \le l_{u,\mathrm{tp}},$$
$$\sum_{s\in\mathbf{F}_u}\sum_{k\in\mathbf{K}_{u,s}} \mathrm{fi}_{u,s,k,\mathrm{tp}} \ge l_{u,\mathrm{tp}} \quad \forall u\in\mathbf{U}_{\mathrm{tatory}},\ \forall s\in\mathbf{F}_u,\ \forall \mathrm{tp}\in\mathbf{TP} \tag{7}$$

Since every operation mode of any given unit can be used to process all its feeds, one can consider all the corresponding sets of operation modes are the same, i.e.,

$$\mathbf{KT}_u = \mathbf{K}_{u,s} \quad \forall u\in\mathbf{U}_{\mathrm{tatory}},\ \forall s\in\mathbf{F}_u \tag{8}$$

Also, since only one of the operation modes in $\mathbf{KT}_u$ can be activated, the following constraints must be incorporated in the mathematical model:

$$\mathrm{fi}_{u,s,k,\mathrm{tp}} = \mathrm{fi}_{u,s',k,\mathrm{tp}} \quad \forall u\in\mathbf{U}_{\mathrm{tatory}},\ \forall s, s'\in\mathbf{F}_u,\ k\in\mathbf{KT}_u,\ \forall \mathrm{tp}\in\mathbf{TP} \tag{9}$$

where $s\neq s'$. Furthermore, the flow ratio between any two feeds of a totary unit is usually fixed under a selected operation mode, i.e.,

$$\mathrm{RT}_{u,s,k}\cdot \mathrm{qfi}_{u,s,k,\mathrm{tp}}=\mathrm{RT}_{u,s',k}\cdot \mathrm{qfi}_{u,s',k,\mathrm{tp}}\qquad \forall u\in \mathbf{U}_{\mathrm{tatory}},\ \forall s,s'\in \mathbf{F}_u,\quad k\in \mathbf{KT}_u,\ \forall \mathrm{tp}\in \mathbf{TP}\qquad (10)$$

where $\mathrm{RT}_{u,s,k}$ and $\mathrm{RT}_{u,s',k}$ are two constants. Finally, the throughput limits in this case should be characterized as

$$\mathrm{QFT}_u^{\mathrm{L}}\cdot l_{u,\mathrm{tp}}\le \sum_{s\in \mathbf{F}_u}\sum_{k\in \mathbf{K}_{u,s}}\mathrm{qfi}_{u,s,k,\mathrm{tp}}\le \mathrm{QFT}_u^{\mathrm{U}}\cdot l_{u,\mathrm{tp}}\qquad \forall u\in \mathbf{U}_{\mathrm{totary}},\ \forall \mathrm{tp}\in \mathbf{TP}\qquad (11)$$

where $\mathrm{QFT}_u^{\mathrm{U}}$ and $\mathrm{QFT}_u^{\mathrm{L}}$ denote, respectively, the maximum and minimum allowable throughputs of totary unit u.

3.2. Separation processes

The separation processes in this study are those in which only separation operations are present, i.e., the aromatics extraction units, the xylene fractionation units and the parex units. On the basis of the flow diagram presented in Fig. 5, the generalized material balances of the separation processes can be written as

$$\begin{aligned}\mathrm{qp}_{u,p,\mathrm{tp}}&=\sum_{s\in \mathbf{F}_u}\mathrm{qf}_{u,s,\mathrm{tp}}\cdot X_{u,s,p}\cdot \mathrm{FC}_{u,s,p}\\&=\sum_{s\in \mathbf{F}_u}\mathrm{qf}_{u,s,\mathrm{tp}}\cdot \mathrm{RF}_{u,s,p}\qquad \forall u\in \mathbf{UB},\ \forall p\in \mathbf{P}_u,\ \forall \mathrm{tp}\in \mathbf{TP}\end{aligned}\qquad (12)$$

where **UB** is the union of the sets of all separation units, i.e., $\mathbf{UB}=\mathbf{U}_{\mathrm{ext}}\cup \mathbf{U}_{\mathrm{xylene}}\cup \mathbf{U}_{\mathrm{parex}}$, $X_{u,s,p}$ and $FC_{u,s,p}$ are the design parameters denoting, respectively, the volume fraction and recovery ratio of product p in feedstock s of unit u and $RF_{u,s,p}$ ($=X_{u,s,p}\cdot \mathrm{FC}_{u,s,p}$) is referred to in this paper as the *recovery efficiency* of product p in feedstock s of unit u. Notice that the definitions of $\mathrm{qf}_{u,s,\mathrm{tp}}$ and $\mathrm{qp}_{u,p,\mathrm{tp}}$ are the same as before. Notice also that the atmospheric distillation units are not incorporated in the BTX supply chain. This is due to the need to simplify model formulation. Otherwise, the scope of present study will have to be expanded to include the supply chains of other downstream products of the atmospheric distillation units, e.g., gasoline, kerosene, ethylene, propylene and butadiene, etc.

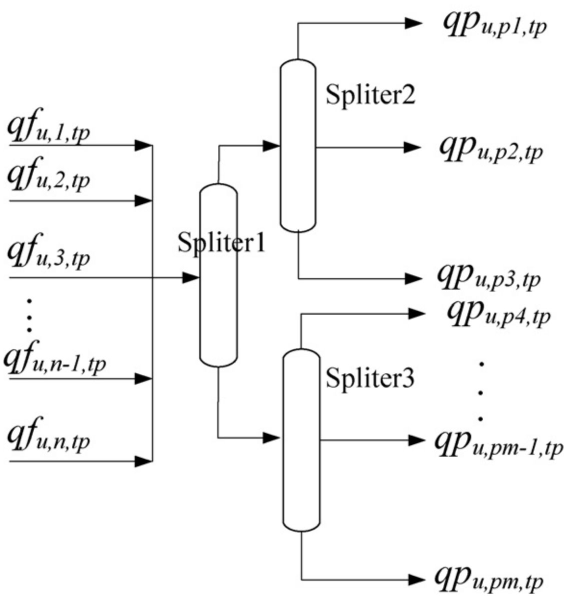

Fig. 5. The generalized separation process.

In order to facilitate normal operation of the supply chain, it is necessary to activate at least one separation unit of each type. In other words, the logic constraint specified in Eq. (4) should also be imposed upon the units in the subsets of **UB**, i.e.,

$$1\le \sum_{u\in \mathbf{U}_{\mathrm{ext}}} l_{u,\mathrm{tp}},\qquad 1\le \sum_{u\in \mathbf{U}_{\mathrm{xylene}}} l_{u,\mathrm{tp}},\qquad 1\le \sum_{u\in \mathbf{U}_{\mathrm{parex}}} l_{u,\mathrm{tp}}\qquad (13)$$

where $l_{u,\mathrm{tp}}\in\{0,1\}$. Since only a single operation mode is implemented in each separation process and mixed feeds are allowed, the throughput limits can be expressed as

$$\mathrm{QFB}_u^{\mathrm{L}}\cdot l_{u,\mathrm{tp}}\le \sum_{s\in \mathbf{F}_u}\mathrm{qf}_{u,s,\mathrm{tp}}\le \mathrm{QFB}_u^{\mathrm{U}}\cdot l_{u,\mathrm{tp}}\qquad \forall u\in \mathbf{UB},\ \forall \mathrm{tp}\in \mathbf{TP}\qquad (14)$$

where $\mathrm{QFB}_u^{\mathrm{U}}$ and $\mathrm{QFB}_u^{\mathrm{L}}$ denote, respectively, the maximum and minimum allowable throughputs of separation unit u.

3.3. Storage processes

As mentioned before, supply-chain planning is usually carried out over a fixed time horizon with multiple periods according to the predictions of feedstock supplies and market demands. Consequently, the material balance model of a generalized storage process (see Fig. 6) should be formulated on the basis of a planning period, i.e.,

$$\mathrm{vin}_{u,m,\mathrm{tp}}=\mathrm{vin}_{u,m,\mathrm{tp}-1}+\mathrm{qti}_{u,m,\mathrm{tp}}-\mathrm{qto}_{u,m,\mathrm{tp}}\qquad \forall u\in \mathbf{U},\ \forall m\in \mathbf{M}_u,\ \forall \mathrm{tp}\in \mathbf{TP}\qquad (15)$$

In the above equation, **U** is the set of all processing units in which storage tanks may be present, i.e.,

$$\mathbf{U}=\mathbf{UA}\cup \mathbf{UB}\cup \mathbf{UT}\cup \mathbf{UD}\qquad (16)$$

where **UT** and **UD** denote, respectively, the sets of all import/export facilities and product distribution terminals. In

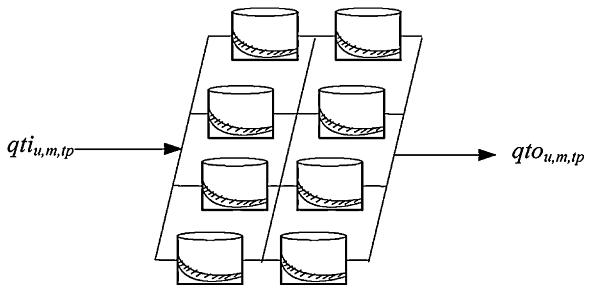

Fig. 6. The generalized storage process.

addition, $\mathbf{M}_u$ is the set of all process materials in unit u, i.e., $\mathbf{M}_u = \mathbf{F}_u \cup \mathbf{P}_u$; $\mathrm{vin}_{u,m,\mathrm{tp}}$ represents the inventory of material m in unit u at the end of planning period tp; $\mathrm{qti}_{u,m,\mathrm{tp}}$ and $\mathrm{qto}_{u,m,\mathrm{tp}}$ denote, respectively, the *total* amounts of material m delivered to and withdrawn from unit u during period tp. This formulation is adopted on the ground that it is often not possible to pump process material simultaneously in and out of a storage tank. Furthermore, it may not be necessary to carry out a particular material transfer operation continuously throughout the whole planning period. For example, the crude oil usually is not transported from a tanker into more than one storage tank at the same time and, thus, these tanks are filled one-by-one at short time intervals. Other limiting constraints on the crude storage processes include jetty availability and the logistics support capability of third party. Finally, it should be noted that more than one input and/or output pipelines are allowed to be connected to a single tank in this model. This is due to the fact that $\mathrm{qti}_{u,m,\mathrm{tp}}$ and $\mathrm{qto}_{u,m,\mathrm{tp}}$ represent the accumulated quantities of *combined* inputs and outputs, respectively. Since in practice the storage capability cannot be unlimited, it is also necessary to impose the following inequality constraints:

$$\mathrm{INV}^{\mathrm{L}}_{u,m} \le \mathrm{vin}_{u,m,\mathrm{tp}} \le \mathrm{INV}^{\mathrm{U}}_{u,m}$$
$$\forall u \in \mathbf{U},\quad \forall m \in \mathbf{M}_u,\quad \forall \mathrm{tp} \in \mathbf{TP} \tag{17}$$

where $\mathrm{INV}^{\mathrm{U}}_{u,m}$ and $\mathrm{INV}^{\mathrm{L}}_{u,m}$ represent, respectively, the upper and lower bounds of the inventory of material m in unit u.

4. Supply-chain structure

To facilitate construction of a comprehensive system structure, let us assume that one buffer-tank system is available for every feedstock and every product in each processing unit of the generalized supply chain. More specifically, the storage processes are attached to the reaction and separation processes according to the frameworks presented in Figs. 7 and 8, respectively. It should be noted that this assumption is by no means restrictive. If a particular buffer system is not present in a practical application, it is only necessary to set the upper and lower bounds of the corresponding inventory in the mathematical

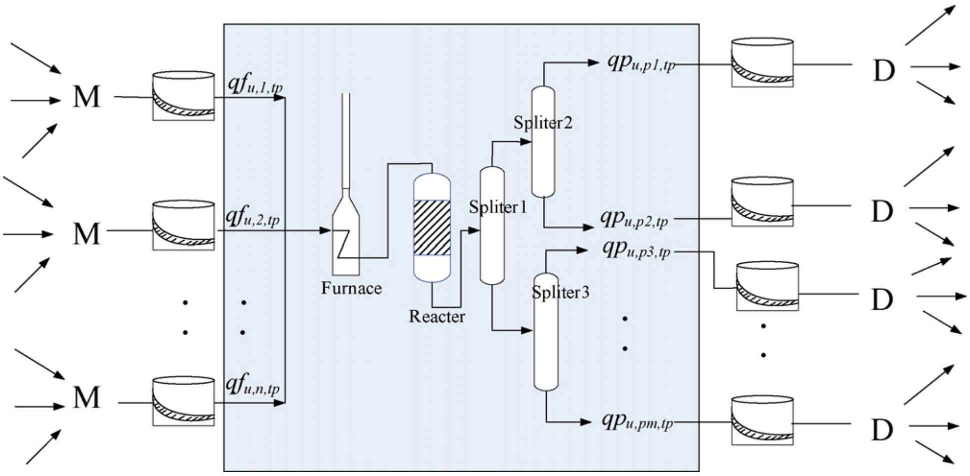

Fig. 7. The flow structure around a reaction process.

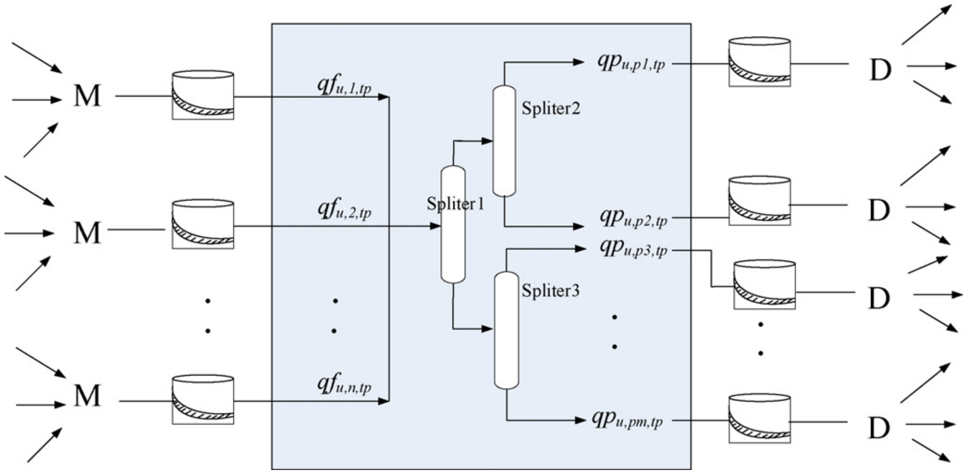

Fig. 8. The flow structure around a separation process.

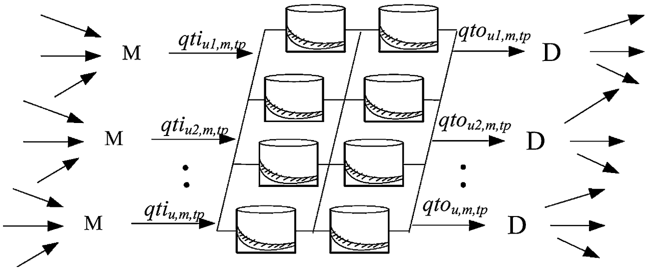

Fig. 9. The flow structure around a storage and transportation terminal.

model to be zeros. On the other hand, there are certainly various storage tanks in the product distribution terminals and also in the import/export facilities for raw materials, intermediates and final products. Usually, their capacities are larger than those in the reaction and separation processes. The general framework of the corresponding storage and transportation processes can be found in Fig. 9.

Notice that the symbols "M" and "D" in all three general structures represent *mixers* and *distributors*, respectively. The inputs of mixers in a processing unit are originated from the distributors in various upstream source units of its feeds and, similarly, the distributors in this unit are linked to the mixers in downstream sink units of its products. The detailed connections in the general configuration of a BTX supply chain are listed in Table 1. For the sake of conciseness, every source or sink unit is represented with a two- or three-letter code and these codes are defined in the first column of this table. The undefined codes OS and OC are the abbreviations of *overseas supplier* and *overseas customer*, and DS and DC denote the *domestic supplier* and *domestic customer*, respectively. In addition, a hyphen indicates that the corresponding sink unit is not modeled in the present study. Finally, notice that the feeds of parex and isomar units are denoted as parexf and isomarf. The former is mainly a mixture of *o*-xylene, *p*-xylene, ethylbenzene and *m*-xylene and the latter consists of *o*-xylene, ethylbenzene and *m*-xylene.

It should be realized that the mixers and distributors may or may not be present physically in the supply chain. They are included to facilitate accurate formulation of the mathematical programming model. Specifically, the material balance around a mixer can be written as

$$\mathrm{qti}_{u,s,\mathrm{tp}} = \sum_{u' \in \mathbf{UI}_{u,s}} q_{u',u,s,\mathrm{tp}}, \quad u \in \mathbf{U}, \quad s \in \mathbf{F}_u, \quad \mathrm{tp} \in \mathbf{TP} \tag{18}$$

where $\mathbf{UI}_{u,s}$ denotes the set of all source units (or suppliers) of feedstock s received by unit u, $\mathrm{qti}_{u,s,\mathrm{tp}}$ denotes the accumulated amount of feedstock s delivered to the buffer tank in unit u during period tp and $q_{u',u,s,\mathrm{tp}}$ represents the accumulated amount of feedstock s transported from unit u' to u during interval tp. On the other hand, the material balance around a distributor can be formulated in a similar fashion, i.e.,

$$\mathrm{qto}_{u,p,\mathrm{tp}} = \sum_{u' \in \mathbf{UO}_{u,p}} q_{u,u',p,\mathrm{tp}}, \quad u \in \mathbf{U}, \quad p \in \mathbf{P}_u, \quad \mathrm{tp} \in \mathbf{TP} \tag{19}$$

where $\mathbf{UO}_{u,p}$ denotes the set of all sink units (or customers) of the product p generated in unit u, $\mathrm{qto}_{u,p,\mathrm{tp}}$ denotes the accumulated amount of product p withdrawn from the buffer tank in unit u during period tp and $q_{u,u',p,\mathrm{tp}}$ represents the accumulated amount of product p transported from unit u to u' during interval tp.

Notice also that, in the cases of reaction and separation processes, the mixers and distributors are attached, respectively, to the feedstock and product buffer tanks. Thus, the outputs of the former tanks should be regarded as the inputs of these processes, i.e.,

$$\mathrm{qto}_{u,s,\mathrm{tp}} = \sum_{k \in \mathbf{K}_{u,s}} \mathrm{qfi}_{u,s,k,\mathrm{tp}}, \quad u \in \mathbf{UA}, \quad s \in \mathbf{F}_u, \quad \mathrm{tp} \in \mathbf{TP} \tag{20}$$

$$\mathrm{qto}_{u,s,\mathrm{tp}} = \mathrm{qf}_{u,s,\mathrm{tp}}, \quad u \in \mathbf{UB}, \quad s \in \mathbf{F}_u, \quad \mathrm{tp} \in \mathbf{TP} \tag{21}$$

On the other hand, the inputs of the product tanks should be considered as the outputs of the reaction and separation processes, i.e.,

$$\mathrm{qti}_{u,p,\mathrm{tp}} = \mathrm{qp}_{u,p,\mathrm{tp}}, \quad u \in \mathbf{U}', \quad p \in \mathbf{P}_u, \quad \mathrm{tp} \in \mathbf{TP} \tag{22}$$

where $\mathbf{U}' = \mathbf{UA} \cup \mathbf{UB}$.

From Eqs. (18) and (19), it is obvious that the process materials must be transferred from on unit to another. The most likely means of transportation within the supply chain should be pumps and pipelines. The transportation methods for importing the raw materials for countries lacking oil resources should be tankers, and the light aromatic compounds could be delivered to domestic customers either via pipelines or by trucks. Since the corresponding transportation capacities should always be limited in practice, the following inequalities are included in our model:

$$Q^{\mathrm{L}}_{v,v',m} \le q_{v,v',m,\mathrm{tp}} \le Q^{\mathrm{U}}_{v,v',m}$$
$$\forall v,\ v' \in \mathbf{USC}, \quad \forall m \in \mathbf{M}, \quad \forall \mathrm{tp} \in \mathbf{TP} \tag{23}$$

and

$$\mathbf{USC{=}U} \cup \mathbf{S} \cup \mathbf{C}, \qquad \mathbf{M} = \bigcup_{u \in \mathbf{U}} \mathbf{M}_u \tag{24}$$

where $\mathbf{S}$ is the set of all suppliers of the raw materials and/or intermediates, $\mathbf{C}$ the set of all customers of the final products and/or intermediates, $Q^{\mathrm{U}}_{v,v',m}$ and $Q^{\mathrm{L}}_{v,v',m}$ denote, respectively, the upper and lower limits of the transportation capacity for delivering material m from unit v to unit v' and $q_{v,v',m,\mathrm{tp}}$ represents the accumulated delivering amount of material m from unit v to unit v' during interval tp.

It is assumed in this study that the crude oil is purchased from the international market and the variations in its quality and quantity can be reasonably predicted over a relatively small number of planning periods (say, three periods). The operation of atmospheric distillation unit can thus be optimized accordingly to satisfy the demands of its *higher-valued* products, e.g., LPG, gasoline, jet fuel and diesel fuel, etc., as much as possible. Consequently, the physical properties and supply rate of light and heavy naphtha and also the generation rate of pyrolysis gasoline in the subsequent naphtha crackers can be regarded as *given* parameters in the mathematical model for BTX supply-chain

Table 1
Connections of processing units in a BTX supply chain

Processing unit	Feedstock	Source unit	Product	Sink unit
Atmospheric distillation (AD)	Crude oil	IEF	C_3/C_4 LPG	–
			Light naphtha	RF
			Heavy naphtha	–
			Kerosene	–
			Light gasoil	–
			Heavy gasoil	–
			Residual oil	–
Reforming (RF)	Light naphtha	IEF, AD	C_3/C_4 LPG	PDT
			C_5 gasoline	PDT
			Reformate	ET
			C_9-aromatic	TT
Extraction (ET)	Reformate	RF	Raffinate	–
	Pyrolysis gasoline	Naphtha cracker	Benzene	PDT, IEF
			Toluene	TT, PDT, IEF
			Mixed xylenes	XF, PDT, IEF
Xylene fractionation (XF)	Mixed xylenes	ET, TT, IM, IEF	*o*-Xylene	PDT, IEF
			C_{9+}gasoline	PDT
			Parexf	PR
Tatory (TT)	Toluene	ET, PDT	Benzene	PDT, IEF
	C_9	RF	Mixed xylenes	XF, PDT, IEF
			C_{10}-aromatic	PDT
Parex (PR)	Parexf	XF	*p*-Xylene	PDT, IEF
			Isomarf	IM
Isomar (IM)	Isomarf	PR	Mixed xylenes	XF, PDT, IEF
Import and export facility (IEF)	Crude oil	OS	Crude oil	AD
	Light naphtha	OS	Light naphtha	RF
	Benzene	ET, TT	Benzene	OC
	Toluene	ET	Toluene	OC
	p-Xylene	PR	*p*-Xylene	OC
	o-Xylene	XF	*o*-Xylene	OC
	Mixed xylenes	OS, ET, TT, IM	Mixed xylenes	OC, XF
Product distribution terminal (PDT)	Benzene	DS, ET, TT	Benzene	DC
	Toluene	DS, ET	Toluene	DC, TT
	p-Xylene	DS, PR	*p*-Xylene	DC
	o-Xylene	DS, XF	*o*-Xylene	DC
	Mixed xylenes	ET, TT, IM	Mixed xylene	DC

planning, i.e.,

$$\mathrm{QLN}^{\mathrm{I}}_{v,m,\mathrm{tp}} = \sum_{v' \in \mathbf{U}_{\mathrm{ref}}} q_{v,v',m,\mathrm{tp}}, \quad v \in \mathbf{S}^{\mathrm{I}}_{\mathrm{litnap}}, \quad m \in \mathbf{P}_v, \quad \mathrm{tp} \in \mathbf{TP} \tag{25}$$

$$\mathrm{QPG}^{\mathrm{I}}_{v,m,\mathrm{tp}} = \sum_{v' \in \mathbf{U}_{\mathrm{ext}}} q_{v,v',m,\mathrm{tp}}, \qquad v \in \mathbf{S}^{\mathrm{I}}_{\mathrm{pyrgas}}, \quad m \in \mathbf{P}_v, \quad \mathrm{tp} \in \mathbf{TP} \tag{26}$$

where $\mathbf{S}^{\mathrm{I}}_{\mathrm{litnap}}$ and $\mathbf{S}^{\mathrm{I}}_{\mathrm{pyrgas}}$ denote, respectively, the sets of suppliers of light naphtha (i.e., the atmospheric distillation units) and pyrolysis gasolines (i.e., the naphtha crakers) inside the refineries, $\mathbf{P}_v$ the set of raw materials produced by supplier v and $\mathrm{QLN}^{\mathrm{I}}_{v,m,\mathrm{tp}}$ and $\mathrm{QPG}^{\mathrm{I}}_{v,m,\mathrm{tp}}$ are two given parameters representing, respectively, the amounts of light naphtha and pyrolysis gasolines delivered by their suppliers inside refineries during period tp. In addition, it is assumed that two intermediates of the BTX supply chain, i.e., light naphtha and mixed xylenes, can be imported for use in the reforming units and xylene fractionation units, respectively. Since the total quantities of these imported intermediates are not required to be fixed in each planning period, it is only necessary to impose the corresponding upper and lower bounds, i.e.,

$$\mathrm{QLN}^{\mathrm{L}}_{v,m,\mathrm{tp}} \leq \sum_{v' \in \mathbf{UT}} q_{v,v',m,\mathrm{tp}} \leq \mathrm{QLN}^{\mathrm{U}}_{v,m,\mathrm{tp}}, \qquad v \in \mathbf{S}_{\mathrm{litnap}}, \quad m \in \mathbf{P}_v, \quad \mathrm{tp} \in \mathbf{TP} \tag{27}$$

$$\mathrm{QXI}^{\mathrm{L}}_{v,m,\mathrm{tp}} \leq \sum_{v' \in \mathbf{UT}} q_{v,v',m,\mathrm{tp}} \leq \mathrm{QXI}^{\mathrm{U}}_{v,m,\mathrm{tp}}, \qquad v \in \mathbf{S}_{\mathrm{mxyl}}, \quad m \in \mathbf{P}_v, \quad \mathrm{tp} \in \mathbf{TP} \tag{28}$$

where $\mathbf{S}_{\mathrm{litnap}}$ and $\mathbf{S}_{mxyl}$ denote, respectively, the sets of overseas suppliers of light naphtha and mixed xylenes, $\mathrm{QLN}^{\mathrm{U}}_{v,m,\mathrm{tp}}$ and $\mathrm{QLN}^{\mathrm{L}}_{v,m,\mathrm{tp}}$ represent, respectively, the upper and lower bounds of the available amount of light naphtha m

from supplier v during period tp and $\mathrm{QXI}^{\mathrm{U}}_{v,m,\mathrm{tp}}$ and $\mathrm{QXI}^{\mathrm{L}}_{v,m,\mathrm{tp}}$ represent, respectively, the upper and lower bounds of the available amount of mixed xylenes m from supplier v during period tp. Finally, it is assumed in this work that the final products of BTX supply chain can also be purchased from domestic suppliers to fulfill contract agreements with customers. A set of similar inequality constraints are thus included in the mathematical model:

$$\mathrm{QBTX}^{\mathrm{L}}_{v,m,\mathrm{tp}} \le \sum_{v' \in \mathbf{UD}} q_{v,v',m,\mathrm{tp}} \le \mathrm{QBTX}^{\mathrm{U}}_{v,m,\mathrm{tp}}, \quad v \in \mathbf{S}_{\mathrm{BTX}}, \quad m \in \mathbf{P}_v, \quad \mathrm{tp} \in \mathbf{TP} \tag{29}$$

where $\mathbf{S}_{\mathrm{BTX}}$ denotes the sets of domestic suppliers of the final products of supply chain and $\mathrm{QBTX}^{\mathrm{L}}_{v,m,\mathrm{tp}}$ and $\mathrm{QBTX}^{\mathrm{U}}_{v,m,\mathrm{tp}}$ represent, respectively, the upper and lower bounds of the available amount of final product m from supplier v during period tp. Notice that the set of all possible inputs of the BTX supply chain can be expressed as: $\mathbf{S} = \mathbf{S}^{\mathrm{I}}_{\mathrm{litnap}} \cup \mathbf{S}^{\mathrm{I}}_{\mathrm{pyrgas}} \cup \mathbf{S}_{\mathrm{litnap}} \cup \mathbf{S}_{\mathrm{mxyl}} \cup \mathbf{S}_{\mathrm{BTX}}$.

The market demands for final products of the supply chain are also assumed to be predictable at least in short term. The actual amounts shipped to the domestic customers during a particular planning period are often allowed to deviate from the requested values. To facilitate representation of the amounts of surplus and backlog, let us introduce two corresponding variables, i.e., $\mathrm{sdq}_{v',m,\mathrm{tp}}$ and $\mathrm{bdq}_{v',m,\mathrm{tp}}$, into the following material balance equations:

$$\mathrm{QPT}^{\mathrm{T}}_{v',m,\mathrm{tp}} + \mathrm{sdq}_{v',m,\mathrm{tp}} - \mathrm{bdq}_{v',m,\mathrm{tp}} = \sum_{v \in \mathbf{UD}} q_{v,v',m,\mathrm{tp}}, \quad v' \in \mathbf{C}_{\mathrm{BTX}}, \quad m \in \mathbf{F}_{v'}, \quad \mathrm{tp} \in \mathbf{TP} \tag{30}$$

where $\mathbf{C}_{\mathrm{BTX}}$ denotes the sets of domestic customers for the final products of supply chain, $\mathbf{F}_{v'}$ the set of materials consumed by customer v', $\mathrm{QPT}^{\mathrm{T}}_{v',m,\mathrm{tp}}$ denotes the *target value* of the amount of material m delivered to customer v' in period tp and $\mathrm{sdq}_{v',m,p}$ and $\mathrm{bdq}_{v',m,p}$ represent, respectively, the surplus and backlog amounts of material m delivered to customer v' in period tp. Notice that Eq. (30) is valid only when the following inequality constraints are imposed:

$$\begin{aligned} &0 \le \mathrm{sdq}_{v',m,\mathrm{tp}} \le n^{\mathrm{s}}_{v',m,\mathrm{tp}} \cdot (\mathrm{QPT}^{\mathrm{U}}_{v',m,\mathrm{tp}} - \mathrm{QPT}^{\mathrm{T}}_{v',m,\mathrm{tp}}), \\ &0 \le \mathrm{bdq}_{v',m,\mathrm{tp}} \le n^{\mathrm{b}}_{v',m,\mathrm{tp}} \cdot (\mathrm{QPT}^{\mathrm{T}}_{v',m,\mathrm{tp}} - \mathrm{QPT}^{\mathrm{L}}_{v',m,\mathrm{tp}}), \\ &n^{\mathrm{s}}_{v',m,\mathrm{tp}} + n^{\mathrm{b}}_{v',m,\mathrm{tp}} \le 1 \end{aligned} \tag{31}$$

where $n^{\mathrm{s}}_{v',m,\mathrm{tp}} \in \{0, 1\}$; $n^{\mathrm{b}}_{v',m,\mathrm{tp}} \in \{0, 1\}$; the design parameters $\mathrm{QPT}^{\mathrm{U}}_{v',m,\mathrm{tp}}$ and $\mathrm{QPT}^{\mathrm{L}}_{v',m,\mathrm{tp}}$ denote, respectively, the upper and the lower bound of the amount of material m delivered to customer v' in period tp. It should be noted that, although the deviations from the desired demand levels are acceptable, the total amounts of delivered products accumulated over a specified number of time periods should still meet every customer's needs exactly, i.e.,

$$\sum_{tp \in \mathbf{TP}} \sum_{v \in \mathbf{UD}} q_{v,v',m,\mathrm{tp}} = \mathrm{SQP}_{v',m}, \quad v' \in \mathbf{C}_{\mathrm{BTX}}, \quad m \in \mathbf{F}_{v'} \tag{32}$$

where $\mathrm{SQP}_{v',m}$ denotes the target value of the total amount of material m delivered to customer v' during all planning periods.

In addition, it is assumed in this work that one of the intermediates of the BTX supply chain, i.e., the mixed xylenes, can be sold to the domestic customers for profit. The corresponding constraints are

$$\mathrm{QXO}^{\mathrm{L}}_{v',m,\mathrm{tp}} \le \sum_{v \in \mathbf{UD}} q_{v,v',m,\mathrm{tp}} \le \mathrm{QXO}^{\mathrm{U}}_{v',m,\mathrm{tp}}, \quad v' \in \mathbf{C}_{\mathrm{mxyl}}, \quad m \in \mathbf{F}_{v'}, \quad \mathrm{tp} \in \mathbf{TP} \tag{33}$$

where $\mathbf{C}_{\mathrm{mxyl}}$ denotes the sets of domestic customers for mixed xylenes and $\mathrm{QXO}^{\mathrm{U}}_{v',m,\mathrm{tp}}$ and $\mathrm{QXO}^{\mathrm{L}}_{v',m,\mathrm{tp}}$ represent, respectively, the acceptable maximum and minimum amounts of material m delivered to customer v' in period tp.

Finally, all intermediate and final products mentioned above should also be allowed to be sold on the overseas market so that the overall performance of the supply chain may be further enhanced. This practice is justifiable if the selling prices and/or demands for some of the products are high enough to compensate for the losses due to the needs to cut down inventories of the other products and to sell them at lower prices and/or higher transportation costs. The delivered quantities to overseas customers should also be subject to similar inequality constraints, i.e.,

$$\mathrm{QOS}^{\mathrm{L}}_{v',m,\mathrm{tp}} \le \sum_{v \in \mathbf{UT}} q_{v,v',m,\mathrm{tp}} \le \mathrm{QOS}^{\mathrm{U}}_{v',m,\mathrm{tp}}, \quad v' \in \mathbf{C}_{\mathrm{ovs}}, \quad m \in \mathbf{F}_{v'}, \quad \mathrm{tp} \in \mathbf{TP} \tag{34}$$

where $\mathbf{C}_{\mathrm{ovs}}$ denotes the sets of overseas customers for the intermediate and final products of BTX supply chains, i.e., benzene, toluene, *p*-xylene, *o*-xylene and mixed xylenes; $\mathrm{QOS}^{\mathrm{U}}_{v',m,\mathrm{tp}}$ and $\mathrm{QOS}^{\mathrm{L}}_{v',m,\mathrm{tp}}$ represent, respectively, the acceptable maximum and minimum amounts of intermediate or final product m delivered to customer v' in period tp. Notice that $\mathbf{C} = \mathbf{C}_{\mathrm{BTX}} \cup \mathbf{C}_{mxyl} \cup \mathbf{C}_{\mathrm{ovs}}$ in the present model.

5. Objective function

The objective function of the proposed optimization problem is chosen to be the total profit realized over a specified number of planning periods, i.e.,

$$\text{total profit} = \sum_{\mathrm{tp} \in \mathbf{TP}} \mathrm{pf}_{\mathrm{tp}} \tag{35}$$

and

$$\mathrm{pf}_{\mathrm{tp}} = \mathrm{rs}_{\mathrm{tp}} - \mathrm{cr}_{\mathrm{tp}} - \mathrm{co}_{\mathrm{tp}} - \mathrm{ct}_{\mathrm{tp}} - \mathrm{ci}_{\mathrm{tp}} - \mathrm{cb}_{\mathrm{tp}} - \mathrm{cd}_{\mathrm{tp}} \tag{36}$$

where $\mathrm{pf}_{\mathrm{tp}}$, $\mathrm{rs}_{\mathrm{tp}}$, $\mathrm{cr}_{\mathrm{tp}}$, $\mathrm{co}_{\mathrm{tp}}$, $\mathrm{ct}_{\mathrm{tp}}$, $\mathrm{ci}_{\mathrm{tp}}$, $\mathrm{cb}_{\mathrm{tp}}$ and $\mathrm{cd}_{\mathrm{tp}}$ denote, respectively, the net profit, the total revenue secured from various product sales, the total cost of raw materials, the total operation cost, the total transportation cost, the total inventory cost, the total backlog cost and the total cost of promotion discount in period tp. The total sale revenue can be expressed as

$$\mathrm{rs}_{\mathrm{tp}} = \sum_{v' \in \mathbf{C}} \sum_{m \in \mathbf{F}_{v'}} \left(\sum_{v \in \mathbf{UC}} q_{v,v',m,\mathrm{tp}} \right) \cdot \mathrm{SP}_{v',m,\mathrm{tp}} \tag{37}$$

where $\mathbf{UC} = \mathbf{UT} \cup \mathbf{UD}$; $\mathrm{SP}_{v',m,\mathrm{tp}}$ represents the selling price of intermediate or final product m sold to customer v' during period tp.

The second term in Eq. (36) is the sum of all costs for producing the raw materials inside refineries (i.e., light naphtha and pyrolysis gasoline), and the costs for purchasing the imported feedstock (i.e., light naphtha and mixed xylenes) and also the final products provided by other domestic suppliers. In particular, this term can be written as

$$\begin{aligned} \mathrm{cr}_{\mathrm{tp}} = {} & \sum_{v \in \mathbf{S}^{\mathrm{I}}_{\mathrm{litnap}}} \sum_{m \in \mathbf{P}_v} \mathrm{QLN}^{\mathrm{I}}_{v,m,\mathrm{tp}} \cdot \mathrm{CLN}^{\mathrm{I}}_{v,m,\mathrm{tp}} \\ & + \sum_{v \in \mathbf{S}^{\mathrm{I}}_{\mathrm{pyrgas}}} \sum_{m \in \mathbf{P}_v} \mathrm{QPG}^{\mathrm{I}}_{v,m,\mathrm{tp}} \cdot \mathrm{CPG}^{\mathrm{I}}_{v,m,\mathrm{tp}} \\ & + \sum_{v \in \mathbf{S}_{\mathrm{litnap}}} \sum_{m \in \mathbf{P}_v} \left(\sum_{v' \in \mathbf{UT}} q_{v,v',m,\mathrm{tp}} \right) \cdot \mathrm{CLN}_{v,m,\mathrm{tp}} \\ & + \sum_{v \in \mathbf{S}_{\mathrm{mxyl}}} \sum_{m \in \mathbf{P}_v} \left(\sum_{v' \in \mathbf{UT}} q_{v,v',m,\mathrm{tp}} \right) \cdot \mathrm{CMX}_{v,m,\mathrm{tp}} \\ & + \sum_{v \in \mathbf{S}_{\mathrm{BTX}}} \sum_{m \in \mathbf{P}_v} \left(\sum_{v' \in \mathbf{UD}} q_{v,v',m,\mathrm{tp}} \right) \cdot \mathrm{CBTX}_{v,m,\mathrm{tp}} \end{aligned} \tag{38}$$

where $\mathrm{CLN}^{\mathrm{I}}_{v,m,\mathrm{tp}}$ and $\mathrm{CPG}^{\mathrm{I}}_{v,m,p}$ denote, respectively, the unit costs for producing light naphtha and pyrolysis gasoline in the refineries and $\mathrm{CLN}_{v,m,\mathrm{tp}}$, $\mathrm{CMX}_{v,m,\mathrm{tp}}$ and $\mathrm{CBTX}_{v,m,\mathrm{tp}}$ denote, respectively, the unit costs for purchasing light naphtha, mixed xylenes and final products. Notice that the first two terms in the above equation can be dropped in actual optimization process since these costs are treated as constants in the present model.

The total operation cost can be considered as the sum of the operation costs for running the reaction and separation processes, i.e.,

$$\begin{aligned} \mathrm{co}_{\mathrm{tp}} = {} & \sum_{u \in \mathbf{UA}} \left(l_{u,\mathrm{tp}} \cdot \mathrm{CXA}_{u,\mathrm{tp}} + \sum_{s \in \mathbf{F}_u} \sum_{k \in \mathbf{K}_{u,s}} \mathrm{qfi}_{u,s,k,\mathrm{tp}} \cdot \mathrm{CVA}_{u,s,k,\mathrm{tp}} \right) \\ & + \sum_{u \in \mathbf{UB}} \left(l_{u,\mathrm{tp}} \cdot \mathrm{CXB}_{u,\mathrm{tp}} + \sum_{s \in \mathbf{F}_u} \mathrm{qf}_{u,s,\mathrm{tp}} \cdot \mathrm{CVB}_{u,s,\mathrm{tp}} \right) \end{aligned} \tag{39}$$

where $\mathrm{CXA}_{u,\mathrm{tp}}$ and $\mathrm{CXB}_{u,\mathrm{tp}}$ denote the fixed operating costs for unit u in **UA** and **UB** during period tp, respectively, $\mathrm{CVA}_{u,k,s,\mathrm{tp}}$ represents the variable operating cost of reaction unit u for processing feedstock s under operation mode k during period tp and $\mathrm{CVB}_{u,\mathrm{tp}}$ is the variable operating cost of separation unit u during period tp.

In general, the overall transportation cost can be expressed as

$$\mathrm{ct}_{\mathrm{tp}} = \sum_{v \in \mathbf{USC}} \sum_{v' \in \mathbf{USC}} \sum_{m \in \mathbf{M}} q_{v,v',m,\mathrm{tp}} \cdot \mathrm{CTP}_{v,v',m,\mathrm{tp}} \tag{40}$$

where $\mathrm{CTP}_{v,v',m,\mathrm{tp}}$ represents the unit transportation cost for moving material m from unit v to unit v' during period tp. The unprocessed inventories remained in the supply chain at the end of each planning period can be penalized by incorporating additional costs, i.e.,

$$\mathrm{ci}_{\mathrm{tp}} = \sum_{u \in \mathbf{U}} \sum_{m \in \mathbf{M}_u} \mathrm{vin}_{u,m,\mathrm{tp}} \cdot \mathrm{CIN}_{u,m,\mathrm{tp}} \tag{41}$$

where $\mathrm{CIN}_{u,m,\mathrm{tp}}$ represents the inventory cost per unit of process material m in unit u during period tp.

The total stockout cost can be computed by summing all backlog penalties, i.e.,

$$\mathrm{cb}_{\mathrm{tp}} = \sum_{v' \in \mathbf{C}_{\mathrm{BTX}}} \sum_{m \in \mathbf{F}_{v'}} \mathrm{bdq}_{v',m,\mathrm{tp}} \cdot \mathrm{CBL}_{v',m,\mathrm{tp}} \tag{42}$$

where $\mathrm{CBL}_{v',m,\mathrm{tp}}$ represent the backlog penalty per unit of product m not delivered to customer v' during time period tp. Similarly, the total cost of promotion discounts can be expressed as

$$\mathrm{cd}_{\mathrm{tp}} = \sum_{v' \in \mathbf{C}_{\mathrm{BTX}}} \sum_{m \in \mathbf{F}_{v'}} \mathrm{sdq}_{v',m,\mathrm{tp}} \cdot \mathrm{CPD}_{v',m,\mathrm{tp}} \tag{43}$$

where $\mathrm{CPD}_{v',m,\mathrm{tp}}$ represent the promotion discount per unit of product m offered to customer v' during time period tp.

6. Case studies

The BTX supply network considered in our case studies is sketched in Fig. 10. Notice that the importation of crude oils and intermediates, i.e., light naphtha and mixed xylenes, are shipped from foreign suppliers by oil tankers via terminal SEADK, and the exportation of intermediate and final products of the supply chain, i.e., mixed xylenes, benzene, toluene, *p*-xylene and *o*-xylene, are delivered to the overseas customers also through the same terminal. The crude oils are transferred from SEADK to three separate refineries, labelled, respectively, as KSR, DLR and LIWR. Each refinery is equipped with an atmospheric distillation unit. It is assumed that the network configuration of this supply chain is fixed and it consists of three (3) reforming units, three (3) aromatic extraction units, two (2) xylene fractionation units, two (2) tatory units, two (2) parex units and two (2) xylene isomar units. These processing units are located in the three separate refineries mentioned above. The first complete set of processing units, i.e., a reforming unit, an aromatic extraction unit, a xylene fractionation unit, a tatory unit, a parex unit and a xylene isomar unit, are situated in the KSR refinery. In addition, this refinery is also equipped with a naphtha cracker. The second reforming unit is installed in the DLR refinery, while all other production units are located in the LIWR refinery. The first aromatic extraction unit contains two processing trains designed for two distinct types of feedstock, i.e., reformer gasoline and pyrol-

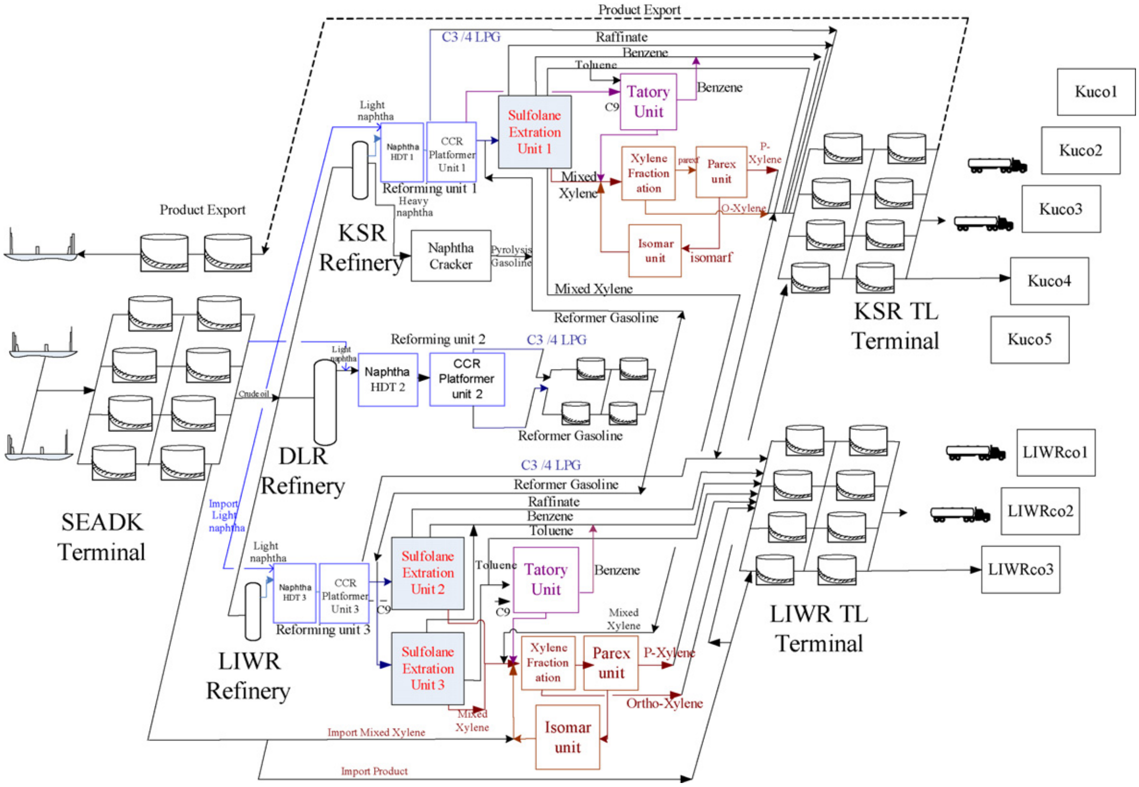

Fig. 10. The BTX supply network.

Table 2

Demand levels and allowable delivery ranges of the intermediate and final products (m^3)

Product	Customer	tp1	tp2	tp3	Total demand
Benzene (bz)	Kuco1	22500–27500	13500–16500	13500–16500	55000
	Kuco3	15300–18700	24300–29700	16200–19800	62000
	LIWRco1	4500–5500	5400–6600	4500–5500	16000
	LIWRco2	12600–15400	5400–6600	34200–41800	58000
Toluene (tl)	Kuco2	4050–4950	36450–44550	8595–10505	54550
	LIWRco1	1800–2200	2700–3300	2250–2750	7500
Mixed xylenes (mx)	Kuco4	900–1100	900–1100	900–1100	3000
p-Xylene (px)	Kuco5	34200–41800	33750–41250	33300–40700	112500
	LIWRco3	18900–23100	18900–23100	19800–24200	64000
o-Xylene (ox)	Kuco4	36450–44550	36450–44550	36000–44000	121000
	LIWRco3	24750–30250	23400–28600	23850–29150	80000

ysis gasoline. The remaining aromatic extraction units are only capable of processing the reformer gasoline. All intermediate and final products of the supply chain are delivered to the local customers from the product distribution terminals KSRTL and LIWRTL via pipelines and/or trucks. The total demand levels of the intermediate and final products and their allowable delivery ranges in every planning period are presented in Table 2. In all our case studies presented here, the target level of every material in each period is set to be the arithmetic mean of the upper and lower bounds of the corresponding range. To facilitate concise presentation, these materials will later be referred to with the two-letter codes specified in the parentheses in this table. For example, the code "bz" denotes benzene and "tl" denotes toluene, etc. The supply rates of light naphtha and pyrolysis

Table 3

Supply rates of light naphtha and pyrolysis gasoline (m^3/month)

Raw material	Source unit	tp1	tp2	tp3
Light naphtha 1 (ln1)	Atmospheric distillation unit 1	69530	46860	20100
Light naphtha 2 (ln2)	Atmospheric distillation unit 2	54040	29560	64980
Light naphtha 3 (ln3)	Atmospheric distillation unit 3	39520	15400	65600
Pyrolysis gasoline (pg)	Naphtha cracker	90000	90000	75000

Table 4
Capacity limits of reforming units (m^3/month)

Unit	ln1		ln2		ln3	
	Lower	Upper	Lower	Upper	Lower	Upper
Reformer 1 (RF-1)	35000	135000	35000	125000	35000	135000
Reformer 2 (RF-2)	45000	145000	50000	156000	55000	160000
Reformer 3 (RF-3)	40000	125000	45000	135000	45000	140000

Table 5
Capacity limits of extraction units (m^3/month)

Unit	Reformer gasoline		Pyrolysis gasoline	
	Lower	Upper	Lower	Upper
Extraction 1 (ET-1)	15000	100000	20000	150000
Extraction 2 (ET-2)	20000	120000	NA	NA
Extraction 3 (ET-3)	20000	120000	NA	NA

Table 6
Capacity limits of the xylene fractionation, tatory, parex and isomar units (m^3/month)

Unit	Lower	Upper
Xylene fraction 1 (XF-1)	25000	110000
Xylene fraction 2 (XF-2)	20000	100000
Tatory 1 (TT-1)	20000	58000
Tatory 2 (TT-2)	35000	80000
Parex 1 (PR-1)	25000	100000
Parex 2 (PR-2)	30000	105000
Xylene isomar 1 (IM-1)	10000	70000
Xylene isomar 2 (IM-2)	12000	100000

Table 7a
Purchasing costs of light naphtha and pyrolysis gasoline (US dollars/m^3)

Material	tp1		tp2		tp3	
	From AD/NC	From OS	From AD/NC	From OS	From AD/NC	From OS
ln1	350	450	370	470	365	465
ln2	375	475	385	485	380	480
ln3	360	480	370	470	370	470
pg	530		550		570	

Table 8
Maximum supply rates and consumption rates of the raw materials, intermediates and final products in each time period (m^3/month)

Material	Supplied by OS or DS	Consumed by OC
ln1	50000	–
ln2	50000	–
ln3	50000	–
bz	25000	25000
tl	65000	35000
mx	100000	15000
ox	25000	25000
px	25000	25000

gasoline in each planning period are provided in Table 3. In this table, the raw materials are also represented with codes given in the parentheses. Notice that, since the composition of light naphtha produced in one distillation unit is usually not the same as that in another, these different grades of materials are thus distinguished with the numerical labels in the codes. The upper and lower limits of the operating capacities of all production units are shown in Tables 4–6. In our case studies, these units are identified on the basis of the codes given in Table 1. Since each reaction or separation process can be carried out in alternative units, these units are numbered according to their locations. In Table 7a, the following two types of cost data are provided: (a) the raw-material costs of light naphtha from atmospheric distillation units (AD) and from overseas suppliers (OS), and (b) the purchasing costs of pyrolysis gasoline obtained from naphtha cracker (NC). In Table 7b, one can find: (a) the selling prices of the intermediate and final products sold to the domestic and overseas customers, i.e., DC and OC, (b) the purchasing costs of final products obtained from domestic suppliers (DS) and (c) the costs of mixed xylenes bought from the overseas suppliers (OS). The largest available quantities of the raw materials, intermediates and final products that can be purchased from the international or domestic markets in each time period are given in the second column of Table 8. In the same table, the maximum amounts of exportable quantities of the products and intermediates are also presented (in the 3rd column). Notice that the lower bounds of these supply and demand rates are all set to zero in our case studies. In addition, all initial inventories of the intermediates and final products are assumed to be zero, and all transportation

Table 7b
Selling prices and purchasing costs of intermediate and final products (US dollars/m^3)

Material	tp1			tp2			tp3		
	To DC	To OC	From DS	To DC	To OC	From DS	To DC		From DS
bz	910	820	1000	850	750	950	880	800	960
tl	650	600	700	670	600	720	700	600	750
mx	538	528	600(OS)	540	500	570 (OS)	550	510	570 (OS)
px	720	610	780	680	630	760	700	650	750
ox	680	610	780	650	540	700	670	560	720
C_3	230			232			235		
C_4	230			232			235		
C_5	310			310			308		
C_9	310			312			315		
C_{10}	312			320			318		

capacities are assumed to be limitless in order to simplify the model formulation. For convenience, let us temporarily assume that the backlog penalties are not assessed and promotion discounts are not offered over the planning horizon of the base case. Finally, for the sake of conciseness, the remaining model parameters are given as the supplementary materials. These parameters include: the performance indices of the reaction and separation processes, i.e., the product yields of the former processes and the recovery efficiencies of the latter, the feed compositions of separation units, the upper limits of all inventories and their costs, and all transportation costs.

There are a total of 1952 constraints (1106 equality constraints and 846 inequalities) and 2227 variables (348 binary variables and 1879 real variables) in the corresponding MILP model. The base case was solved with module CPLEX of the commercial software GAMS in 0.094 s (CPU time) on a personal computer with Pentium IV 3.0 CPU and 1024 KB RAM. The optimal throughputs of all production units can be identified from the solution and summarized in Table 9a and Tables 9b and 9c. Notice that the codes “ro1”, “ro2” and “ro3” are used here to represent different grades of reformates produced by reforming units RF-1, RF-2 and RF-3, respectively. It can be observed that the units (and also the network configurations of the supply chain) chosen in the three planning periods are not the same. Other than the raw materials supplied

Table 9a
Optimal throughputs of all production units in time period 1 (m^3/month)

Unit	Feedstock	Mode	Source unit	Throughput
RF-1	ln1	K1	AD-1	69530
			IEF	50000
RF-2	ln2	K2	AD-2	54040
			IEF	1430
ET-1	pg		Naphtha cracker	90000
	ro1		RF-1	79727
ET-2	ro1		RF-1	3944
	ro2		RF-2	16056
ET-3	ro2		RF-2	20000
XF-1	mx		ET-1	38910
			IM-1	2705
			TT-1	12940
			IEF	55445
XF-2	mx		ET-2	6600
			ET-3	5700
			IM-1	63795
			TT-2	23905
TT-1	tl	K1	IEF	23232
TT-2	tl	K2	ET-1	12300
			ET-2	2600
	C_9		ET-3	2600
			RF-1	11953
			RF-2	5547
PR-1	Parexf		XF-1	72185
PR-2	Parexf		XF-2	55454
IM-1	Isomarf		PR-1	53055
			PR-2	16945

Table 9b
Optimal throughputs of all production units in time period 2 (m^3/month)

Unit	Feedstock	Mode	Source unit	Throughput
RF-1	ln3	K2	AD-3	35000
RF-2	ln1	K1	AD-1	45000
ET-1	pg		Naphtha cracker	90000
	ro1		RF-1	22750
ET-3	ro2		RF-2	24750
	ro3		RF-3	20250
XF-1	mx		ET-1	18741
			TT-1	16529
			IEF	74730
XF-2	mx		ET-3	8168
			IM-1	59363
			IM-2	7200
			IEF	25270
TT-1	tl	K3	ET-1	9600
			IEF	2500
	C_9		RF-1	1750
			RF-2	10350
PR-1	Parexf		XF-1	79251
PR-2	Parexf		XF-2	56565
IM-1	Isomarf		PR-1	64109
			PR-2	5747
IM-2	Isomarf		PR-2	12000

Table 9c
Optimal throughputs of all production units in time period 3 (m^3/month)

Unit	Feedstock	Mode	Source unit	Throughput
RF-1	ln3	K2	AD-3	76000
RF-2	ln1	K1	AD-1	20100
			IEF	24900
RF-3	ln2	K2	AD-2	94540
ET-1	pg		Naphtha cracker	75000
	ro1		RF-1	49400
ET-3	ro2		RF-2	24750
	ro3		RF-3	47270
XF-1	mx		ET-1	27168
			IM-1	44324
			IEF	38508
XF-2	mx		ET-3	22667
			TT-2	45157
			IM-1	27176
			IM-2	3000
TT-2	tl	K3	ET-1	8095
			ET-2	2400
	C_9		ET-3	18295
			IEF	4268
			RF-1	3800
			RF-2	10350
			RF-3	18908
PR-1	Parexf		XF-1	73653
PR-2	Parexf		XF-2	61362
IM-1	Isomarf		PR-1	37134
			PR-2	32866

Table 10
Optimal supply rates of the purchased materials in the base case (m^3/month)

Material	tp1	tp2	tp3	Total
ln1	50000		23040	73040
ln2	1430			1430
ln3				
bz		19807		19807
tl	45178			45178
mx	55445	100000	38508	193953
px				
ox		5663		5663

Table 11
Product inventories at the end of every planning period in the base case (m^3)

Terminal	Product	tp1	tp2	tp3
KSRTL	bz		2712	
	tl	15800		
	mx			
	px			
	ox		1950	
LIWRTL	bz		9007	
	tl	9328		
	mx			
	px			
	ox			

by the production units within the refineries, i.e., the light naphtha from the atmospheric distillation units and the pyrolysis gasoline from the naphtha crackers, additional materials must be purchased from external sources. The optimal supply rates of these purchased materials can be found in Table 10. Notice that the total amounts of purchased benzene and mixed xylenes in three months are 19,807 and 193,953 m^3, respectively. The inventories of the final products at the end of every planning period are presented in Table 11. It can be observed that all inventories are reduced to the lowest possible level (zero) at the end of the 3-month horizon. This is obviously due to the need to minimize the storage costs. The suggested amounts of intermediate and final products to be delivered to the customers in each planning period are shown in Table 12. According to this table, the optimal amounts of benzene shipped to the customers should be close to the upper bounds in the first month, the lower bounds in the second month and the targets in the final period. This is due to the fact that the selling price of benzene is the highest in the first month (910 US dallar/m^3), while the price drops to its lowest level in the second month (850 US dallar/m^3). Similarly, since the prices of toluene and mixed xylenes are at the highest levels in the third planning period, the suggested amounts of delivery in this period should be close to their maximum allowable values. Finally, the largest total profit in this case can be predicted to be 61,526,390 US dollars.

Table 12
Suggested amounts of intermediate and final products to be delivered in the base case (m^3)

Product	Customer	tp1	tp2	tp3	Total
bz	Kuco1	27500	13500	14000	55000
	Kuco3	18700	24300	19000	62000
	LIWRco1	5100	5400	5500	16000
	LIWRco2	15277	5400	37323	58000
tl	Kuco2	4050	39995	10505	54550
	LIWRco1	1800	2950	2750	7500
mx	Kuco4	900	1000	1100	3000
px	Kuco5	38000	33800	40700	112500
	LIWRco3	19639	20161	24200	64000
ox	Kuco4	36450	40550	44000	121000
	LIWRco3	27302	23548	29150	80000

Several different scenarios have been studied with the proposed model. In the first case, we assumed that the extraction unit ET-1 is not operable in the second time period due to scheduled maintenance. Notice that only this extraction unit is capable of processing pyrolysis gasoline in the present supply network. Consequently, the pyrolysis gasoline produced in the naphtha cracker during the second time period has to be stored temporarily in a buffer tank, and this extra inventory cannot be consumed completely later in the third time period. More specifically, the inventory of pyrolysis gasoline in the buffer tank of ET-1 reaches 90,000 m^3 after the second month and then lowered to 15,000 m^3 at the end of the 3-month horizon. This additional inventory inevitably causes a significant variation in the consumption of light naphtha. Consequently, the amounts of purchased intermediate and final products, i.e., mixed xylenes and benzene, must be higher than those in the base case. Under these circumstances, it was found that the total profit is about 11.4 million US dollars less than that achieved with the complete set of production units in the base case. The supply rates of the purchased materials identified in this case are shown in Table 13. The suggested amounts of intermediate and final products to be delivered to the domestic customers in each planning period are presented in Table 14.

In the second scenario, it was assumed that no suitable benzene and toluene could be purchased during all time periods. Thus, the quantities of raw materials consumed in this case must be larger than those used in the base case. The optimal supply rates of the purchased materials can be identified from the MILP solution (see Table 15). It can be observed that the total amount of purchased light naphtha (a raw material) is more than that required in the base case by 296,949 m^3 (a 398.7% increase). But the imported amount of mixed xylenes (an intermediate) is less due to the fact a larger quantity of raw material is con-

Table 13
Optimal supply rates of the purchased materials when the first extraction unit is not operable in the second time period due to scheduled maintenance (m^3/month)

Material	tp1	tp2	tp3	Total
ln1	14077			14077
ln2				
ln3		15080		15080
bz	18573	25000		43573
tl	42202			42202
mx	83756	100000	34876	218632
px				
ox		4242		4242

Table 14
Suggested amounts of intermediate and final products to be delivered to the local customers when the first extraction unit is not operable in the second time period due to scheduled maintenance (m^3)

Product	Customer	tp1	tp2	tp3	Total
bz	Kuco1	25000	13500	16500	55000
	Kuco3	17900	24300	19800	62000
	LIWRco1	5100	5400	5500	16000
	LIWRco2	12600	5400	40000	58000
tl	Kuco2	4050	39995	10505	54550
	LIWRco1	1800	2950	2750	7500
mx	Kuco4	900	1000	1100	3000
px	Kuco5	37010	34790	40700	112500
	LIWRco3	20900	18900	24200	64000
ox	Kuco4	39959	37041	44000	121000
	LIWRco3	24850	26000	29150	80000

Table 15
Optimal supply rates of the purchased materials when no suitable benzene and toluene could be obtained from external sources (m^3/month)

Feed/product	tp1	tp2	tp3	Total
ln1	50000	50000	50000	150000
ln2	50000	50000	50000	150000
ln3	17419	4000	50000	71419
bz				
tl				
mx	31014	73804		104818
px	2537		4339	6876
ox		14940		14940

sumed. The optimal throughputs of all production units in this case are shown in Table 16. When compared with Table 9a and Tables 9b and 9c, it can be observed that more production units are utilized to satisfy the customers' demands and, also, their throughputs are almost all larger than those in the base case. Profit in this case is reduced to 51,763,386 US dollars.

The third scenario is concerned with a modified forecast of the selling prices and purchasing costs of the intermediate and final products. Let us assume that the predicted purchasing costs of imported light naphtha have all been increased by 200 US dollars per cubic meter. In other words, each new prediction is approximately 44.4% higher than the base-case cost. Additional modifications in the forecasts of the selling prices and purchasing costs of intermediate and final products are described in Table 17. Notice that the base-case predictions are only partially changed and the modified figures are underlined here. In addition, since the prices/costs of benzene, C_3, C_4, C_5 and C_{10} are the same as those listed in Table 7b, these data are not repeated for the sake of brevity. As a result of the aforementioned changes in forecasts, it is not beneficial to operate the tatory unit since the difference in market values between its inputs (i.e., toluene and C_9) and outputs (i.e., benzene and mixed xylenes) becomes too small. In addition, the amounts of purchased light naphtha and toluene are bound to be reduced due to the cost increases mentioned above. Under this situation, the total amounts of purchased benzene and mixed xylenes are increased to 60,855 m^3 (307.2% of the base level) and 248,228 m^3 (128.0% of the base level), respectively, during the 3-month period. The processing rates of all production units are presented in Table 18. It can be observed that fewer production units are utilized and, also,

Table 16
Optimal throughputs of all production units when no suitable benzene and toluene could be purchased from external sources (m^3/month)

Time period	Unit	Feed-stock	Mode	Through-put	Unit	Feed-stock	Mode	Through-put
Tp1	RF-1	ln1	K1	119530	XF-1	mx		110000
	RF-2	ln2	K2	104040	XF-2	mx		95914
	RF-3	ln3	K1	56939	TT-1	tl	K3	10551
						c_9		10551
	ET-1	pg		90000	TT-2	tl	K3	17500
		ro1		83671		c_9		17500
	ET-2	ro2		20000	PR-1	Parexf		70591
	ET-3	ro2		47626	PR-2	Parexf		55822
		ro3		25622	IM-1	Isomarf		70000
Tp2	RF-1	ln1	K1	88249	XF-1	mx		110000
	RF-2	ln2	K2	79560	XF-2	mx		89703
	ET-1	pg		90000	TT-1	tl	K3	16781
		ro1		61774		c_9		16781
	ET-3	ro2		51714	PR-1	Parexf		74747
					PR-2	Parexf		47903
					IM-1	Isomarf		70000
Tp3	RF-1	ln3	K2	135000	XF-1	mx		110000
	RF-2	ln2	K2	114980	XF-2	mx		100000
	RF-3	ln1	K1	78711	TT-1	tl	K3	14125
						c_9		14125
	ET-1	pg		75000	TT-2	tl	K3	29311
		ro1		87750		c_9		29311
	ET-3	ro2		74737	PR-1	Parexf		68627
		ro3		25975	PR-2	Parexf		61934
					IM-1	Isomarf		70000

Table 17
Modified forecast in the selling prices and purchasing costs of intermediate and final products in scenario 3 (US dollars/m^3)

Material	tp1			tp2			tp3		
	To DC	To OC	From DS	To DC	To OC	From DS	To DC	To OC	From DS
tl	900	830	1050	900	860	980	870	860	980
mx	680	528	780 (OS)	640	500	770 (OS)	650	510	770 (OS)
px	720	610	880	680	630	860	700	650	850
ox	680	610	880	650	540	800	670	560	820
C_9	710			712			715		

Table 18
Optimal throughputs of all production units in scenario 3 (m^3/month)

Time period	Unit	Feed-stock	Mode	Through-put	Unit	Feed-stock	Mode	Through-put
Tp1	RF-1	ln3	K2	39520	XF-1	mx		110000
	RF-2	ln1	K1	53295	XF-2	mx		86250
	ET-1	pg		90000	PR-1	Parexf		79092
		ro1		15000				
	ET-2	ro1		10688	PR-2	Parexf		45702
		ro2		9312				
	ET-3	ro2		20000	IM-1	Isomarf		70000
Tp2	RF-1	ln1	K1	38195	XF-1	mx		110000
	RF-2	ln2	K1	59560	XF-2	mx		85868
	ET-1	pg		90000	PR-1	Parexf		82278
		ro1		26737	PR-2	Parexf		45461
	ET-3	ro2		26802	IM-1	Isomarf		70000
Tp3	RF-1	ln3	K2	81000	XF-1	mx		110000
	RF-2	ln1	K1	45000	XF-2	mx		44256
	RF-3	ln2	K2	89020	PR-1	Parexf		100000
	ET-1	pg		75000	IM-1	Isomarf		59365
		ro1		52650				
	ET-3	ro2		24750				
		ro3		44510				

their throughputs are in general smaller than those in the base case. The optimal supply rates of the purchased materials are presented in Table 19. Notice that, due to a large increase in the purchasing cost of light naphtha, the best strategy is to avoid using any imported raw material and to buy extra amounts of benzene and xylenes instead. The profit in this case is 43,915,489 US dollars.

The impacts of demand variations are examined in the fourth case study. Let us assume that all orders of *p*-xylene from customer Kuco5 are cancelled unexpectedly just before the first planning period due to its equipment problems. As a result, the total demand for *p*-xylene drops to 37% of the original level. This reduction in product demand in turn forces all production units in the supply chain to lower their processing rates and, consequently, the total amounts of purchased light naphtha and mixed xylenes must be decreased accordingly. On the other hand, since the production rates of the other final products, i.e., benzene and *o*-xylene, are also reduced as a result, it becomes necessary to make up the resulting backlog by increasing their purchase levels. The optimal supply rates of all purchased materials in this scenario are presented in Table 20. Notice that the amounts of light naphtha and mixed xylenes are indeed less than those in the base case by 10,950 m^3 (14.7%) and 65,872 m^3 (33.96%),

Table 19
Optimal supply rates of the purchased materials in scenario 3 (m^3/month)

Material	tp1	tp2	tp3	Total
ln1				
ln2				
ln3				
bz	17300	25000	18555	60855
tl		60		60
mx	100000	100000	48228	248228
px	4155		19176	23331
ox		25000	1825	26825

Table 20
Optimal supply rates of the purchased materials if customer Kuco5 cancels all orders of *p*-xylene (m^3/month)

Feed/product	tp1	tp2	tp3	Total
ln1	50000		8040	58040
ln2				
ln3	5480			5480
bz		25000	1051	26051
tl	30022			30022
mx	36795	78842	12444	128081
px				
ox		25000	22352	47352

respectively, and, in addition, extra quantities of benzene and *o*-xylene (i.e., 6244 m^3 and 41,689 m^3) must be bought from the local suppliers. The corresponding total profit is about 10.9 million US dollars less than that of the base case.

The effects of backlog penalties and/or promotion discounts are evaluated in this last set of case studies. Let us first consider the scenario when only the backlog penalties are assessed. If these penalties are set to be 20% of the selling prices, the resulting maximum profit realized over the entire planning horizon can be found by solving the corresponding MILP model. This value, i.e., 61,375,188 US dollars, is slightly lower than that in the base case. From the corresponding optimal solution, it can be observed that there are only two deliveries which are different from their target levels, i.e., the amounts of *p*-xylene delivered to Kuco5 is lower than the target by 484 m^3 (1.29%) in the second period and higher by 484 m^3 (1.3%) in the third period. Next, let us assume that a 10% promotion discount is offered in every sale. The overall profit in this situation is lowered to 60,730,985 US dollars. This result is expected since the total amount of each material delivered to the customers in three months is required to be maintained at a fixed level in the present mathematical programming model. From the optimal solution of the corresponding MILP model, one can see that there are 5 off-target deliveries. For customer Kuco4, there is a 9.4% (3824 m^3) shortage of *o*-xylene in the first period and a 9.6% (3824 m^3) surplus in the last period. In the case of customer Kuco5, the delivered amounts of *p*-xylene are lower than the targets by 1089 m^3 (2.7%) and 186 m^3 (0.5%) respectively in the first two periods and higher by 1275 m^3 (3.4%) in the last period. Finally, if the above backlog penalties and promotion discounts are both applied, the optimal profit should be further reduced to 60,566,563 US dollars. This is due to the fact that, in order to avoid penalties and discounts, the amount of any intermediate or final product delivered to a customer in each month is forced to match the target level. Consequently, the flexibility in operating and managing the supply chain is somewhat reduced.

7. Conclusions

A generic MILP model is developed in this work for the purpose of devising the optimal planning strategy for the BTX supply chains. Various realistic scenarios can be efficiently examined accordingly. From the results we obtained so far, it is clear that the proposed approach can be used not only to generate the most economic production schedule on the basis of given supply and demand rates, but also select the best process configuration in a multi-train supply chain to implement such a schedule. This capability is not available in the traditional LP-based production planning software.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2007.04.016.

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