SITE-WIDE AND SUPPLY CHAIN OPTIMISATION FOR CONTINUOUS CHEMICAL PROCESSES

By

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To my wife, Susanna

Abstract

Petrochemical manufacturing is a typical example of a continuous chemical process, which usually involves several interconnected process units. The unit interactions introduce many degrees of freedom for process operation, and also complicate supply chain management. Optimisation is therefore brought in to support decision-making on both process operation and supply chain aspects.

In order to enhance operational feasibility and model accuracy, the optimisation should in principle be executed directly in a site-wide fashion and employing rigorous process representations. This however results in an extremely large-scale site-wide model. This hinders the continuous process from obtaining the utmost benefit from the optimisation. This thesis hence aims to remove the obstacle by developing a practical direct optimisation method for site-wide supply chain problems.

The thesis employed an ethylene process as an example of a continuous process for the solution method development. Based on the process, four types of problems with different complexities were established. They are (i) single-site single-period; (ii) single-site multi-period; (iii) multi-site single-period and (iv) multi-site multi-period.

A novel direct optimisation technique, namely gPROMS-Based Application (gBA) Approach, was developed and examined using the example problems. It overcame the difficulty of the large problem size by separating the optimiser from the process simulator, gPROMS. This allowed gPROMS to simulate each site and each period in the supply chain one-by-one, and send the required information to the

optimiser individually. This avoided computer memory shortage problems, which could be triggered by a simultaneous optimisation of the complete supply chain.

Other solution approaches were also investigated in the thesis to compare with the gBA Approach. For example, Successive Linear Programming (SLP) was used for the single-site single-period problem. A Rolling Horizon technique was used to handle the multi-period problem and a Site/Market Decomposition approach was employed to tackle the multi-site problem. Adopting a "feasible process operation table" in a mixed-integer linear programming (MILP) model was also tested for multi-site/-period problems. Nonetheless, the gBA Approach was always able to find the best solution in the test examples.

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1 Introduction

1.1 Continuous Process and Supply Chain Planning

The term "continuous processes" usually refers to chemical processes which operate under continuous material flow. They are designed to operate continuously for a very long period (e.g. a year) before preventive maintenance is carried out. They are therefore favourable for production with large and broadly constant annual demands. Petrochemical manufacturing and oil refining are two typical examples of continuous processes. Due to the stable product demands and commodity nature of the products, their gross margins are relatively slim. To secure the business in such an adverse situation, it is necessary to have an effective production strategy. Supply chain planning is a useful tool for achieving this.

A supply chain is a network of infrastructures involving the raw material suppliers, the production facilities and the product delivery units. Supply chain planning is a technique to obtain an economic overall allocation of different resources within the infrastructure network. This can be accomplished by choosing suitable raw materials, determining efficient inventory policies, optimising production and estimating cost-effective product delivery routes. Optimisation has always found viable applications here. As different components are engaged in the supply chain, the planning optimisation results greatly depend on the type and accuracy of the component representations in the optimisation model.

The representation type in any supply chain planning model inevitably relates to the characteristics of the process. Batch processes usually involve "recipe-based" representations. They only follow the fixed conditions recorded in the recipe to produce specific products. Planning with this kind of model becomes a process of

recipe selection and sequencing, and can be easily done by a mixed integer linear programming (MILP) model. This recipe-based planning is useful for processes requiring precise product specifications due to regulations (e.g. pharmaceuticals). This is also practical for processes with relatively small demands which need to share facilities with other productions (e.g. fine chemicals). Poor process knowledge is also a possible factor that pushes the processes towards "recipe-based" operation (e.g. food processing). On the other hand, continuous processes (e.g. refining and petrochemicals) can accept a wide range of operating conditions. The "recipe-based" representations might not be good enough to exploit all the degrees of freedom in the processes. This leads the continuous processes to "property-based" representations. The process models handle different operating conditions via considering the physical properties directly. This gives the models capability to explore more opportunities for the process. The significantly improved knowledge of chemical process in the past decades also makes the implementation of rigorous process formulations easier. This provides very accurate "property-based" representations for continuous process units. Consequently, this introduces the potential to improve the continuous process profits by combining detailed process modelling with supply chain optimisation.

Operators in the process industry conventionally tend to plan a continuous process supply chain in a discrete manner. A continuous process has numbers of operation units. The operators usually optimise the operations of different units individually by some reasonably accurate models (e.g. nonlinear steady-state models). After that, they integrate the resulting operational data into an approximated planning model (e.g. linear yield model) to estimate the most suitable supply chain strategy.

The discrete approach does result in some benefits, however, mismatches among the modelling results of different process units are also easily incurred. This is because the discrete approach does not take account of the site-wide interactions among the process units. The result mismatches might worsen the overall solution accuracy, overlook potential opportunities, or even induce process operational infeasibility. Hence, a holistic approach to continuous process supply chain planning is more desirable.

The holistic approach should model all the process units in a site-wide supply chain model framework. Inside the framework, the site-wide unit operations and the supply chain considerations can be optimised simultaneously. This helps to eliminate the drawbacks of the discrete approach. To enhance model accuracy and operational feasibility, rigorous "property-based" representations should also be used for the unit operations. Combining the above efforts, supply chain planning should be able to ensure the competitiveness of a continuous process in a slim profit margin environment.

1.2 Thesis Aim

The holistic approach to continuous process supply chain planning has the potential to bring in attractive benefits, but it has been seldom practised so far. This is because the holistic approach results in a large-scale nonlinear mathematical model, which is very difficult to solve. Making the holistic approach practically solvable is a target of the thesis.

The thesis aims to develop a technique to tackle site-wide supply chain optimisation problems for continuous processes, where the process models are

constructed by rigorous "property-based" representations. The thesis first defines examples of continuous processes, and explores different techniques to solve different supply chain problems of the example processes. Eventually, the most efficient optimisation technique is determined. Although the technique is only tested using the examples described in this thesis, it is believed that the technique is generic to many other continuous processes.

1.3 Thesis Outline

The remaining chapters of the thesis include a literature review, investigations of potential optimisation techniques, and a discussion of future work. They are summarised as follows.

Chapter 2 presents a comprehensive literature review on supply chain planning and site-wide optimisation. The detailed objectives of the thesis are also defined in the chapter according to the literature review.

Chapter 3 chooses an ethylene production process as the study example of the thesis. It provides reasons for the decision and develops two example processes based on ethylene production. The chapter also explains the model formulations of the unit operations, which are the basic elements to assemble the site-wide supply chain models.

Chapter 4 investigates the performance of different solution approaches to solve the single-site single-period problem. The problem is just a standalone site-wide optimisation problem. The approaches investigated include some site-wide methods (Simultaneous Approach, "Base + Delta" Approach, Hybrid Approach) and a decomposition method (Separate Approach). The chapter aims to determine the

most promising approach for the problem studied.

Chapter 5 studies the single-site multi-period problem. Material inventories during a planning horizon are considered in this chapter. As the large problem size is the major barrier to solve the site-wide methods for this type of problem, the chapter concentrates on using a decomposition method (Rolling Horizon Approach) and a simplification method (Feasible Operation Table Approach). The results obtained are important references to develop an executable site-wide approach.

Chapter 6 develops a novel technique to handle the single-site multi-period problem in a site-wide fashion, namely the gPROMS-based application (gBA) Approach. It tries to overcome the site-wide optimisation difficulty caused by the large problem size. Eventually, the approach intends to apply the same idea to solve all different types of site-wide supply chain optimisation problems.

Chapter 7 considers a different type of supply chain problem, the multi-site single-period problem. It takes account of material transfer among different geographical locations. The chapter employs decomposition methods (Site/Market Decomposition, Rolling Site), the simplification method (Feasible Operation Table), and the site-wide method (gBA) to tackle the problem.

Chapter 8 examines the multi-site multi-period problem, which imitates an enterprise supply chain network. The problem encounters both the inventory control and the material transfer issues. It is one of the most complicated forms of supply chain problem. The chapter aims to investigate the reliability of the novel gBA approach about solving such complicated problems.

Finally, Chapter 9 presents the conclusions and future work. The chapter suggests the most efficient solution technique based on the results found in the

previous chapters. It also discusses some possible improvements to the suggested techniques.

2 Literature Review

2.1 Introduction

This chapter presents a literature review on different areas of the process industry supply chain. Firstly, it provides definitions for the supply chain and supply chain management. Secondly, it introduces the concepts of the process industry supply chain. The chapter then classifies process industry supply chain problems into three types. They are Network Design, Analysis and Policy Formulation, and Planning. After that, the chapter discusses the application of site-wide optimisation for continuous processes. Finally, objectives of the thesis are defined according to the literature findings.

2.2 Supply Chain and Supply Chain Management

A supply chain can be used to refer to a network of facilities in an industry. The earliest supply chain study was applied to logistic network design, although the term of "supply chain" was not mentioned (Ganeshan & Harrison, 1995). As the benefits had been recognised, enterprises started to integrate the studies of their own procurement, manufacturing and product distribution together. "Supply chain" has then gradually been adopted to describe an integrated network of "*sourcing, materials handling, and logistics which process a product goes through from manufacture to selling point, and beyond*" (Murphy, 2008). This has eventually evolved as today's most accepted supply chain definition.

In a supply chain network, facilities can belong to just a single company or a group of multiple companies, such as suppliers' suppliers or customers' customers.

The supply chain deals with resource allocations among the facilities within the network, in order to produce products from raw materials and deliver them to end customers. The product of the supply chain can be a real material product or just a service. Supply chain complexity varies with each industry and each company, but it basically follows a typical format as shown in Figure 2.1

After the concept of the supply chain arose, techniques to handle supply chain management have also been developed. In previous decades, individual enterprises took major control of their part of the supply chain. They solely decided the manufacturing details and the distribution details. Mismatches between the manufacturing unit and the distribution unit easily induced a serious time lag between the customer orders and the product delivery, but customers could not influence the situation. As the economy has undergone globalisation in recent years, enterprises have to compete with their rivals all over the world. Customers have

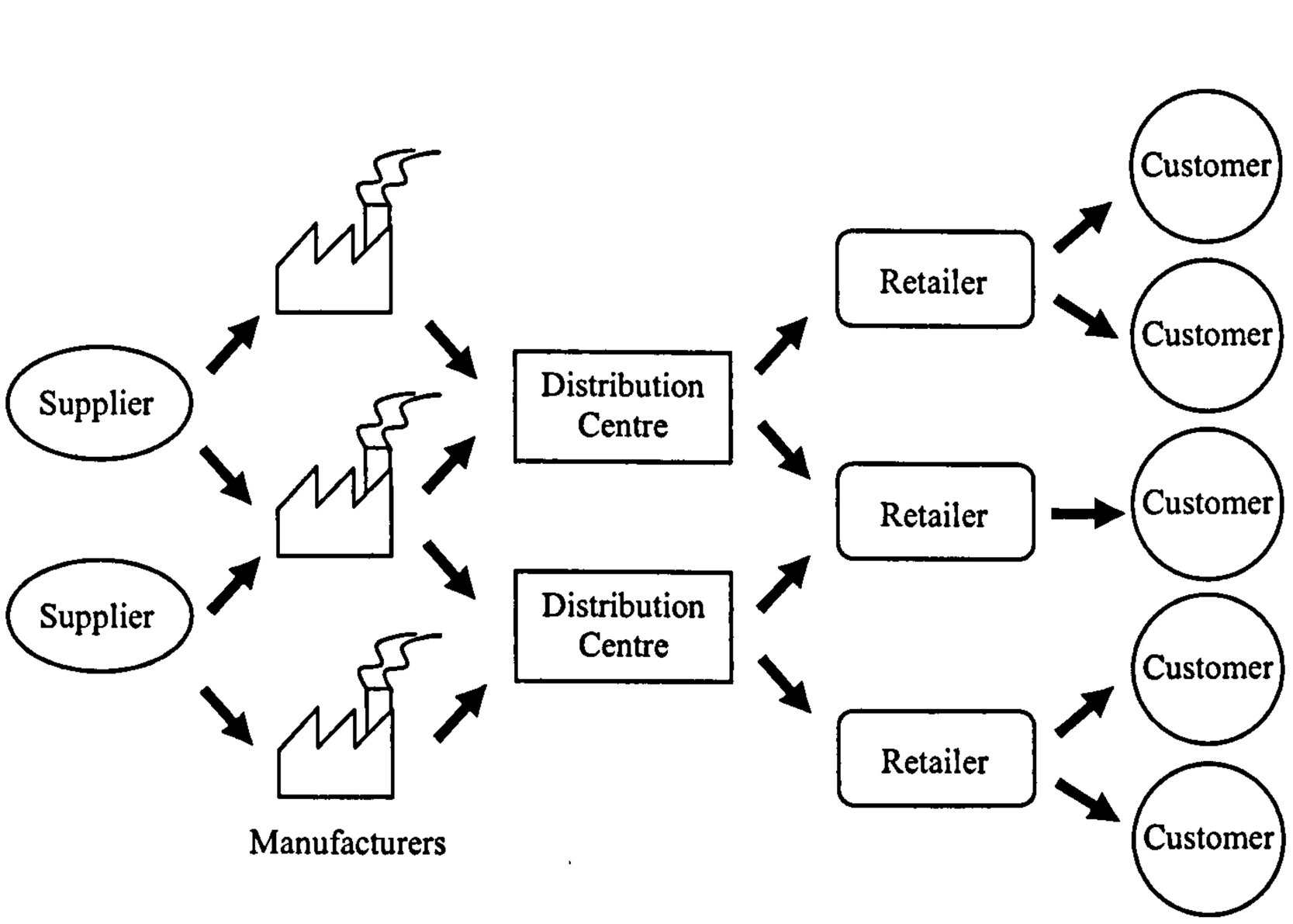

Figure 2.1: A typical supply chain.

more choices of product providers. To gain enough market share and remain competitive, enterprises have to meet customer demands as soon as possible. This has consequently driven enterprises to focus on having effective supply chain management.

Supply chain management is a strategy to incorporate various activities in the supply chain and hence to minimise overall supply cost. According to the Supply-Chain Council, those activities include managing supply and demand, sourcing raw materials, manufacturing, storing inventory and product delivery to customers (Anon, ca. 1996). The activities have their own objectives, and some of them in fact conflict with each other. For instance, the production sector tends to maximise the throughput with the possible lowest cost. It takes little consideration of the inventory level and distribution capacity. The distribution sector in contrast wants to lower the inventory level and minimise the delivery time lag. It exerts pressure back on the production sector to have a quick response to customer demands. It is only therefore possible to achieve effective supply chain management when all the sectors in the supply chain are viewed together in a bigger picture. Based on that, needs of different sectors can be balanced and sectors can co-operate with each other. Anderson *et al.* (1997) therefore suggested some principles to integrate the supply chain sectors. They include grouping customers into segments based on their service needs, designing the logistic network based on customer segments, monitoring the market to forecast the demand accordingly, sourcing strategically to reduce costs, making decisions that optimise the whole supply chain, and measuring the supply chain performance from the view of the end customer.

The principles indicate the philosophy of managing the supply chain, however,

they do not provide explicit methods for implementation. Lambert and Cooper (2000) presented a conceptual framework of supply chain management. The framework includes three strongly interrelated components, the supply chain network structure, the supply chain business processes, and the supply chain management components. The network structure refers to the members of the supply chain and the way they connect. The business processes are the linking activities among the chain members, which usually add value or provide services to the output. The management components are the controls over the process links, such as operation planning, and information management. With the framework, operators of the supply chain can easily decide what kind of management action is required for each process inside the supply chain.

A similar conceptual model for supply chain management was also proposed by Webster (2002). The model is in a pyramid format. The supply chain structure is the base of the pyramid. On the top of it, the author placed business processes and management components together into a single category of management. The author also believed that all management activities would be executed only if they could support good supply chain performance. Therefore, the author placed the performance at the apex of the pyramid, which is not a main component in Lambert and Cooper's framework.

Based on the idea of those supply chain management models, different types of studies have been established. Some researchers extended the supply chain from individual companies to multi-company networks. Chapman and Corso (2005) reviewed some literature about inter-company collaboration in supply chain management. They also discussed the management idea of continuous innovation

to improve the long-term performance of the inter-company network. Some researchers even reversed the supply chain idea to introduce the concept of "demand chain" (Jüttner *et al.*, 2007). They start the chain from customers and work backward to the raw material suppliers. They believe that management decisions made in that way would be more responsive to individual customers' needs and would increase satisfaction from customers.

As various management strategies have been developed, researchers need a systematic measurement to compare how well the strategies perform in the supply chain. These performance measures could be in a qualitative format or in a quantitative format (Beamon, 1998). The former measures objectives which do not explicitly provide numerical results, such as customer satisfaction and supplier reliability. The results obtained might be subjective, so, some researchers prefer the latter. Gunasekaran and Kobu (2007) skipped the qualitative measures and simply defined a performance measure as a process to quantify efficiency or effectiveness of a management action applied on the supply chain. In addition, they summarised different studies about quantitative performance measures. With systematic performance measurements, researchers could easily identify promising management strategies and ensure the supply chain is operated efficiently.

2.3 Process Industry Supply Chains

The chemical industry is sometimes referred as the process industry. This is because chemical manufacturing and oil refining usually involve series of production processes. The processes use huge amounts of energy to physically and/or chemically transform raw materials into products. In terms of process formats, the

process industry could be categorised into continuous process and batch process. The former produces specific products in a large and stable volume with continuous material flows. The latter on the other hand produces a wide range of products in batches with multi-purpose equipment.

There could be different methods to define the process industry supply chain. The products of the process industry are mainly consumed in other manufacturing industries. This naturally places the process industry in the middle of an integrated supply chain. Most of researchers hence consider a process industry supply chain in a company-centric view (Lambert *et al.*, 1998). The process industry enterprise acts as the central entity of the supply chain and connects with some peripheral entities, such as first-tier suppliers and customers. This view integrates the production and logistics sectors inside the enterprise, and results in better global network planning.

Unlike other industries, the process industry involves huge amounts (usually in tonnes) of materials moving along the supply chain. Although the material unit cost is relatively low, the large scale together with the process inherent capital and the operating cost inevitably magnify the economic tension in the supply chain (Braithwaite, 2002). Maintaining a smooth material flow, storing suitable amounts of inventory, and maintaining efficient customer delivery are vital to release the economic tension. Coincidentally, they are objectives of effective supply chain management. To achieve them, researchers basically have divided supply chain problems of the process industry into three types and tackle them one by one (Shah, 2005). They are (i) supply chain network design, (ii) supply chain analysis and policy formulation, and (iii) supply chain planning.

2.3.1 Supply Chain Network Design

A supply chain network indicates connections of facilities, such as production plants, warehouses and distribution channels, in a supply chain. Geoffrion and Powers (1995) suggested that a successful network design should achieve some of the following objectives: locating new facilities in the supply chain, retrofitting existing facilities, sourcing materials or services for facilities and allocating facilities to form production routines.

The network design problem has been investigated since the 1970s. Studies mainly focused on logistics issues at that time. Elson (1972) proposed a multi-period mixed-integer linear programming (MILP) model to locate warehouses in a distribution network. The network model only considers plants, warehouses and customers. Despite its simplicity, it is able to take account of different factors, like warehouse construction cost, warehouse capacity, material transportation cost, and customer demands. Geoffrion and Graves (1974) attempted a more complicated problem, which aimed to optimise locations of intermediate distribution centres in a multi-product distribution network. They formulated the problem in an MILP model and adopted the Benders Decomposition technique to solve it. The solution approach was proved to be efficient.

Since the end of 1980s, researchers have recognised the benefits of combining logistics and production in the supply chain network design. Brown *et al.* (1987) investigated the biscuit division of Nabisco and optimised the production-distribution network. The representation of production used in the study however was only simple product-facility yield correlations. A decade later, Vidal and Goetschalckx (1997) presented a detailed review on production-distribution modelling. They

fully acknowledged the applications of MILP models in the field.

Some researchers have also implemented the production-distribution idea to design a global supply chain. Verter and Dincer (1995) studied the global configuration of an enterprise with multi-national organisations. The authors emphasised that coordination among international components could reinforce the enterprise's competitiveness. Goetschalckx *et al.* (2002) employed the concept of transfer price to tackle global supply chain design. Transfer price is a price charged by an entity for supplying materials or services to other entities in the same enterprise. The authors suggested that the simultaneous consideration of transfer price and material flows was able to benefit the enterprise significantly. Laínez *et al.* (2007) however pointed out that previous studies did not include financial considerations in the supply chain design rigorously enough. They adopted the "Discount-Free-Cash-Flow" method to tackle the problem and obtained some encouraging results. The authors also described the potential of including uncertainty considerations in the research.

Uncertainty has drawn attention in network design research for some time. Applequist *et al.* (2000) employed a polytope integration method to represent the demand uncertainty and the corresponding risk in a deterministic supply chain model. They then compared the proposed method to the conventional stochastic programming method. Tsiakis *et al.* (2001) instead applied a scenario approach to capture discrete possible outcomes caused by the demand uncertainty. They included the scenarios in a multi-period model, and used it to optimise the distribution network layout as well as the material flows. Other uncertainty handling methods include solving the stochastic model by Lagrangean relaxation

(Miranda & Garrido, 2004; 2008) and setting up suitable safety inventory levels (Jung *et al.*, 2004). Some researchers also addressed the uncertainty using multi-objective optimisation. Sabri and Beamon (2000) used the approach to cope with the uncertain lead times and demands during network design. Guillén *et al.* (2005) developed a multi-objective stochastic model to manage the financial risks associated with different design options. Santoso *et al.* (2005) also proposed a stochastic model for realistic scale design problems. The authors applied some approximations and a modified Benders Decomposition algorithm to provide a practical optimisation method for the huge scale stochastic problems.

2.3.2 Supply Chain Analysis and Policy Formulation

The long-term performance of the supply chain mainly depends on the operating policy. Due to intrinsic uncertainties, for instance, material supply reliability and market conditions, supply chain performance could vary from time to time. The performance variations are described as the supply chain dynamics. To formulate a policy with least adverse dynamic behaviours, supply chain simulations are carried out to analyse the relationships between policies and outcome performance.

Deterministic models have been used in supply chain simulation although some uncertainty considerations might need to be neglected. Ishii *et al.* (1988) developed a deterministic model to estimate the suitable base stock levels and lead times for an integrated infrastructure of production, inventory and distribution. Cohen and Lee (1989) proposed a mixed-integer nonlinear programming (MINLP) model to simulate a global production-distribution network. The model maximised the global after-tax profit by designing an operation policy, such as workload allocation

of production units and usages of delivery channels. Cohen and Moon (1990) continued the work in a constrained optimisation model to examine effects of different strategies on the supply chain cost. They concluded that the effects were basically dominated by the transportation cost in most strategies. Voudouris (1996) designed a mathematical model to simulate the efficiency and the responsiveness of a supply chain. That was achieved by measuring the spare capacities of inventory storage and material transportation. The model was also able to provide suitable production and delivery schedules, and inventory levels in terms of the supply chain flexibility.

In order to verify uncertain parameters in the supply chain operation, stochastic simulation plays an important role in supply chain analysis. Cohen and Lee (1988) integrated four stochastic sub-models to evaluate existing production and distribution strategies, and to suggest alternatives. Each sub-model only represents one of four supply chain stages, (i) material sourcing, (ii) production, (iii) inventory, and (iv) product distribution. Pyke and Cohen (1993) developed a stochastic model based on the Markov Chain technique. The model was at first limited to a single product and a simple network of a production unit, a warehouse and a retailer only. They later expanded the model to allow a more complicated network and multiple products (Pyke & Cohen, 1994). Alptekinoğlu and Tang (2005) also launched a stochastic model for multi-channel systems. Due to the large scale of the problem, the authors only searched for a near optimal distribution policy using a decomposition scheme.

Venkateswaran and Son (2004) attempted to quantify the relationship between the model representation details and the simulation accuracy. The study was based on a three-echelon network. The authors applied different approximations and

assumptions to adjust the model's level of detail. They then compared the supply chain performance caused by different settings. It was not surprising that a more detailed model resulted in a more accurate simulation. In addition, the work provided a basic idea about the trade-off between the model accuracy and the model efficiency in practical uses.

The studies reviewed so far mainly concentrated on logistics and inventory aspects. Production was only represented simply or even neglected. Perea-López *et al.* (2001) tried to include more detail of production in a supply chain simulation. They studied the supply chain of a polymer manufacturer, which involved production, distribution and customers. The production facility was represented by a multi-product batch reactor model. It considered recipes, processing time, yield and associated cost for each polymer product. The study treated the supply chain as a decentralised system, where individual components could make their own decisions. The study then used the decentralised model to simulate the supply chain dynamics caused by different operation heuristics. However, the model was incapable of providing an optimal operational decision. The authors followed this up by introducing a model predictive control optimisation framework (Perea-López *et al.*, 2003). To compare with the previous study, the authors also took account of a centralised system. An example in the article showed that the centralised approach could generate more profit than the decentralised approach.

Although centralised coordination might bring some benefits, the idea of the decentralisation is closer to practical reality. A technique of agent-based simulation has been developed recently to handle decentralised systems. An agent-based system consists of agents, messages, activities, hosts and environments (Julka *et al.*,

2002). An agent is an individual object, which executes tasks described by activities and communicates with other agents through messages. It makes its own autonomous decisions according to the information available. A message is a piece of information shared among agents. An activity defines a particular behaviour performed by an agent, for instance, production, keeping inventory and delivering products. A host is responsible for message transmission among agents. An environment is a group of agents. Agents inside an environment cannot communicate with those located outside. Applications of the technique for inventory management, production evaluation (Gjerdrum *et al.*, 2000; García-Flores & Wang, 2002) and refinery operation (Julka *et al.*, 2002) have already been reported. van der Zee and van der Vorst (2005) further developed the idea in an object-oriented model framework. Due to the object-oriented characteristics, the model framework can be easily connected to a graphical interface. This lets users build and interact with their own simulation models more easily. The latest applications of agent-based systems in supply chain have been reviewed by Lee and Kim (2008).

2.3.3 Supply Chain Planning

Supply chain planning is the main study area of this thesis. Optimisation is widely utilised in this area. Therefore, the term of "supply chain optimisation" used in the thesis basically only refers to supply chain planning. It tackles problems with fixed supply chain infrastructures in both the medium and short-term. Medium-term planning is tactical level planning. It plans the usage of resources including production, storage and distribution over a planning period, in order to meet forecasted demands efficiently and economically. Short-term planning is

operational level planning, and sometimes is described as scheduling. It concentrates on the production sector. It schedules the sequence of manufacturing processes constrained by limited resources. It is useful to manage customer order changes, material shortages and other supply chain disruptions (Lapide, 1998).

The representations of the production process in the supply chain planning model could be classified as recipe-based and property-based (Shah, 2005). The recipe-based representation is more desirable for batch processes. This is because batch processes produce specific products according to fixed conditions recorded in recipes. Continuous processes instead suit the "property-based" representation. The processes do not have obvious production recipes, and they are capable of tolerating a range of operating conditions. To study precisely the effects of condition variations on continuous processes, the process model should consider material physical properties directly.

2.3.3.1 Recipe-based Planning

Batch processes are applicable to different kinds of production, including processes with (i) precise product specifications (e.g. pharmaceuticals), (ii) small demands but relatively large profit margin (e.g. fine chemicals), and (iii) poor process knowledge (e.g. food production). They have to follow their own recipes during production. A recipe usually describes the details of material balance, resource requirements, and processing time/rate of a batch process. This could be easily implemented into a set of linear equations. This makes recipe-based planning a major discipline in supply chain optimisation.

Wilkinson *et al.* (1996) optimised a production-distribution system planning for

a continent-wide enterprise, which used recipe-based models for the production sector. The problem involved many factories and large varieties of end products. The enterprise had two options to satisfy different product demands. First, it could produce different products in each factory but with a high operational complexity. Second, it could produce a particular set of products in each factory but with a higher distribution cost. The aim of the study was hence to balance the trade-off. Timpe and Kallrath (2000) developed an MILP model for international supply chain planning. The model was developed in a multi-period framework, where time intervals in the early periods were shorter than those in the later periods. The configuration intended to allow a finer recipe for production in the beginning, and set up an appropriate planning resolution for distribution at the end. Bok *et al.* (2000) studied continuous flexible process planning in a similar manner, but where production recipes were replaced by production schemes. The authors proposed a bilevel decomposition algorithm to speed up the solution time for the large-scale problem. Dogan and Grossmann (2006) also modelled continuous flexible processes in a bilevel format, but they targeted planning and scheduling simultaneously. The approach was believed to obtain better consistency between the planning and scheduling results. A similar idea to combine supply chain design and planning was also adopted by Moreno and Montagna (2007).

Planning problems involving uncertainties have been investigated in the past few years. Gupta and Maranas (2003) separated the production and distribution sectors into a bilevel framework to handle demand uncertainty. The production sector was represented by a set of deterministic linear equations. The demand uncertainty was only involved in the logistics part in a wait-and-see fashion. Ryu

and Pistikopoulos (2004) also adopted a bilevel model to manage demand uncertainty. They formulated the problem as a single parametric problem and solved it using a parametric programming approach. Chen and Lee (2004) tackled demand uncertainty together with price uncertainty and several other conflicting objectives. They illustrated the problem through a multi-echelon supply chain network and solved it in a multi-period stochastic model. Li *et al.* (2004) extended uncertainty considerations from demand to raw material supply and utility supply. The authors developed a probabilistic programming model to evaluate different optimal solutions under various confidence levels of probabilistic variables. The study aimed to estimate the reliability of supply chain planning in an uncertain market. Besides a traditional gradient-based algorithm, a hybrid evolutionary algorithm has also been applied to a stochastic batch scheduling problem (Till *et al.*, 2007).

2.3.3.2 Property-based Planning

A continuous process, such as in an oil refinery or petrochemical site, usually has a slim profit margin because of its large volume, commodity nature and relatively stable demands. To explore opportunities for profitability, the process operating conditions are varied from time to time. A recipe-based representation is not flexible enough to describe the variations accurately. A property-based representation, which simulates process operation via unit operation and stream properties, hence has to be used to model the process. However, a property-based representation involves complicated nonlinear equations. This makes the planning model computationally expensive. This has also discouraged researchers from paying too much attention to property-based planning.

In those limited published studies, property-based representations have been mostly used in refinery planning although that is not strictly a "supply chain" application. Moro *et al.* (1998) and Pinto *et al.* (2000) employed nonlinear process models and blending relations to tackle refinery production planning problems. The studies indicated that commercial optimisers are basically powerful enough to solve industrial scale problems and provide considerable benefits to the refinery. Neiro and Pinto (2004) extended the work to model a petroleum complex. The complex included several refineries, terminals and a pipeline network. The planning was performed by an MINLP model, and which determined stream flowrates, stream properties, inventory levels and facility assignments for the complex. A similar study was also carried out by the same authors (Neiro & Pinto, 2005), but they emphasised handling uncertainties inside the refinery this time. To boost the model accuracy, Li *et al.* (2005) placed empirical nonlinear process representations in an integrated refinery planning model. Later, the authors (Li & Hui, 2007) introduced marginal value analysis to interpret the planning model result. They showed that the technique should be useful for process debottlenecking and retrofitting. A simulation-based planning model, which involved rather rigorous process models, was also proposed by Chryssoloris *et al.* (2005).

2.4 Site-wide Optimisation

Not too many property-based supply chain planning studies have been reported so far, because continuous processes always consist of multiple operation units. Property-based representations of the operations, such as reaction and distillation, are mathematically nonlinear and very complicated. As the operations are

interconnected in the process, supply chain planning should be executed in a site-wide fashion. This results in a huge holistic model. Unfortunately, the huge model size together with the complexity of the property-based formulations make the site-wide optimisation problem very difficult to solve. This hinders the development of property-based planning for continuous processes, as well as site-wide optimisation.

Researchers conventionally utilised separate models to deal with individual units in the process. For instance, Lim *et al.* (2006) and Schulz *et al.* (2006) independently developed optimisation models to schedule cracking furnace decoking, and Grossmann *et al.* (2005) concentrated on complex distillation synthesis. The separate models undoubtedly bring in certain benefits to those particular operations, but they cannot provide a complete picture for the overall process operation. If results of the separate models were blindly combined, the outcome could not ensure an overall optimum. In the worst case, that might even incur operational infeasibility. To obtain the best operational strategy, site-wide optimisation seems to be necessary.

Researchers have tried to use decomposition to handle site-wide optimisation. They introduced strategies to break up the site-wide model into different sub-models, so that the sub-models could be solved easily and the combined result of the sub-models is relatively near to the true optimum. Lagrangean decomposition is a very popular decomposition strategy. Some of the earliest applications could be found in the 1960s (Everett, 1963). Throughout the years, the strategy has been successfully adopted in different planning problems (Gupta & Maranas, 1999; Jackson & Grossmann, 2003). The strategy is popular because it is theoretically

possible to obtain the optimal solution. In addition, it is capable to provide feasible intermediate solutions. This potentially can save a lot of computational time, as the strategy can be terminated once a result with the desired accuracy has been reached.

Jose and Ungar (2000) developed a novel decomposition strategy, namely the "slack auction". The strategy treated units in a chemical process as independent objects. They have to compete with each other for the limited resources presented in the inter-process streams via pricing them, as in an auction. Usually within several rounds of the auction, the resource prices would reach equilibrium as would the amounts of resources in the streams. This indicates that an optimal operation has just been achieved for the process.

Zhang and Zhu (2006) proposed another decomposition method to tackle site-wide optimisation. The method is a two-level strategy. The upper level is called the site level. It allocates resources including materials and utilities to different process units inside the site using a successive linear programming (SLP) technique. The allocations are sent to the lower level (process level) where process unit operations are optimised individually according to the fixed resource allocations. The result of the process level is then fed back to the site level to update the resource allocations. The site and process level optimisations continuously iterate until a satisfactory overall result obtained. A refinery case study had been carried out to demonstrate the application of the strategy. Although the details of the refinery model were not clearly shown in the article, the authors suggested that the decomposition method is capable of offering accurate results by capturing rigorous process representations at the process level.

Besides decomposition, researchers have also attempted some methods to solve

site-wide problems in a holistic fashion. Sadhukhan *et al.* (2004) proposed a method of analytical optimisation, namely value analysis. The method does not execute any mathematical programming optimisation for the site-wide problem. Instead, it systematically calculates the value of each stream in the site-wide model based on product prices, raw material costs and operating costs. Through some predefined analytical procedures, researchers can eventually identify the best operation strategy for the whole process. The proposed method offers an alternative to mathematical optimisation. It also gives more understanding on the background of the decision-making, but the optimality of its result has no guarantee.

Simplification is another method to tackle the site-wide optimisation as a whole, but in a mathematical programming way. Due to technology limitations, such as, computer CPU speed and memory capacity, researchers usually do not use property-based process representations in the site-wide model. They substitute the detailed process model with simplified nonlinear or even linear correlations. This aims to reduced the model size without losing too much accuracy, and hence to make a site-wide optimisation feasible.

One of the most commonly-adopted simplification methods in refinery planning is the setting up of operation "modes" (Göthe-Lundgren *et al*, 2002; Zhang & Hua, 2007). Researchers set up a list of operation modes for process units. The modes define operational details of the units, including yield, material usage and utility consumption. With the operation modes, researchers can easily reformulate a planning problem into an operation mode selection problem using an MILP model. This eliminates the non-linearity in the process units, and greatly reduces the complexity of the resulting model as well as the required computational effort.

A few optimisation studies on holistic petrochemicals planning have been reported in recent years. Al-Sharrah *et al.* (2003) focused on planning petrochemical production, and they involved a detailed petrochemical network in their model. On the other hand, Lababidi *et al.* (2004) paid more attention on material logistics, and clearly defined the transportation network from production to market. Although both studies employed integrated models to deal with the optimisation, the production representations in the models were only simplified linear material balance correlations. This inevitably affected the accuracy of the final result obtained. In order to enhance the accuracy, Gubitoso and Pinto (2007) employed nonlinear expressions to formulate flowrates and component compositions in process streams. The authors used the model to optimise production planning of an ethylene plant, and provided encouraging results.

Schulz *et al.* (2005) also endeavoured to solve petrochemicals supply chain problems. The authors took on a petrochemical complex, which included two ethylene plants and other downstream processes. They applied nonlinear correlations among raw material flowrates, operating pressures, temperatures and production yields to represent one of the ethylene plants. They used another set of simplified linear equations for another ethylene plant as a comparison. Both ethylene process models were required to coordinate production rates, customer demands and inventory management in the site-wide supply chain. The result showed that the two models produced similar trends of the production rates. However, the nonlinear one obtained a more uniform production profile. The authors suggested that the failure to handle a wide operation range caused the discrepancy in the simplified model result. This clearly illustrated the effect of

model details on result accuracy. This also gave an important insight into optimising a site-wide supply chain for continuous processes, which is to apply precise property-based process representations.

2.5 Concluding Remarks and Research Objectives

The production process is usually placed in the middle of a supply chain. An accurate production representation, such as a property-based representation, is therefore essential for supply chain optimisation to obtain a reliable result. In addition, continuous processes consist of interconnected operation units. Simultaneous optimisation of all units is the most straightforward way to explore benefits from mathematical programming techniques. Less advanced technologies in the past, like inefficient optimisation algorithms, slow CPU and shortage of computer memory unfortunately constrained the applications of property-based optimisation and site-wide optimisation.

Throughout the years, researchers had to investigate different solution alternatives to avoid the technological obstacles. They included decomposition, analytical optimisation and simplification. Each of them has some advantages and offers some benefits. Decomposition provides a practical way to handle those hardly solvable site-wide models. Analytical optimisation even totally skips the computational difficulty caused by solving large-scale mathematical programming models. Simplification is also able to reduce the site-wide model size to a solvable level without losing too much accuracy. However, they all share the same shortcoming, which is no optimality guarantee for their final results. Some site-wide opportunities might still be hidden due to mismatches in decomposition,

human error in analytical optimisation or poor approximation in simplification. As continuous processes usually only have a slim profit margin, a little improvement in the supply chain operation could be critical to sustain the business. It is necessary to explore the best possible opportunity. To achieve that, a direct optimisation of the property-based site-wide model should be explored.

Up to current knowledge, no report of combining the property-based planning and site-wide optimisation for continuous chemical processes has been found. Furthermore, continuously improving computing technology and chemical process knowledge in recent years have made employing a holistic property-based model in continuous process supply chain optimisation feasible. Joining the facts together, this has revealed a research gap to improve the overall supply chain operation by developing novel optimisation techniques for large-scale property-based planning models. In order to fill up the research gap, three research objectives have been defined for the thesis.

1. **Define an example continuous process, and construct a holistic model to represent the process unit operations and the supply chain.**

   The example process acts as a reference point for comparing different studies performed in the thesis. This is important to define clearly at the beginning of the research. Based on the example process, a holistic model of both unit operations and supply chain operations can be constructed. In order to ensure a high level of accuracy in the holistic model, the process unit models have to be formulated using property-based representations. For instance, detailed

reaction kinetics and rigorous vapour-liquid-equilibrium data in distillation should be included.

2. **Develop a holistic approach to solve the site-wide supply chain model.**

   According to the literature review, a direct optimisation technique should be the best way to exploit benefits from a holistic supply chain model. However, limitations on the technology may obstruct the application of direct optimisation. It is therefore fundamental to develop techniques to overcome the obstacles and optimise the site-wide supply chain model in a holistic approach.

3. **Verify the significance of the holistic approach.**

   As the holistic approach is newly developed in the thesis, its performance should be compared with other solution approaches, such as decomposition and simplification. This verifies whether the holistic approach is truly the most promising method among other available approaches.

3 Ethylene Process Description and Modelling

3.1 Introduction

The thesis aims to explore different site-wide supply chain optimisation approaches for continuous processes. It is essential to define a study example before any approach can be examined. Ethylene production is a technically well-known and economically vital process. It is thus chosen as the example, and it is employed throughout the thesis. In this chapter, the reasons for selecting the ethylene process are presented. The chapter also provides a general background on a typical ethylene process. Finally, the chapter describes the example processes used in the research and explains the model formulations of the process units.

3.2 Reasons for Selecting the Ethylene Process

3.2.1 Technical Reason

Ethylene is the lightest olefin and has the chemical formula, $H_2C{=}CH_2$. Its double bond gives it a relatively high reactivity. It is involved in a variety of reactions including polymerisation, oxidation, halogenation and alkylation (Kniel *et al.*, 1980). This makes ethylene a basic raw material of many petrochemicals, such as polyethylene, ethylbenzene, ethylene oxide and ethylene dichloride (Figure 3.1) (Anon, ca. 2006). Most of the ethylene derivatives contribute to manufacture other polymers (Speight, 2002).

As ethylene is such a vital raw material, chemical engineers have spent a lot of time to study and improve the production process over past decades. Steam cracking followed by a distillation sequence has eventually emerged as the most

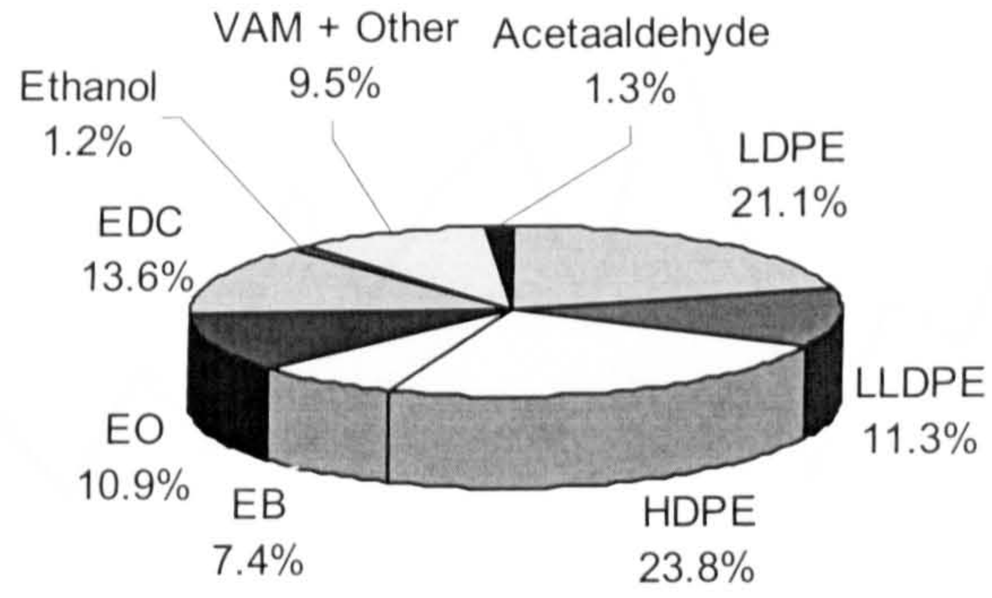

Figure 3.1: Western European ethylene consumptions by derivatives in 2005.

common ethylene production method. It has also become one of the most familiar continuous processes to chemical engineers. The cracking reaction kinetics and the distillation theory have been well documented in the literature. This makes rigorous models for the ethylene process possible without further studies on the reactions and distillations. This leads to a useful starting point for constructing the supply chain model based on those rigorous process representations. The ethylene production process is hence a good technical example for the study of a continuous process supply chain optimisation.

3.2.2 Economic Reason

Due to the important role of ethylene in commodity polymer manufacturing, the ethylene market is severely influenced by the global economic situation. Between 2000 and 2001, the global economic downturn decelerated the ethylene demand growth. Some petrochemical companies shut down their plants in response to the weak market at the time. In 2004-2005, the global economy started to recover and

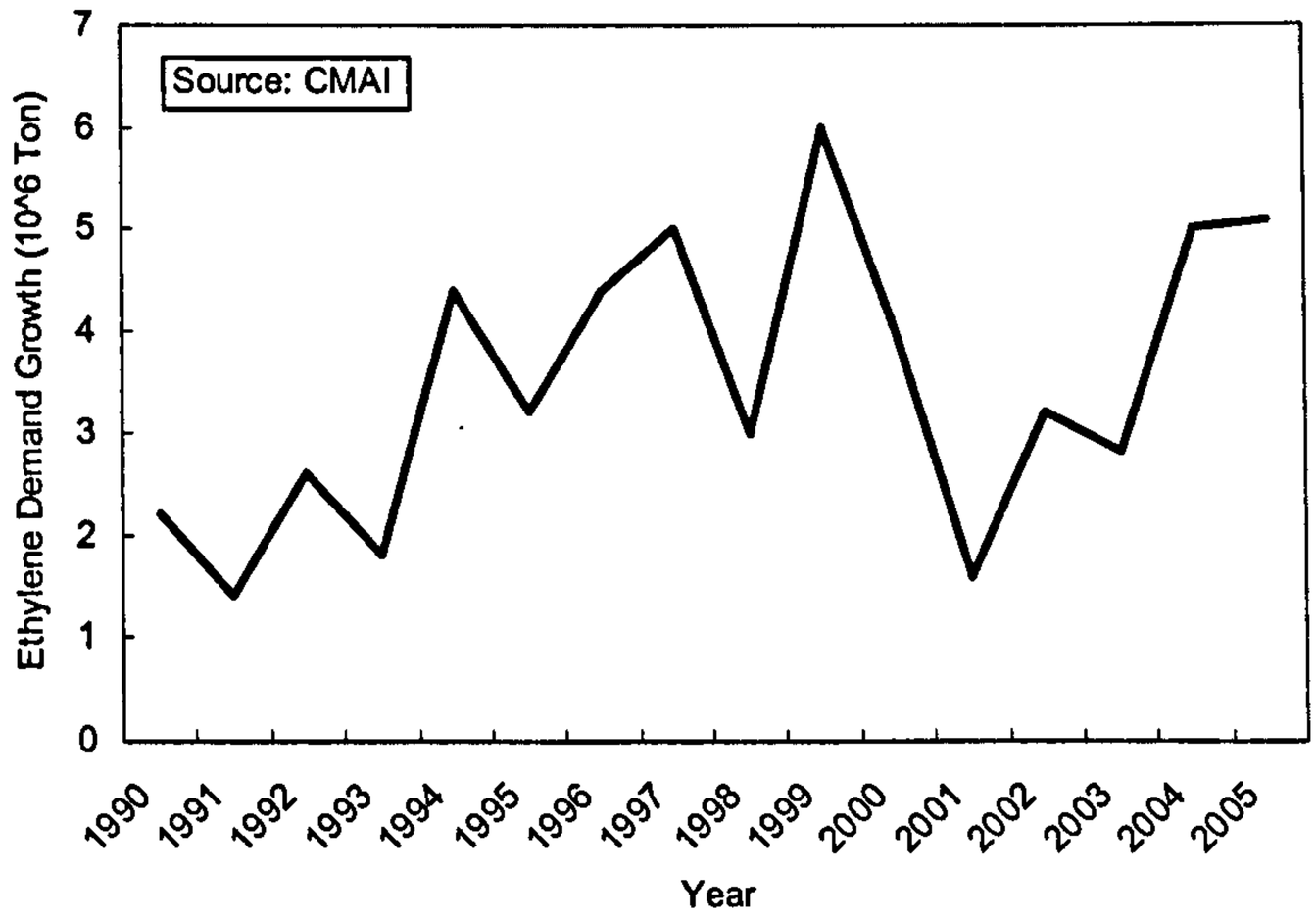

Figure 3.2: Global ethylene demand growth (1990-2005).

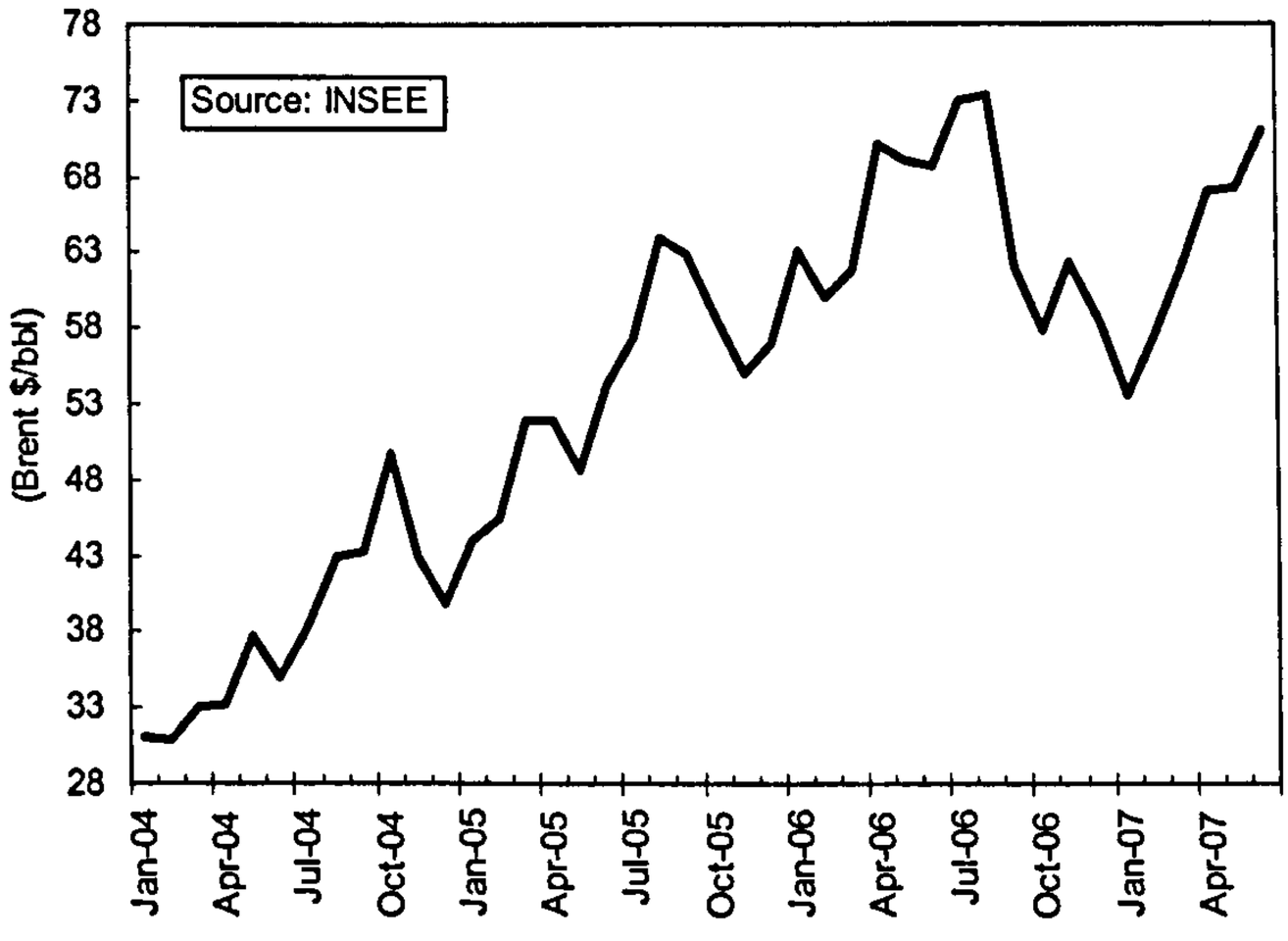

Figure 3.3: Brent oil price trend (January-2004 to April-2007).

the ethylene demand growth rose again (Figure 3.2) (Brown, 2005). Some analysts predicted that the ethylene demand growth would be 4-5% per year (CMAI, 2006) and the trend would hold until 2011 (Anon, 2007). This encouraged the petrochemical companies to restart their idle plants and invest in new capacity (Sim,

2005). The ethylene market has become very competitive once again.

The current high crude oil price (Figure 3.3) (Hadhri & Weigel, 2007), however, brings uncertainties to the market. Global economic growth and ethylene demand growth might slow down. Expensive crude oil also hints at a high raw material price for the ethylene production. This will result in a slim ethylene profit margin.

In order to survive in the highly competitive and low profit margin market, ethylene plants have to improve their profitability in all possible ways. Effective supply chain management is an inevitable element for achieving the task. This indicates that ethylene production is also a good economic example in the study.

3.3 Ethylene Production Process

3.3.1 General Process Description

Ethylene can be produced from a wide range of feedstocks, for example, ethane, propane, naphtha and gas oil. The possible manufacturing routes include catalytic pyrolysis, ethane dehydrogenation with a membrane reactor, and coal gasification followed by Fischer-Tropsch process (Sundaram *et al.*, 2001). However, the choices above are not generally economically viable. The conventional industrial practice for ethylene production is in fact steam cracking without catalysts. The process also produces valuable by-products like propylene and butadiene.

Steam cracking refers to a hydrocarbon feedstock being chemically cracked in the present of steam at a very high temperature. The steam serves as a coking inhibitor inside the reactor and an enhancer for high ethylene selectivity. A variety of steam cracking processes have been commercialised for ethylene production (Anon, 2003). Although they are designed for different feedstocks and various

advantages, they share the same basic features. They are basically divided into two parts, the hot side and the cold side.

The overall process starts at the hot side, and the steam cracking reactor is the main component there. The feedstock and the steam are fed into the reactor and processed at a high temperature. The reactor inlet temperature and the outlet temperature can vary from 850 K to 950 K and from 1050 K to 1200 K respectively (Moulijn *et al.*, 2001). The dilution ratio between the steam and the hydrocarbon feedstock varies between 0.3 and 0.9 kg-steam per kg-hydrocarbons, which is proportional to the feedstock molecular weight (Speight, 2002). After the cracking reaction, water is directly added to quench the cracker effluent. It stops further cracking in order to maintain the ethylene selectivity. The stream leaving the quench tower is immediately compressed. Besides ethylene, undesired acid gas can also be found in the reactor effluent due to impurities in the raw material. It should be removed from the process stream to enhance final product purity as well as to prevent corrosion of downstream equipment. The cleaned and compressed process stream then passes through a sequence of drying and cooling. The stream is finally ready for the cold side, the distillation system.

The distillation system contains several columns to recover individual products. The number of columns depends on the product specifications. Due to the very light components (e.g. hydrogen and methane), the distillations operate at relatively low temperatures and are described as the cold side of the process. The basic distillation trains in the ethylene process consist of five columns. The first column is the demethaniser, which removes hydrogen and methane from the main hydrocarbons stream. The second column is the deethaniser, which picks up the

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bottom stream from the demethaniser and separates C2 components (ethane, ethylene) from other hydrocarbons. The C2 components are then recovered as the main product ethylene and the recycle ethane in the third column, the C2 splitter. The fourth column, the depropaniser, takes the hydrocarbons stream and removes the C3 components (propane, propylene). The C3 components are further split into the product propylene and the recycle propane in the fifth column, the C3 splitter. If the C4 product is desirable, a debutaniser column can be placed after the depropaniser for the separation of the C4 and the pyrolysis gasoline. A diagram of the general ethylene process is shown in Figure 3.4.

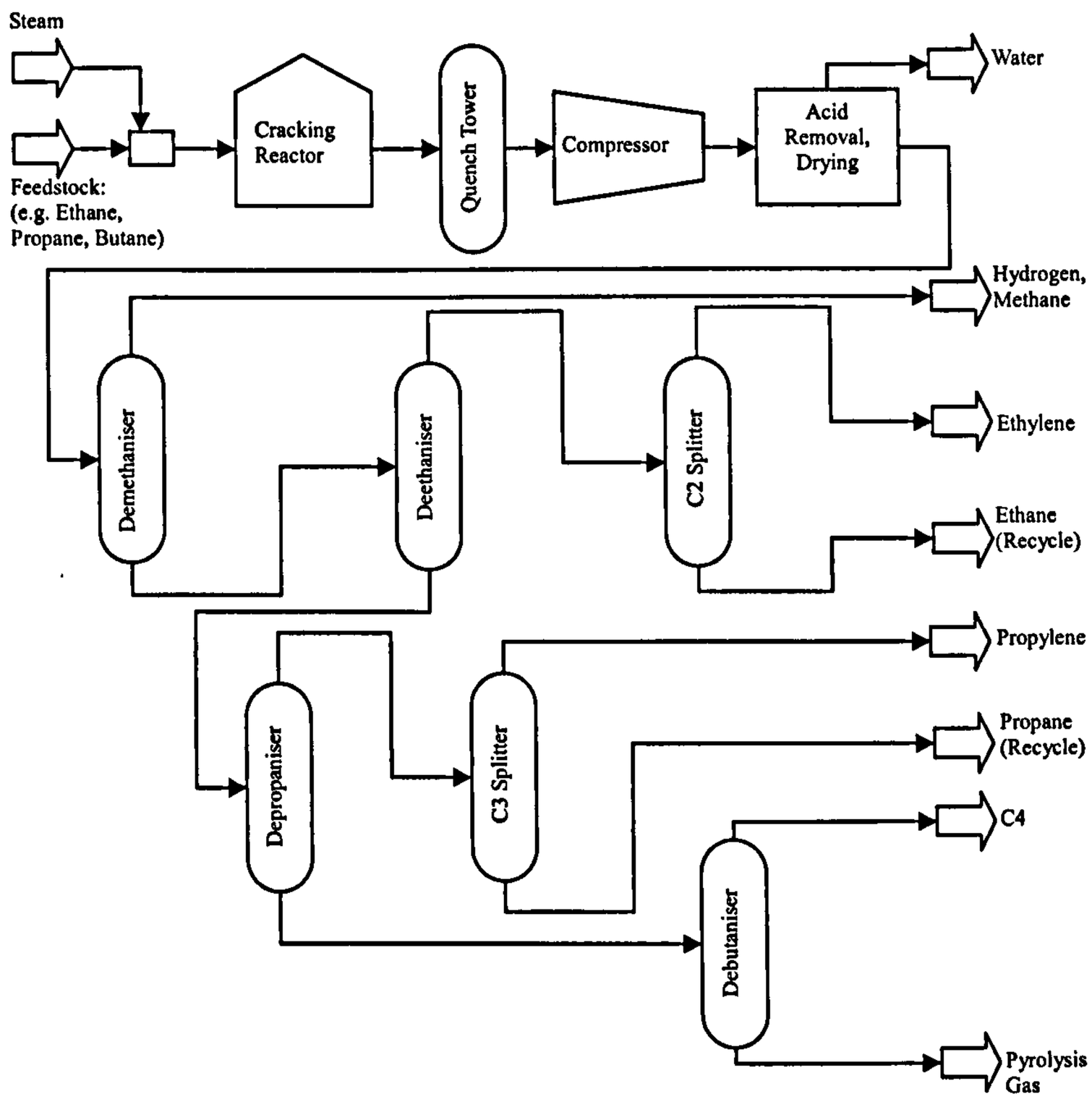

Figure 3.4: General ethylene production process.

3.3.2 Example Process Description

Using rigorous property-based representations in the site-wide supply chain optimisation is the main objective of this research. The details of the process are not the first concern in model building. Instead, the rigour of the process unit models is more important. As long as the major process components are modelled rigorously, some process simplifications should not affect the research results.

Two simplified example processes based on the general description are designed for the case studies in the following chapters of the thesis. The cracking reaction and the distillation are the two major operations in the whole process. Hence, both the example processes have detailed models for these steps. The simplifications only occur in between the two major operations. The quench tower is replaced by a quench cooler. The presence of the acid gas is ignored in the process stream as the assumption of clean raw material is made. The drying process is simulated via a black box model.

With sharing the same process simplifications, the only difference between the two processes is the number of distillation columns. The first process has three columns, the demethaniser, the deethaniser and the C2 splitter (Figure 3.5). It recovers ethylene as the only main product. The C3+ chemicals are only grouped as a single by-product. This process is only used in Chapter 4 for the single-site single-period study, the simplest form of the site-wide optimisation. The second process has five columns in total (Figure 3.6). It adopts two more columns, the depropaniser and the C3 splitter, to recover ethylene as well as propylene. The C4+ chemicals are also treated as a valuable product. This enables the supply chain model to model multiple products better. The process is used after Chapter 4.

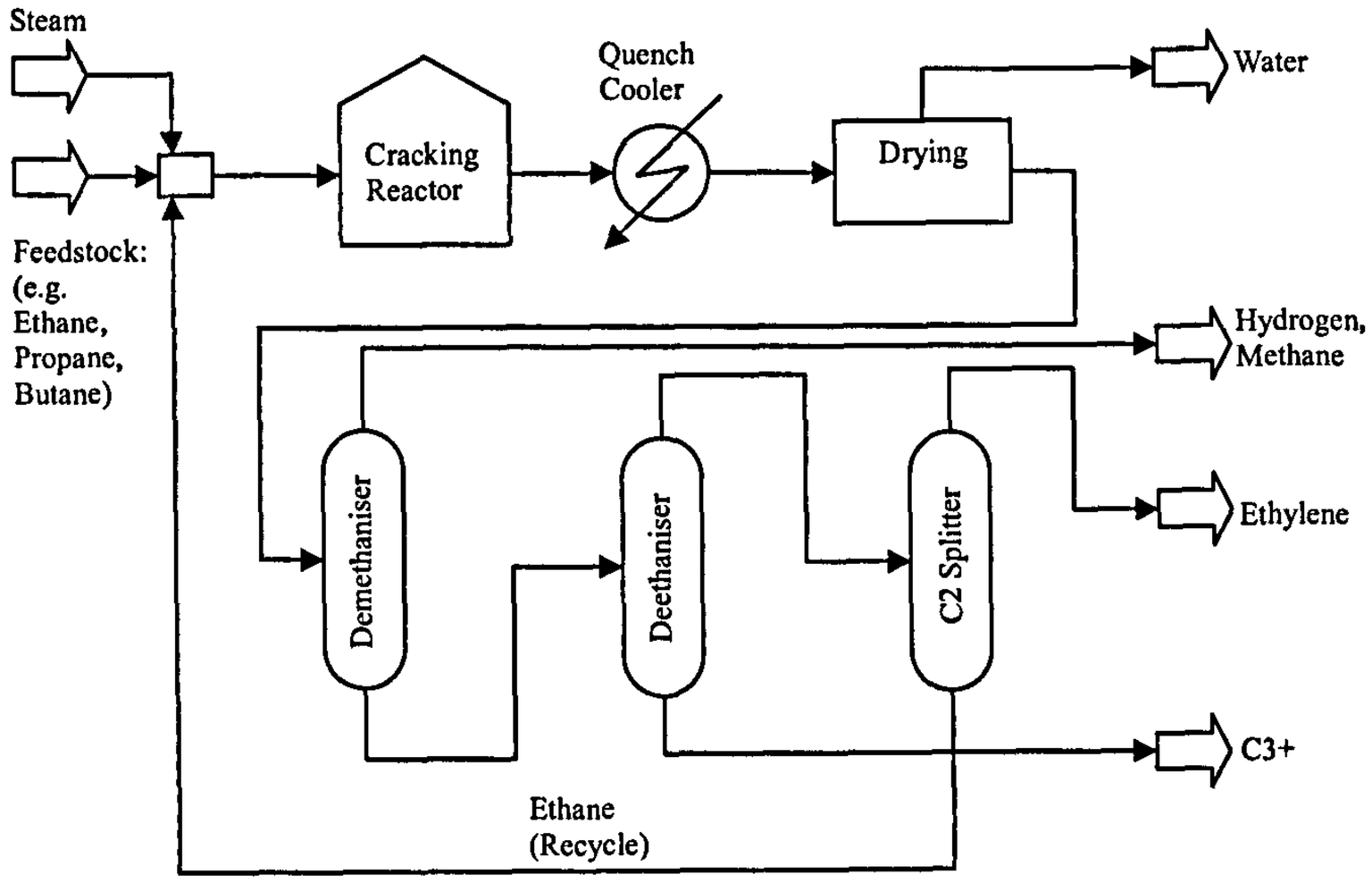

Figure 3.5: 3-Column ethylene process.

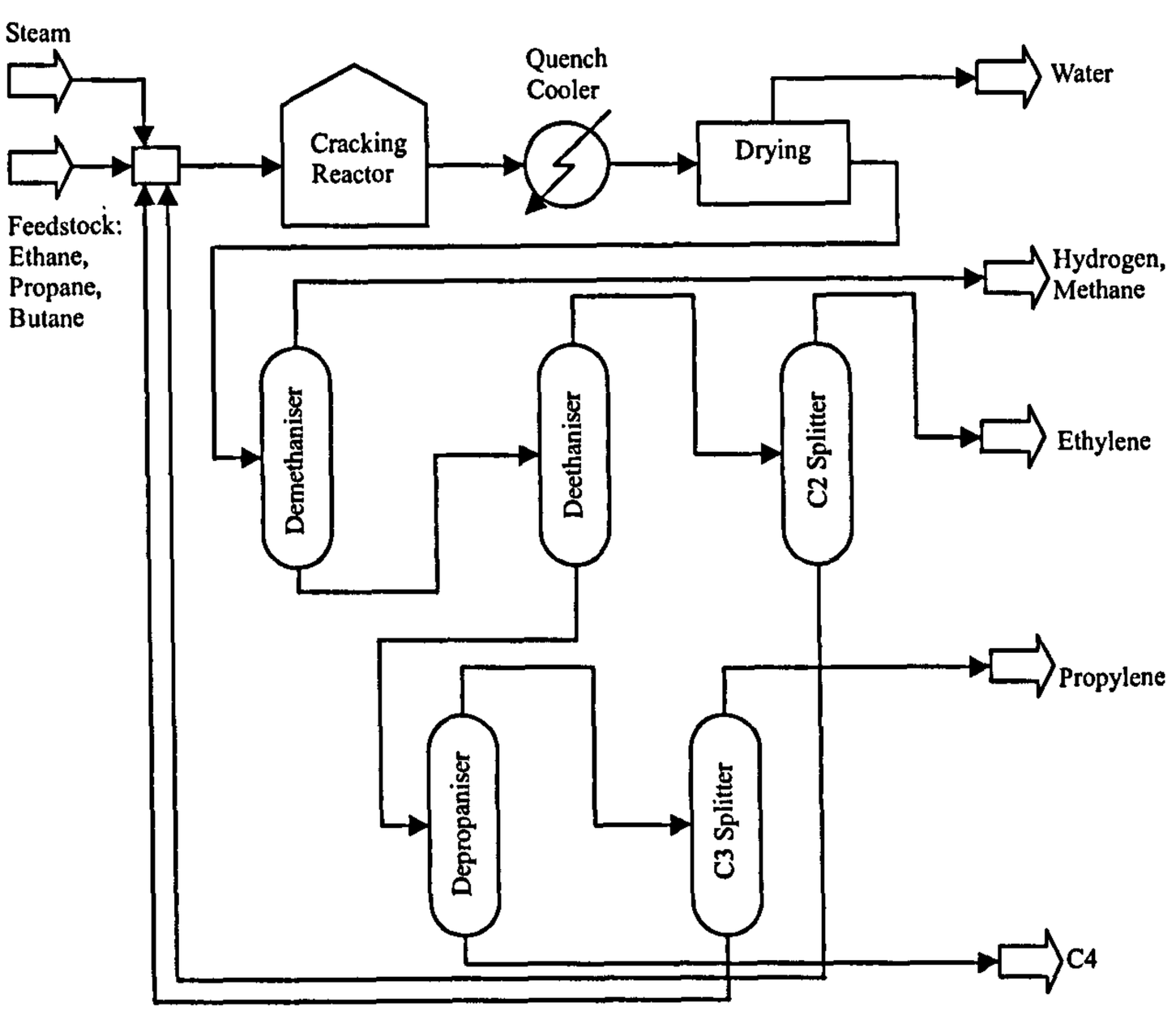

Figure 3.6: 5-Column ethylene process.

3.4 Process Units Modelling

Based on the example processes described in the previous section, there are five different types of units. They are the mixer, the cracking reactor, the quench cooler, the drying black box and the distillation column. The reactor and the distillation column are modelled using detailed physical property-based representations. The others are only simplified models; they also follow the basic material balances. Once the unit models are ready, they can be connected to form the site-wide model of the process. In the thesis, the unit models are built using the software package gPROMS (PSE, 2008). It also helps in integrating the site-wide model through its hierarchical modelling structure. All the process unit operations are assumed to be at a steady-state, so, the site-wide model is also a steady-state model. Problems with time consideration, like inventory control, can be tackled by casting the steady-state model into a multi-period framework. The key formulations of the individual process units are presented below.

3.4.1 Mixer Model

The mixer is used to mix different feed streams and recycle streams together, and feed the mixed stream to the reactor. This characteristic is simply carried out by the mass balance equations.

Stream Component Mass Balance:

$$\sum_{s} Fin_{s,i} = Fout_{i} \qquad \text{(Eq. 3.1)}$$

Total Inlet/Outlet Mass Flowrates:

$$TFin_s = \sum_i Fin_{s,i} \qquad \text{(Eq. 3.2)}$$

$$TFout = \sum_i Fout_i \qquad \text{(Eq. 3.3)}$$

where

i	=	Chemical component index.
s	=	Inlet stream index of the mixer.
$Fin_{s,i}$	=	Component i mass flowrate in inlet stream s (kg/s).
$Fout_i$	=	Component i mass flowrate in outlet stream (kg/s).
$TFin_s$	=	Total mass flowrate of inlet stream s (kg/s).
$TFout$	=	Total mass flowrate of outlet stream (kg/s)

3.4.2 Steam Cracking Reactor Model

The steam cracking process takes place inside a tubular furnace. The furnace accommodates several parallel reactor tubes. To save some computational effort, the reactor model only formulates a single reactor tube. In order to match the flowrate in the main process stream, the tube inlet and outlet flowrates are scaled according to the number of the tubes.

The mathematical model of the steam cracking process mainly involves three types of differential equations along the tube. They are the energy balance equation, the pressure balance equation and the continuity equations for the reaction components (Froment, 1992). The energy balance equation handles the heat flux (Q_{rxn}) applied by the cracking furnace. The pressure balance equation deals with

the reactor tube pressure drop, which is caused by the tube wall friction. The continuity equations take care of the material balances based on the reaction kinetics.

Energy Balance Equation:

$$\frac{dH}{dz} = Q_{rxn} \cdot \pi \cdot Dia \qquad \text{(Eq. 3.4)}$$

Pressure Balance Equation:

$$-\frac{dP}{dz} = \frac{4 \cdot fr \cdot v^2 \cdot \overline{\rho}}{2 \cdot Dia} \qquad \text{(Eq. 3.5)}$$

Continuity Equations:

$$\frac{dF_i}{dz} = \pi \cdot \frac{Dia^2}{4} \cdot \sum_j (\eta_{ij} \cdot r_j) \qquad \text{(Eq. 3.6)}$$

where

i	=	Chemical component index
j	=	Reaction index
η_{ij}	=	Reaction stoichiometric coefficients
$\overline{\rho}$	=	Mass density (kg/m^3)
Dia	=	Diameter of the reactor tube (m)
F_i	=	Component i molar flowrate (mol/s)
fr	=	Friction factor, $fr = 0.092/Re^{0.2} \cdot Dia$
H	=	Energy in the reactor tube (J/s)
P	=	Pressure inside the reactor tube

Q_{rxn} = Heat flux to the reactor tube (J/m^2-s)

Re = Reynolds number

r_j = Rate of reaction j (sec or m^3/mol-s)

v = Process gas velocity (m/s)

z = Axial coordinate of the reactor tube (m)

The reaction kinetics (the stoichiometric coefficients η_{ij} and the reaction rates r_j) are available from various literature studies (Froment, 1981; Joo *et al.*, 2001; Belohlav *et al.*, 2003). The thesis has employed a molecular reaction kinetic scheme, which is modified from (Sundaram & Froment, 1977a, b). The scheme can manage ethane, propane, *n*-butane, *iso*-butane and their mixtures as the feedstock. There are a total of 16 species (Table 3.1) and 22 reactions (Table 3.2) in the scheme. Their corresponding reaction rate equations are given in Table 3.3. Physical properties involved in the model (e.g. heat of formation, enthalpy) are calculated by the gPROMS built-in physical property subroutine (IPPFO) in order to minimise the model complexity.

Table 3.1: Chemical components in the reaction scheme.

No.	Chemical		No.	Chemical	
1.	Hydrogen	(H_2)	9.	Propane	(C_3H_8)
2.	Methane	(CH_4)	10.	1,3-Butadiene	(C_4H_6)
3.	Water	(H_2O)	11.	1-Butene	(1-C_4H_8)
4.	Acetylene	(C_2H_2)	12.	*iso*-Butene	(*iso*-C_4H_8)
5.	Ethylene	(C_2H_4)	13.	*trans*-2-Butene	(*trans*-2-C_4H_8)
6.	Ethane	(C_2H_6)	14.	*n*-Butane	(*n*-C_4H_{10})
7.	Methyl Acetylene	(C_3H_4)	15.	*iso*-Butane	(*iso*-C_4H_{10})
8.	Propylene	(C_3H_6)	16.	C_6	

Table 3.2: Steam cracking reaction scheme.

No.	Reaction	Arrhenius' Constant	Activation Energy (J/mol)
1.	$C_2H_6 \leftrightarrow C_2H_4 + H_2$	4.652E+13	273021.23
2.	$2C_2H_6 \rightarrow C_3H_8 + CH_4$	3.750E+12	273188.70
3.	$C_3H_6 \leftrightarrow C_2H_2 + CH_4$	3.794E+11	248654.05
4.	$C_2H_2 + C_2H_4 \rightarrow C_4H_6$	1.026E+09	172747.37
5.	$C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$	7.083E+10	253008.32
6.	$C_3H_8 \rightarrow C_2H_4 + CH_4$	4.692E+10	211852.08
7.	$C_3H_8 \leftrightarrow C_3H_6 + H_2$	5.888E+10	214740.97
8.	$C_3H_8 + C_2H_4 \rightarrow C_2H_6 + C_3H_6$	2.536E+10	247272.41
9.	$2C_3H_6 \rightarrow 3C_2H_4$	1.514E+11	233623.44
10.	$2C_3H_6 \rightarrow 0.5C_6 + 3CH_4$	1.423E+09	190499.40
11.	$C_3H_6 + C_2H_6 \rightarrow 1\text{-}C_4H_8 + CH_4$	1.000E+11	251249.87
12.	*iso*-$C_4H_{10} \leftrightarrow$ *iso*-$C_4H_8 + H_2$	3.046E+11	227761.92
13.	*iso*-$C_4H_{10} \rightarrow C_3H_6 + CH_4$	5.000E+11	227887.52
14.	*iso*-$C_4H_{10} + C_2H_4 \rightarrow$ *trans*-2-$C_4H_8 + C_2H_6$	7.320E+05	126608.83
15.	$C_3H_6 + H_2 \rightarrow C_2H_4 + CH_4$	5.770E+06	146538.00
16.	*iso*-$C_4H_8 \rightarrow C_3H_4 + CH_4$	6.374E+15	309823.20
17.	$C_3H_4 \rightarrow 0.5C_6 + 2H_2$	3.504E+04	60708.60
18.	*n*-$C_4H_{10} \rightarrow C_3H_6 + CH_4$	7.000E+13	249700.75
19.	*n*-$C_4H_{10} \rightarrow 2C_2H_4 + H_2$	7.000E+14	295923.02
20.	1-$C_4H_8 \rightarrow (2/3)C_6 + 4H_2$	7.685E+06	124934.11
21.	*n*-$C_4H_{10} \rightarrow C_2H_4 + C_2H_6$	4.099E+12	256692.71
22.	*n*-$C_4H_{10} \leftrightarrow$ 1-$C_4H_8 + H_2$	1.637E+12	261088.85

Table 3.3: Reaction rate equations.

No.	Reaction Rate	No.	Reaction Rate
1.	$r_1 = k_1\left(C_6 - \frac{C_1 C_5}{Keq_1}\right)$	12.	$r_{12} = k_{12}\left(C_{15} - \frac{C_1 C_{12}}{Keq_{12}}\right)$
2.	$r_2 = k_2 C_6$	13.	$r_{13} = k_{13} C_{15}$
3.	$r_3 = k_3\left(C_8 - \frac{C_2 C_4}{Keq_3}\right)$	14.	$r_{14} = k_{14} C_5 C_{15}$
4.	$r_4 = k_4 C_4 C_5$	15.	$r_{15} = k_{15} C_1 C_8$
5.	$r_5 = k_5 C_5 C_6$	16.	$r_{16} = k_{16} C_{12}$
6.	$r_6 = k_6 C_9$	17.	$r_{17} = k_{17} C_7$
7.	$r_7 = k_7\left(C_9 - \frac{C_1 C_8}{Keq_7}\right)$	18.	$r_{18} = k_{18} C_{14}$
8.	$r_8 = k_8 C_5 C_9$	19.	$r_{19} = k_{19} C_{14}$
9.	$r_9 = k_9 C_8$	20.	$r_{20} = k_{20} C_{11}$
10.	$r_{10} = k_{10} C_8$	21.	$r_{21} = k_{21} C_{14}$
11.	$r_{11} = k_{11} C_6 C_8$	22.	$r_{22} = k_{22}\left(C_{14} - \frac{C_1 C_{11}}{Keq_{22}}\right)$

Keq_j = Equilibrium constant of equilibrium reaction j

$$Keq_1 = 5.480\times10^7 \exp\left(-1.364\times10^5/RT\right)$$

$$Keq_3 = 1.910\times10^7 \exp\left(-1.263\times10^5/RT\right)$$

$$Keq_7 = 74\cdot\exp\left(\frac{-\Delta H_{rxn}\left(1/T - 1/1048.15\right)}{R}\right)$$

$$Keq_{12} = 1.110\times10^8 \exp\left(-1.152\times10^5/RT\right)$$

$$Keq_{22} = 9.190\times10^7 \exp\left(-1.259\times10^5/RT\right)$$

r_j = Reaction rate of reaction j (sec or m^3/mol-s)

k_j = Rate constant of reaction j, $k_j = k_{0j}\exp\left(-Ea_j/RT\right)$

k_{0j} = Arrhenius' Constant of reaction j

Ea_j = Activation energy of reaction j (J/mol)

C_i = Concentration of component i (mol/m^3)

R = Gas constant, 8.31447 (J/mol-K)

T = Temperature (K)

$\Delta Hrxn$ = Heat of Reaction 7 (J/mol)

3.4.3 Quench Cooler Model

The cooler is placed after the reactor to cool down the process stream, in order to stop further cracking and maintain high ethylene selectivity. Its cooling duty is calculated by Eq. 3.7.

$$Q_{CW} = \sum_i F_i \cdot \Delta Cp_i (Tin - Tout) \qquad \text{(Eq. 3.7)}$$

where

i	=	Chemical component index.
F_i	=	Component i molar flowrate (mol/s).
ΔCpi	=	Heat capacity of component i (J/mol-K), a polynomial function in terms of temperature.
Q_{CW}	=	Cooling duty of the cooler (J/s).
Tin	=	Process stream inlet temperature (K).
$Tout$	=	Process stream outlet (target) temperature (K).

3.4.4 Drying Black Box Model

The black box after the cooler is used to simulate the drying process. The water in the process stream is removed according to a user-defined input parameter. The quantities of other components are kept unchanged.

Black Box Main Outlet Component Flowrates:

$$Fout_{i\neq water} = Fin_{i\neq water} \quad \text{(Eq. 3.8)}$$

$$Fout_{i=water} = Fin_{i=water} \times (1 - Df) \quad \text{(Eq. 3.9)}$$

Black Box Water Outlet Flowrate:

$$WFout = Fin_{i=water} \times Df \quad \text{(Eq. 3.10)}$$

where

i	=	Chemical component index.
Df	=	Water removal fraction ($0 \leq Df \leq 1$).
Fin_i	=	Component i inlet mass flowrate (kg/s).
$Fout_i$	=	Component i mass flowrate in the main outlet (kg/s).
$WFout$	=	Water flowrate in the water outlet (kg/s).

3.4.5 Distillation Model

A general distillation model class is built for all columns in the process. The model adopts a rigorous approach, which tackles the distillation calculation stage by stage (Wankat, 1988). With suitable input parameters (e.g. number of stages, feed temperature, feed pressure, reflux and boil-up ratios), the model should be able to satisfy different distillation duties in the process and characterise the product streams. The major equations are shown from Eq. 3.11 to Eq. 3.22. The physical properties involved, like enthalpies (H^{liq}, H^{vap}) and equilibrium K values, are provided by the subroutine IPPFO in gPROMS.

Internal Material Balance Equations:

Feed Stage: $$Fz_i + L_{Nf-1}x_{i,Nf-1} + V_{Nf+1}y_{Nf+1} = L_{Nf}x_{i,Nf} + V_{Nf}y_{i,Nf} \quad \text{(Eq. 3.11)}$$

Other Stages: $$L_{k-1}x_{i,k-1} + V_{k+1}y_{i,k+1} = L_k x_{i,k} + V_k y_{i,k} \quad \text{(Eq. 3.12)}$$

External Material Balance Equations:

Each Component: $$Fz_i = Dy_{i,distillate} + Bx_{i,bottom} \quad \text{(Eq. 3.13)}$$

Reflux Ratio: $$R = L_1/D \quad \text{(Eq. 3.14)}$$

Boil-up Ratio: $$Bup = V_N/B \quad \text{(Eq. 3.15)}$$

Mole Fraction Summations:

Vapour: $$\sum_i y_{i,k} = 1 \quad \text{(Eq. 3.16)}$$

Liquid: $$\sum_i x_{i,k} = 1 \quad \text{(Eq. 3.17)}$$

Energy Balance Equations:

Feed Stage: $$F \cdot H_{Feed} + L_{Nf-1}H_{Nf-1}^{Liq} + V_{Nf+1}H_{Nf+1}^{Vap} = L_{Nf}H_{Nf}^{Liq} + V_{Nf}H_{Nf}^{Vap} \quad \text{(Eq. 3.18)}$$

Partial Condenser: $$L_1H_1^{Liq} + V_1H_1^{Vap} = V_2H_2^{Vap} + Qc \quad \text{(Eq. 3.19)}$$

Partial Reboiler: $$L_{N+1}H_{N+1}^{Liq} + V_{N+1}H_{N+1}^{Vap} = V_NH_N^{Vap} + Qr \quad \text{(Eq. 3.20)}$$

Other Stages: $$L_{k-1}H_{k-1}^{Liq} + V_{k+1}H_{k+1}^{Vap} = L_kH_k^{Liq} + V_kH_k^{Vap} \quad \text{(Eq. 3.21)}$$

Equilibrium Equations:

$$y_{i,k} = x_{i,k}K_{i,k} \quad \text{(Eq. 3.22)}$$

where

i	=	Chemical component index
k	=	Column stage index (1 = condenser, N = Reboiler)
Bup	=	Column Boilup Ratio
B	=	Column bottom flowrate (mol/s)
D	=	Column distillate flowrate (mol/s)
F	=	Column feed flowrate (mol/s)
H_{Feed}	=	Column feed enthalpy (J/mol)
H_k^{Liq}	=	Total liquid enthalpy at stage k (J/mol)
H_k^{Vap}	=	Total vapour enthalpy at stage k (J/mol)
$K_{i,k}$	=	Equilibrium K constant of component i at stage k
L_k	=	Column liquid flowrate at stage k (mol/s)
N	=	Number of stage
Nf	=	Feed stage number
Q_c	=	Condenser duty (J/s)
Q_r	=	Reboiler duty (J/s)
R	=	Column reflux ratio
V_k	=	Column vapour flowrate at stage k (mol/s)
$x_{i,k}$	=	Component i liquid mole fraction at stage k
$y_{i,k}$	=	Component i vapour mole fraction at stage k
z_i	=	Component i mole fraction at feed stream.

3.5 Process Model Validation

Validations should be performed to ensure that the models are able to simulate the process as expected. This can be done by simulating different situations using the model to examine whether the model can respond accordingly. As the 5-column process includes the whole 3-column process and two addition columns, only the validation of the 5-column process model is discussed in this section.

To complete the process model, values must be given to the parameters of the process units. These include the reactor dimensions and the numbers of stages of the columns. The values of the parameters will not be changed throughout the validation, and they will also be used in the following chapters of the thesis. The parameters and their values are listed in Table 3.4.

Table 3.4: Unit model parameters.

Parameter	Value	Parameter	Value
Reactor		***Deethaniser***	
Length of reactor tube (m)	60.00	No. of stages	14
Diameter of reactor tube (m)	0.10	Feed stage	7
No. of reactor tube	90		
		C2 Splitter	
Quench Cooler		No. of stages	40
Target temp. (K)	303.15	Feed stage	20
Drying Black Box		***Depropaniser***	
Water removal (%)	99.99	No. of stages	20
		Feed stage	10
Demethaniser			
No. of stages	10	***C3 Splitter***	
Feed stage	5	No. of stages	40
		Feed stage	20

Both the 3-column and 5-column processes are designed to accept three types of feedstock (ethane, propane and butane) in order to produce high purity ethylene. Therefore, three cases each using different raw material combinations are tested in the 5-column process model. The operating conditions of the three cases, reactor heat flux and distillation reflux and boil-up ratios, are also adjusted. This aims to verify that the process model is capable of producing high purity ethylene from all three raw materials. The feedstock flowrates and the process operating conditions of the three cases are shown in Table 3.5.

Table 3.5: Input data of the validation cases.

	Case 1	Case 2	Case 3
Ethane feed (kg/s)	12.50	2.50	2.50
Propane feed (kg/s)	2.95	15.00	2.50
Butane feed (kg/s)	2.50	2.50	14.49
Process steam feed (kg/s)	9.12	9.26	9.26
Reactor heat flux ($kJ/m^2/s$)	44.31	39.94	38.49
Demethaniser boil-up	0.96	1.15	3.00
Demethaniser reflux	2.81	2.52	2.24
Deethaniser boil-up	3.00	2.02	1.80
Deethaniser reflux	1.12	0.90	1.12
C2 splitter boil-up	4.44	3.69	3.87
C2 splitter reflux	1.48	1.23	1.29
Depropaniser boil-up	2.02	0.62	2.69
Depropaniser reflux	1.43	0.52	1.22
C3 splitter boil-up	2.72	5.00	5.00
C3 splitter reflux	5.00	3.66	4.44

The cracking reactor is the unit that converts raw materials into products. The chemical compositions at the reactor outlet are directly affected by the raw material choice. Light raw materials (e.g. ethane) should manufacture light products (e.g. ethylene), vice versa. Case 1 uses ethane as its major feedstock. As not too much propane and butane are available in the system, only small amounts of heavy olefins, propylene and butylene, are expected at the reactor outlet. From the Figure 3.7, it is observed that the reactor is able to convert most of ethane into ethylene, and only little propylene and butane are produced as predicted. Propane is the major raw material in Case 2. Although ethylene is still the main product there, more propylene is found at the reactor outlet (Figure 3.8). In Case 3, butane (50% *n*-butane, 50% *i*-butane) is the main fresh feedstock. During the butane cracking, ethane is also formed and un-reacted ethane will be recycled back to the reactor. This makes the actual reactor inlet contain a large portion of ethane. Nevertheless, the butanes still dominate the system and significant amounts of propylene and butylene can be found at the reactor outlet (Figure 3.9). This suggests that both results of Cases 2 and 3 match their raw material choices as it occurs to Case 1.

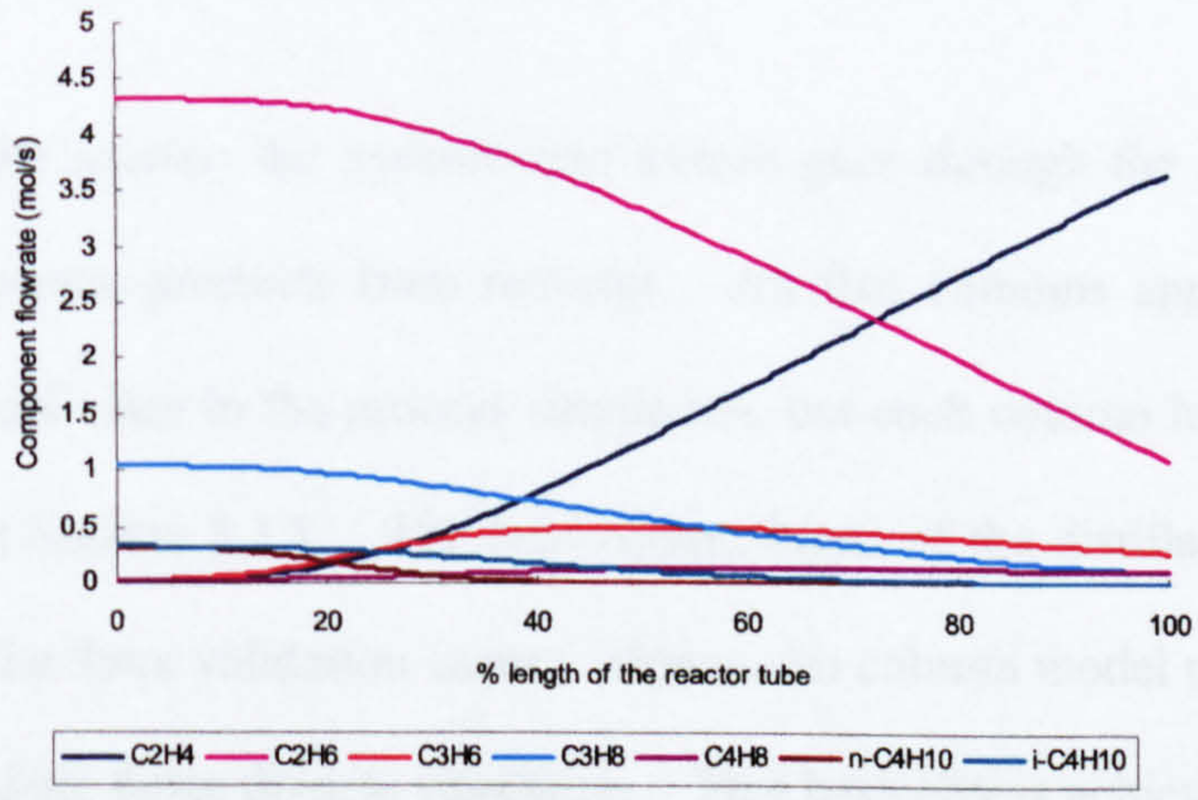

Figure 3.7: Selected component flowrates across a reactor tube in Case 1.

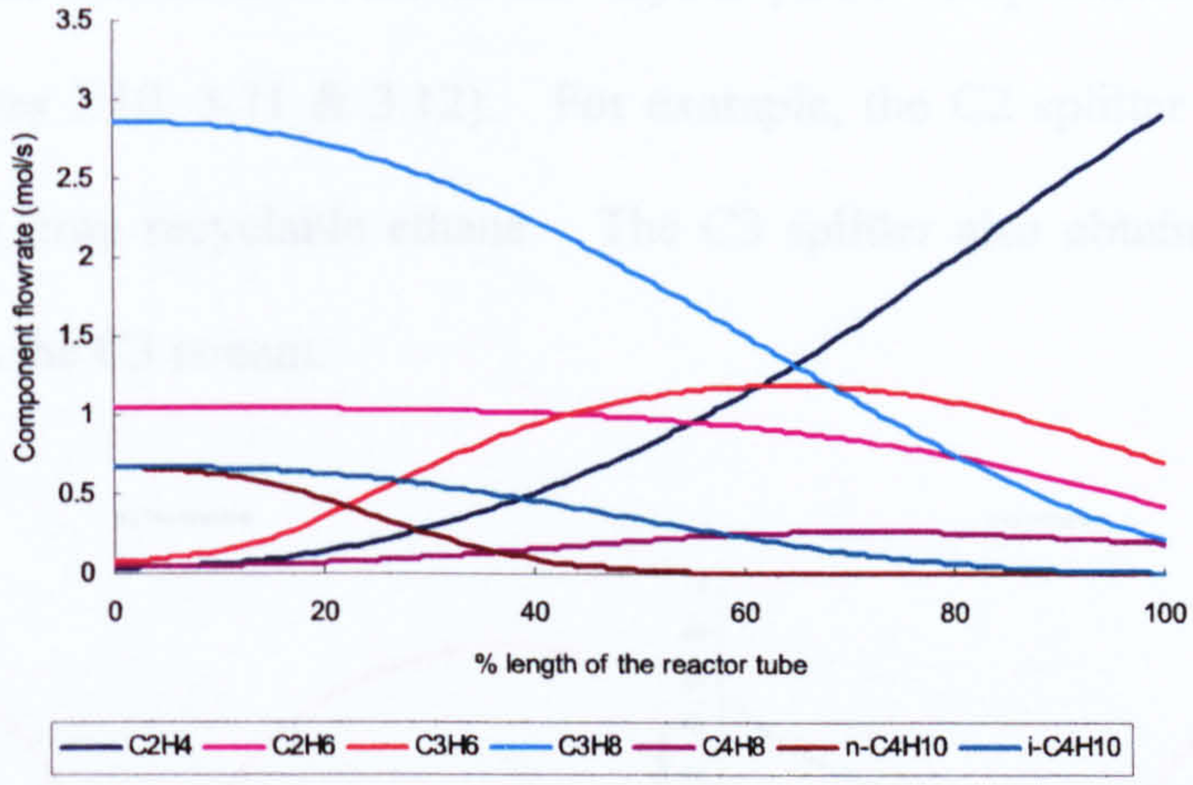

Figure 3.8: Selected component flowrates across a reactor tube in Case 2.

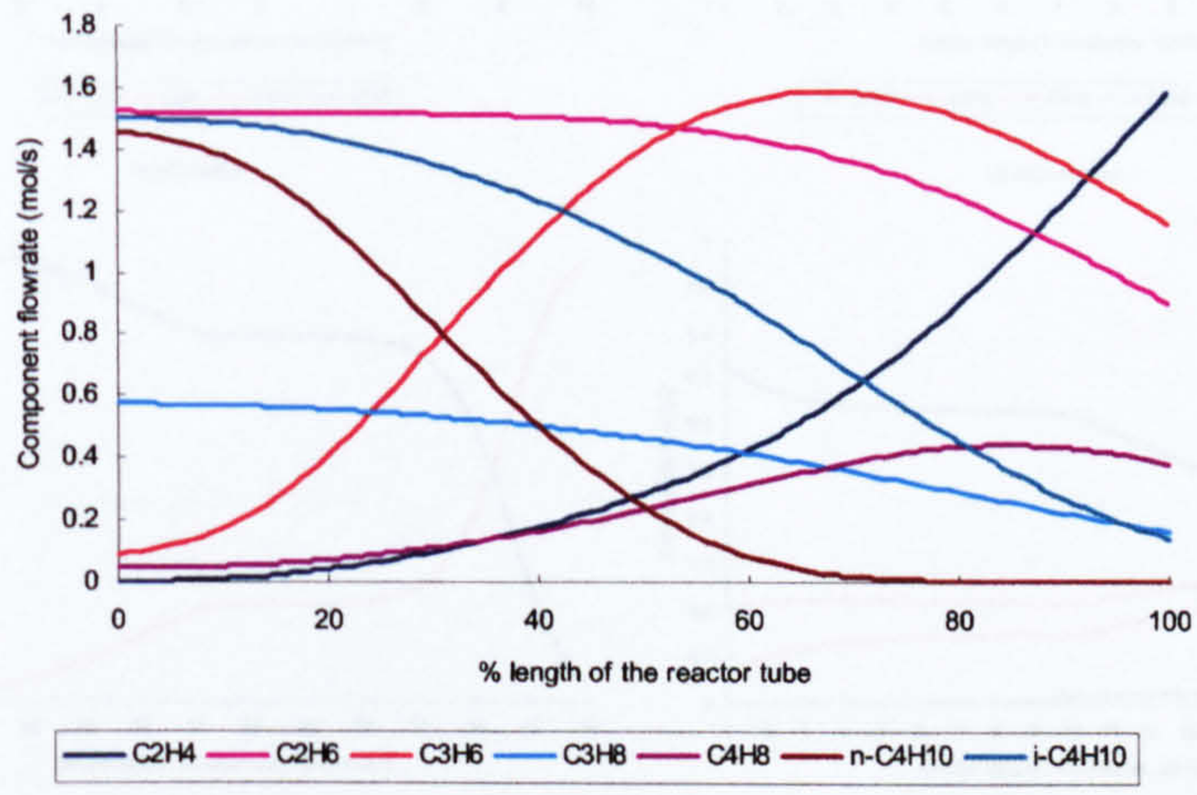

Figure 3.9: Selected component flowrates across a reactor tube in Case 3.

Leaving the reactor, the hydrocarbon stream goes through the five distillation columns to separate products from recycles. All five columns apply an identical distillation model class in the process simulation, but each column has its own duty as described in Section 3.3.1. The feed compositions of the distillation system are also varied in the three validation cases. Hence, the column model must be flexible enough to simulate those diverse situations. This basically is achieved by carefully adjusting the column reflux and boil-up ratios in different cases (Table 3.5). The

successful results can be observed in the vapour phase composition profiles of the columns (Figures 3.10, 3.11 & 3.12). For example, the C2 splitter separates high purity ethylene from recyclable ethane. The C3 splitter also obtains good quality propylene from the C3 stream.

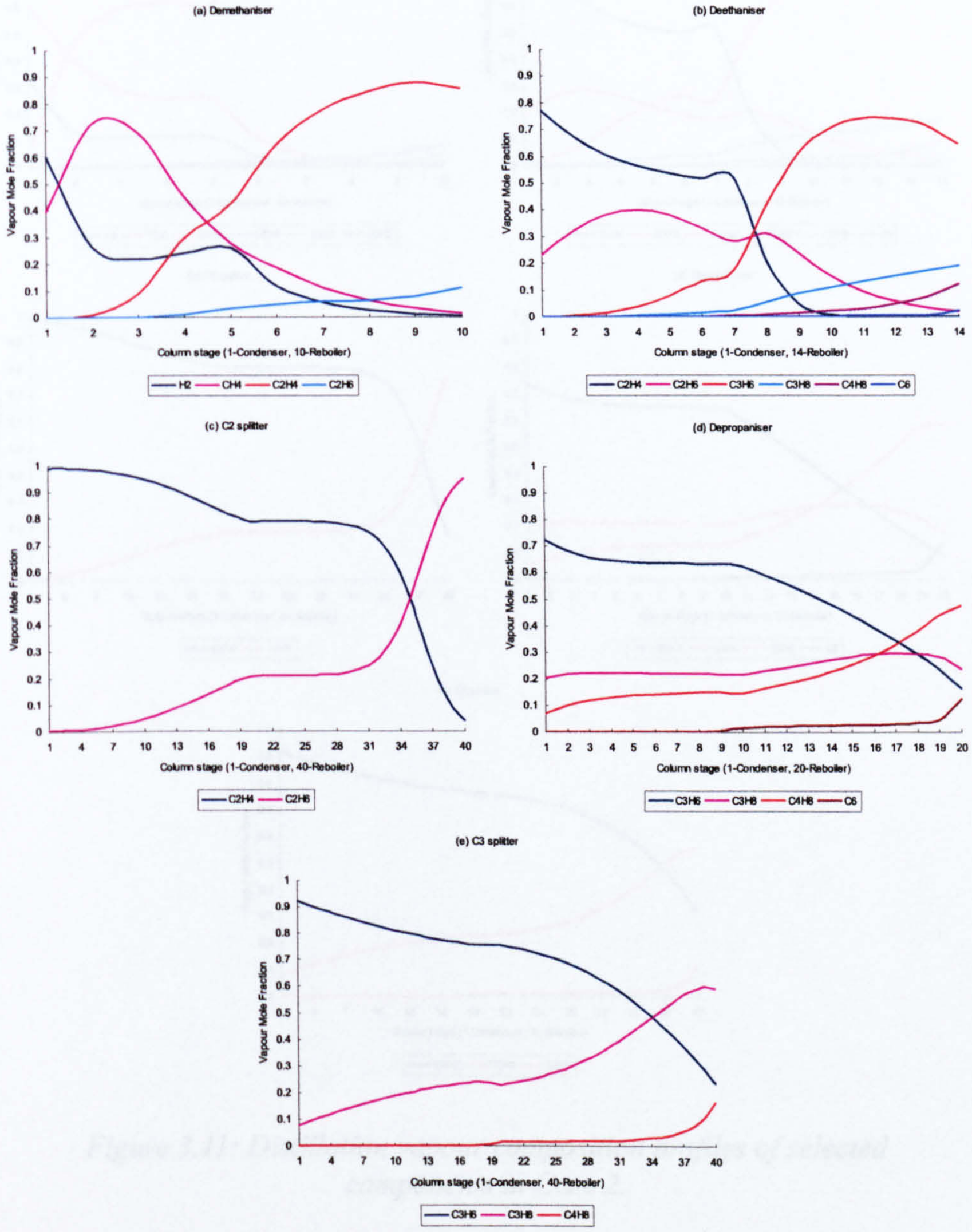

Figure 3.10: Distillation vapour composition profiles of selected components in Case 1.

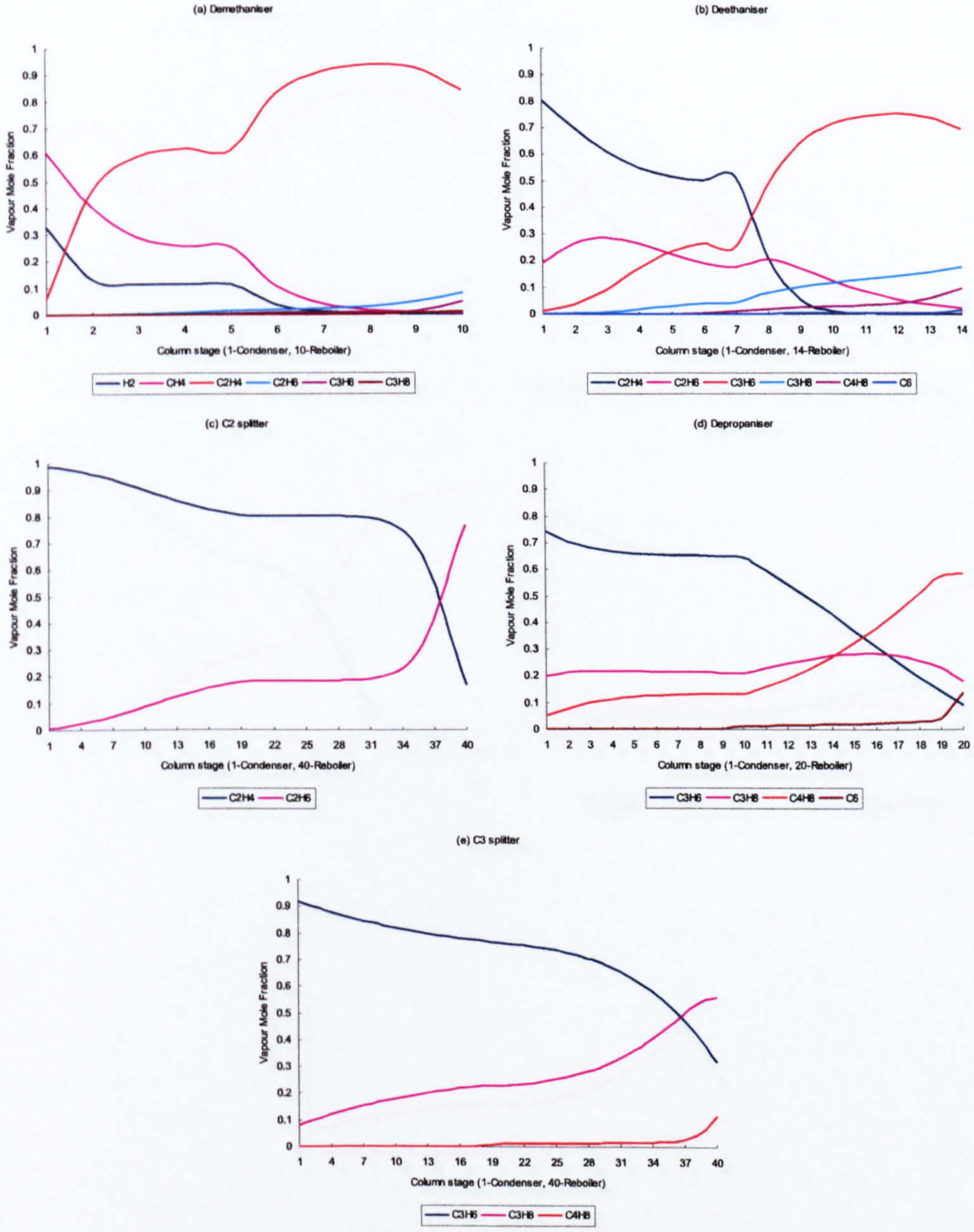

Figure 3.11: Distillation vapour composition profiles of selected components in Case 2.

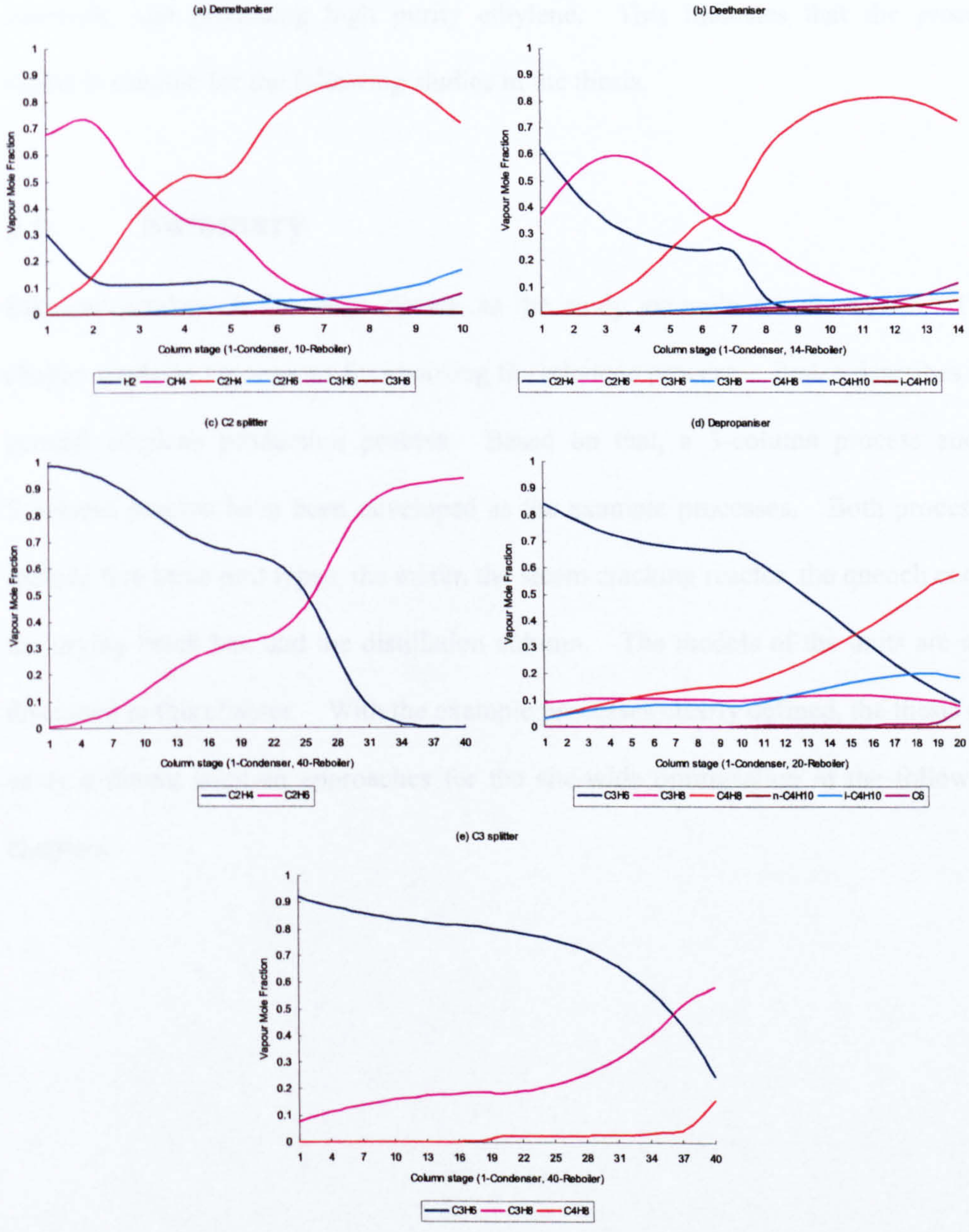

Figure 3.12: Distillation vapour composition profiles of selected components in Case 3.

Based on the validation case results, the reactor model and the column models are found to be reliable on different simulation situations. In general, the process model also fulfils its design criteria; accepting ethane, propane and butane as raw materials, and producing high purity ethylene. This indicates that the process model is suitable for the following studies in the thesis.

3.6 Summary

Ethylene production has been chosen as the study example for the thesis. This chapter explains the reasons for choosing the ethylene process. It also describes the general ethylene production process. Based on that, a 3-column process and a 5-column process have been developed as the example processes. Both processes include five basic unit types; the mixer, the steam cracking reactor, the quench cooler, the drying black box and the distillation column. The models of the units are also discussed in this chapter. With the example processes clearly defined, the thesis can study different solution approaches for the site-wide optimisation in the following chapters.

4 Single-site Single-period Problem

4.1 Introduction

The single-site single-period problem is the simplest form of site-wide optimisation problem. The single-site single-period model is essentially just a process model. It only tackles the operation of a single plant site at a particular time. It does not consider any supply chain information such as inventory control or material flow among different plant sites. Nonetheless, a supply chain model is literally a collection of single-site single-period models. It is hence necessary to understand this type of problem before moving on to more complicated supply chain optimisation.

The simplest form of the site-wide problem is not necessarily easy to solve. The continuous chemical process usually contains several process units. The site-wide optimisation problem aspires to find the optimal of the whole process, instead of optimising individual unit operations. It requires the solution of a large-scale model, which contains all process units. It is recognised that the model will become more difficult to solve as the model size increases. The model complexity is another influence that is proportional to the solution difficulty. Unfortunately, most chemical processes are mathematically nonlinear and complicated. Researchers conventionally reduced the complexity by applying approximate formulations in the site-wide model (Diaz & Bandoni, 1996; Tjoa *et al.*, 1997). The model reliability inevitably depends on the accuracy of the approximation. The benefit from the site-wide optimisation could be negated by the poor approximation. Rigorous property-based unit representations should therefore be used in site-wide optimisation despite the increase in complexity.

This chapter has two goals. First, it explores an effective solution approach for the single-site single-period site-wide optimisation, which involves rigorous unit representations. Second, it decides which solution approach should be used in the following thesis chapters for the more complicated site-wide optimisation problems. The chapter employs the 3-column ethylene process described in Chapter 3 as the basis. Four different solution approaches are examined in the chapter. They are the Simultaneous Approach, Separate Approach, "Base + Delta" Approach, and Hybrid Approach combining Simultaneous and "Base + Delta" approaches. The chapter begins with the problem statement, which is followed by the explanations of the solution approaches. After that, the chapter describes two case studies derived from the 3-column process and uses different approaches to solve them. Their results are also analysed. Finally, conclusions are drawn on the two goals.

4.2 Problem Statement

The problem tackled in this chapter is the single-site single-period optimisation. A chemical plant site with a pre-defined continuous process is given in the problem. The 3-column ethylene process described in Chapter 3 (Figure 4.1) represents the continuous process in this chapter. The problem only considers the plant site operating at steady state over a single time period.

The continuous process contains a number of process units and they are represented by individual model formulations. Rigorous property-based formulations are desirable for the unit models, especially the major process units, because of the anticipated high accuracy. To compose the whole process model, the

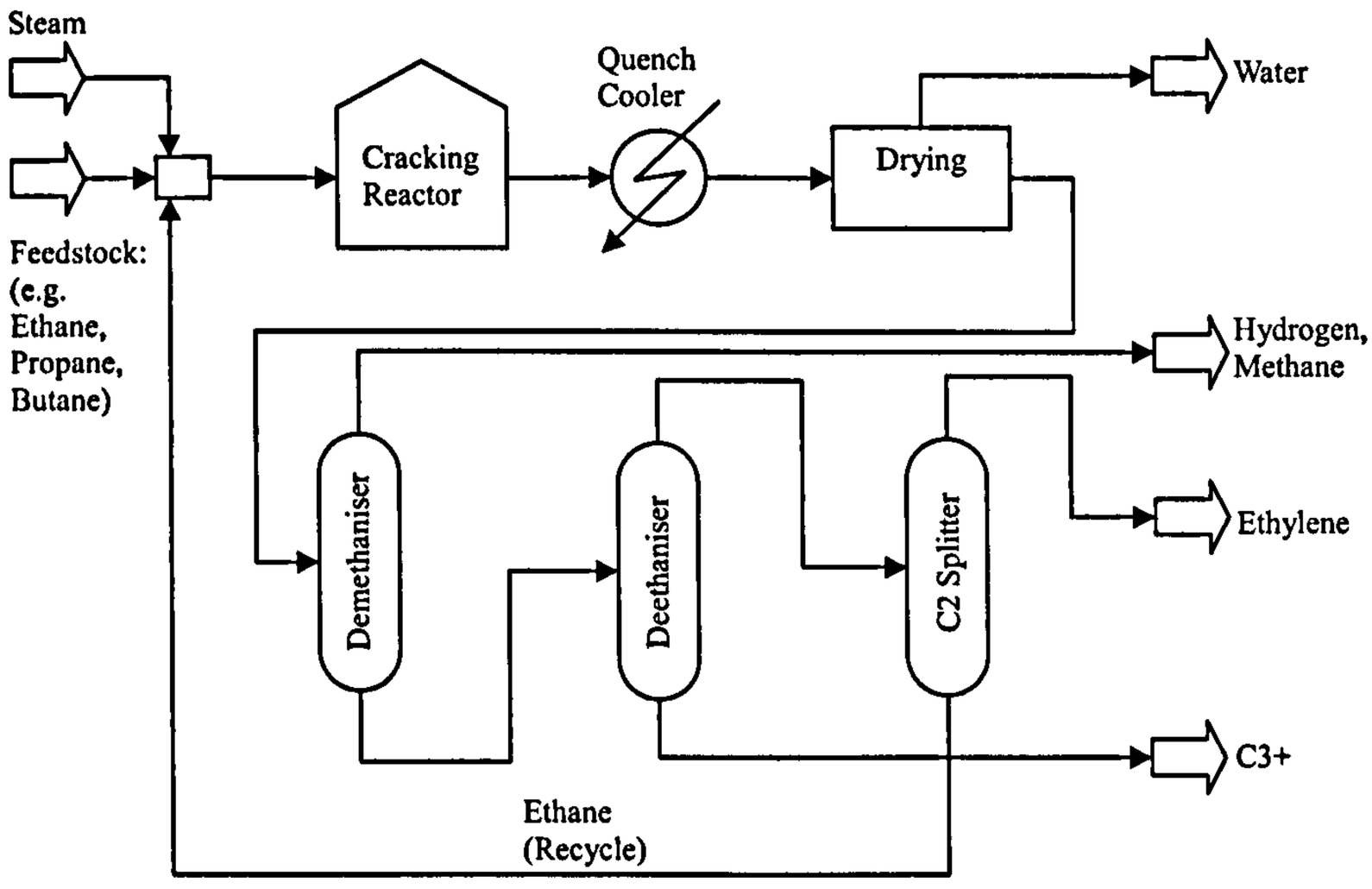

Figure 4.1: 3-Column ethylene process.

unit models are connected according to the process configuration. That configuration would not be changed throughout the problem.

As the overall process model is a collection of unit models, it involves a large number of variables. Not all the variables are in fact directly related to the optimisation. Variables, which are constrained by bounds and/or contribute to the optimisation objective, are counted as the "related" variables. Others are unrelated variables. The related variables are divided into two groups, the input variables (u) and the output variables (y). By placing the unrelated variables in the background, the output variables are apparently controlled by the input variables only. The process model can then be generalised as a set of equations, $y = f(u)$. Also, the objective can be calculated solely by the variables u and y.

The optimisation is basically a nonlinear programming (NLP) problem, as some of the process operations are mathematically nonlinear. The objective of the optimisation is to maximise the plant site's profit within a particular time period by

varying the input variables. In addition, the input and the output variables must lie within their bounds in the final solution. The mathematical representation of the problem is presented below.

Indices:

i	Process model input variable index.
j	Process model output variable index.

Variables:

u_i	Process model input variable.
y_j	Process model output variable.
P	Profit of the plant site.

Parameters:

α_i^u	Price/cost associated with variables u_i.
α_j^y	Price/cost associated with variables y_j.
u_i^{min}	Lower bound of input variable u_i.
u_i^{max}	Upper bound of input variable u_i.
y_j^{min}	Lower bound of output variable y_j.
y_j^{max}	Upper bound of output variable y_j.
I	The total number of input variables.
J	The total number of output variables.
PD	Duration of the time period.

Equations:

f_j Mathematical relations of y_j in terms of $\forall u_i$, both linear and nonlinear.

Objective: Profit

$$\max\left(P = \left(\sum_i \alpha_i^u \cdot u_i + \sum_j \alpha_j^y \cdot y_j\right) \cdot PD\right) \quad \text{(Eq. 4.1)}$$

Subject to: Process model

Eq. 4.2 is a generalisation of the 3-column process model, which is formulated according to the model formulations described in Chapter 3.

$$y_j = f_j(u_1, u_2, u_3, \ldots, u_I) \quad \text{(Eq. 4.2)}$$

$$u_i^{\min} \le u_i \le u_i^{\max} \quad \text{(Eq. 4.3)}$$

$$y_j^{\min} \le y_j \le y_j^{\max} \quad \text{(Eq. 4.4)}$$

4.3 Solution Approaches

The site-wide optimisation problem is very difficult to solve. Although the optimisation only takes account of the input (u) and output (y) variables, the calculations in between the optimisation iterations cannot ignore those unrelated variables. Otherwise, no accurate output variables can be obtained. The computational time of the optimisation is still greatly influenced by the process model size. As the attempted problems include rigorous unit model formulations, the total number of model variables is large. For instance, the 3-column ethylene process model involves more than 26,000 variables. In order to control the

optimisation solution time within an acceptable range, special solution strategies might be required. This chapter investigates four different solution approaches. They are the Simultaneous Approach, Separate Approach, "Base + Delta" Approach, and Hybrid Approach. They are tested on the case studies, and are compared on the solution quality as well as the solution time.

4.3.1 Simultaneous Approach

The Simultaneous Approach is a direct optimisation approach, which solves the whole site-wide model at once by exploiting the optimisation ability of gPROMS. Basically, gPROMS applies the successive quadratic programming (SQP) technique to optimise the problems. It is one of the most widely used NLP algorithms. In brief, SQP obtains the optimal solution by solving a sequence of quadratic programming problems, which are derived from the NLP master problem. By developing the process model in gPROMS, the built-in simultaneous technique and the SQP optimiser can be directly applied to perform the process optimisation. With a robust optimiser, this approach should be able to provide a good quality solution. On the other hand, its solution time might be long due to the computational effort of handling the large-scale model. A more detailed explanation of SQP can be found in (Chen & Macchietto, 1989; Sargent & Ding, 2001), and a brief comparison among SQP and other NLP algorithms has been discussed by Biegler & Grossmann (2004).

4.3.2 Separate Approach

The Separate Approach applies a decomposition procedure to the problem. Decomposition is a conventional method to tackle the site-wide problem. The basic idea is to disconnect the units in the process, and optimise them individually. After that, the individual optimal results are combined to obtain an overall solution. The advantage of the decomposition is a reduced solution time, as the individual sub-problems are smaller than the original problem. However, the integration of the sub-problem results does not guarantee a good overall solution. Mismatches among sub-problem results can easily occur due to the lack of any site-wide consideration in the individual optimisations. The challenge of the Separate Approach is hence to make individual sub-problems communicate throughout the optimisation process, and it can be achieved by an iterative procedure. The Separate Approach collects related units in the process to form sub-groups. The sub-groups are then optimised in cycles. By doing so, the "downstream" sub-group can utilise the "upstream" sub-group's intermediate results to adjust its own optimisation. The optimisations are executed repeatedly until the sub-groups converge to a final solution.

The Separate Approach reported below is tailor-made for the example process, the 3-column ethylene process. In the example process, the approach places the mixer, the reactor and the quench cooler in the "Reaction System". A black box splitter that simulates the distillations with a linear yield model is also added (Figure 4.2). The drying process and the three distillation columns are grouped into the "Distillation System" (Figure 4.3).

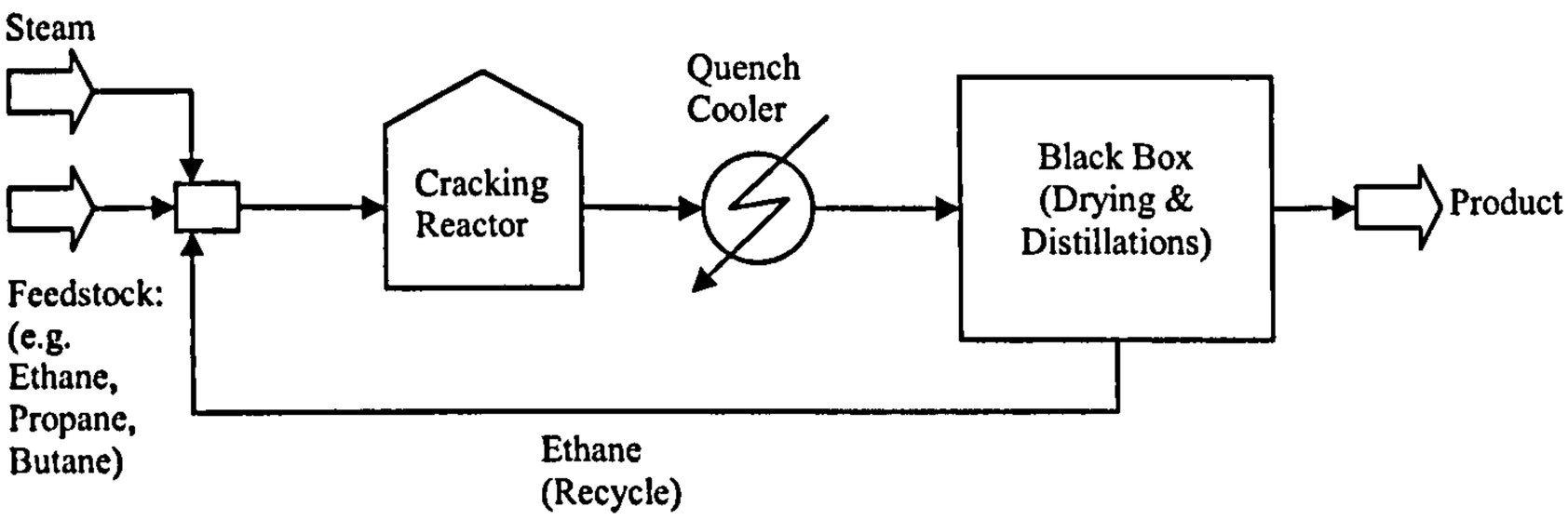

Figure 4.2: Reaction system in Separate Approach.

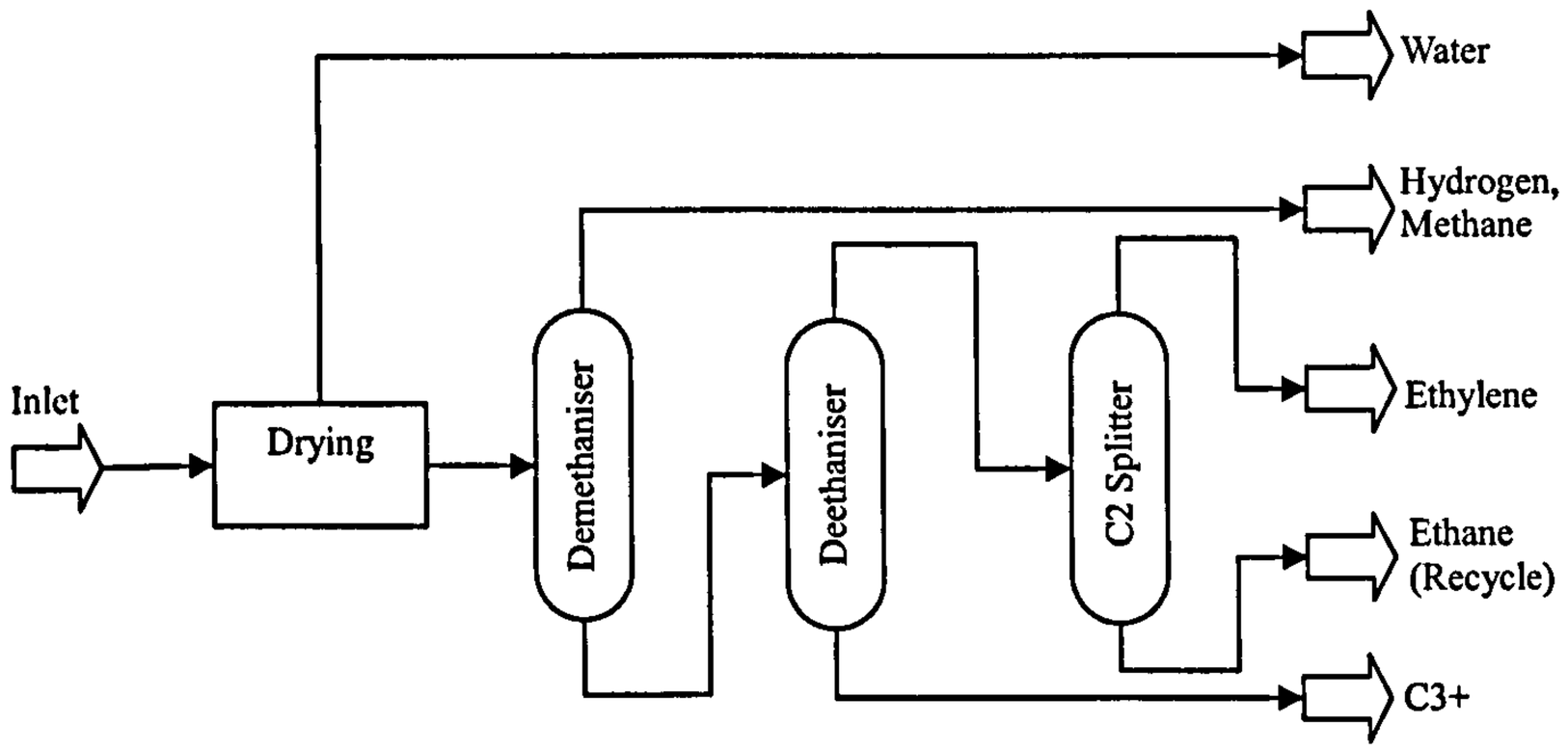

Figure 4.3: Distillation system in Separate Approach

In the Reaction System, the black box splitter divides the chemical component flowrates into the recycle stream and the product stream according to user-specified recovery fractions (RS_{ci}) (Eq. 4.5 and Eq. 4.6). The objective function of the system is equal to the product revenue obtained from the product stream less the raw material cost and the reactor operating cost.

In the Distillation System, the distillation model recovers the products based on rigorous calculations rather than simple recovery models. The system then

back-calculates the actual recovery fractions of each component (DS_{ci}) (Eq. 4.7). Since the Distillation System does not contain any first hand information about the raw material usage and the reactor operation, two constant parameters are added to the objective of the system. They represent the raw material cost and the reactor operating cost respectively. The objective function is equal to the product revenue less the column utility cost, the constant raw material and reactor costs.

The recycle component flowrate in the Reaction System:

$$RF_{ci}^{RS} = MF_{ci}^{RS} \times RS_{ci} \qquad \text{(Eq. 4.5)}$$

The product component flowrate in the Reaction System:

$$PF_{ci}^{RS} = MF_{ci}^{RS} \times (1 - RS_{ci}) \qquad \text{(Eq. 4.6)}$$

The component recovery fraction in the Distillation System:

$$DS_{ci} = RF_{ci}^{DS} / MF_{ci}^{DS} \qquad \text{(Eq. 4.7)}$$

where:

ci	=	Chemical component species.
RS_{ci}	=	Recovery fractions of component *ci* in Reaction System (user-input).
RF_{ci}^{RS}	=	Recycle component flowrate of component *ci* in Reaction System.
PF_{ci}^{RS}	=	Product component flowrate of component *ci* in Reaction System.
MF_{ci}^{RS}	=	Black box splitter inlet component flowrate of component *ci* in

Reaction System.

DS_{ci} = Recovery fraction of component *ci* in Distillation System.

RF_{ci}^{DS} = Recycle component flowrate of component *ci* in Distillation System.

MF_{ci}^{DS} = System inlet component flowrate of component *ci* in Distillation System.

With the two systems defined, the Separate Approach can execute its algorithm procedures to locate the optimal solution. The algorithm begins by optimising the Reaction System. Initial guess values of RS_{ci} are assigned to every component in the first iteration. After the Reaction System optimisation, the resulting reactor outlet component flowrates are sent to the Distillation System as the system inlet component flowrates. The intermediate raw material and reactor operating costs from the Reaction System are also fixed as constants in the objective function calculation of the Distillation System. The Distillation System objective function is then optimised and the component recovery fractions (DS_{ci}) are determined. The DS_{ci} values are transferred to the Reaction System to assign the RS_{ci} and the procedures start over again.

The fractions of RS_{ci} and DS_{ci} are indicators for notifying whether the optimal solution is found. To obtain the best possible result, their values should be as close as possible for all components. In spite of that, only the ethane and ethylene fractions are actually important in the example process. This is because the first two columns in the example process have already removed other components away from the C2 splitter. The recycle stream mainly contains ethane and ethylene, and

only has trace amounts of other species. Therefore, if both the differences of the ethane and ethylene recovery fractions between the two systems are less than the tolerance, the overall optimal solution is found. This also stops the algorithm (Figure 4.4). The optimisations of the two sub-systems are carried out directly by the gPROMS built-in optimiser, which has been discussed in the Simultaneous Approach.

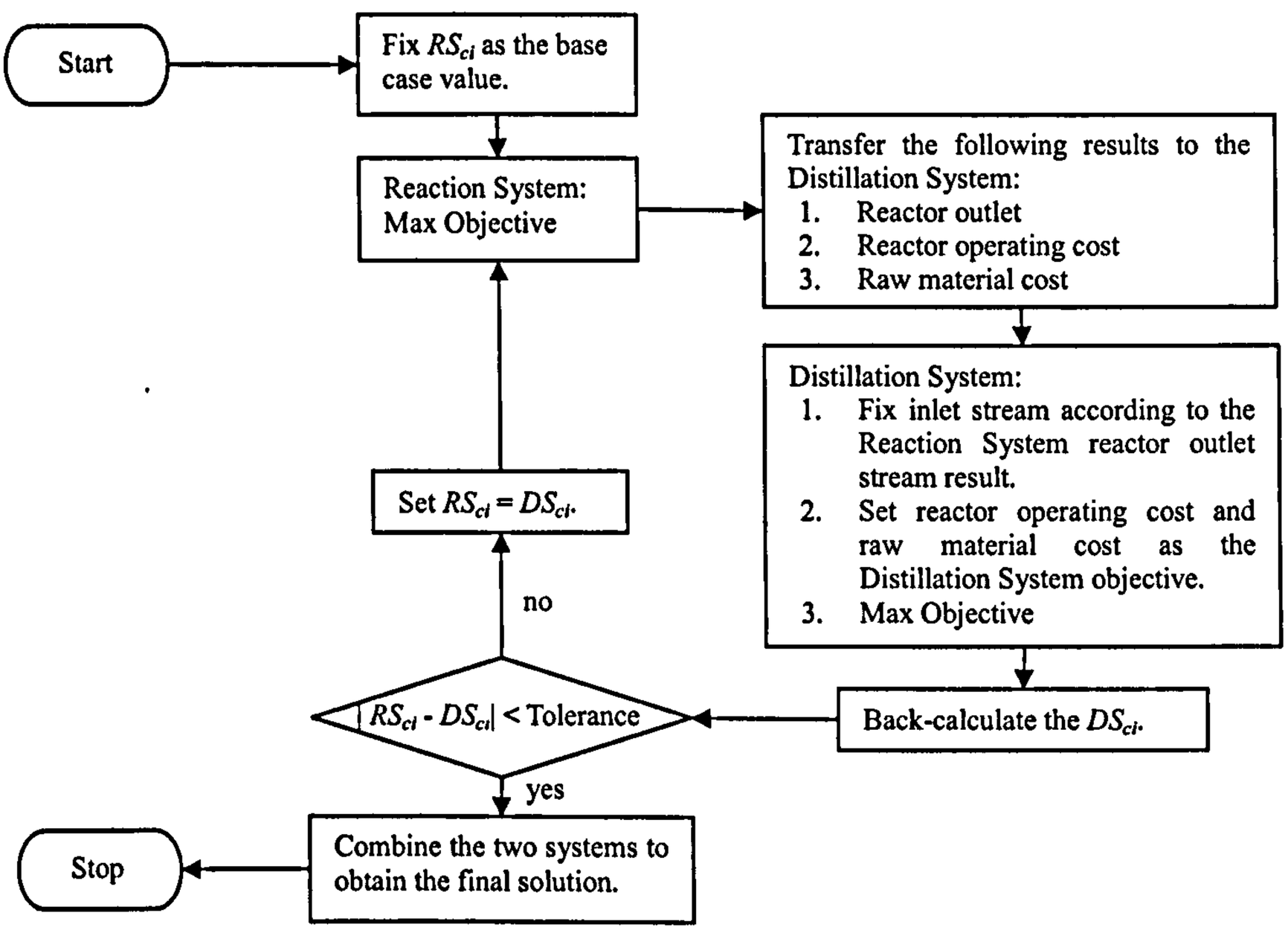

Figure 4.4: Separate Approach algorithm.

4.3.3 "Base + Delta" Approach

The "Base + Delta" Approach uses a successive linear programming (SLP) algorithm to solve the problem. One of the earliest applications of SLP in the process industry was proposed by Griffith and Stewart (1961). Although further studies on large-scale problems were also reported by Palacios-Gomez *et al.* (1982), the algorithm has not received much attention outside blending applications. In contrast to SQP, SLP linearises the NLP problem to a linear (LP) sub-problem at a base point. The sub-problem is only allowed to locate an optimal solution within a small region surrounding the base point called the "step bound" (Δ). This is because the LP is only accurate near the base point. Once the LP is optimised, the nonlinear model is simulated based on the LP result (the new point) for an actual solution. The objective difference between the LP prediction and the NLP simulation are then compared, in order to decide whether the new point is accepted or not. If it is accepted, the new point becomes the base point. The NLP model is then linearised at the new base point and the LP step bound also moves along. If rejected, the previous LP is solved again with a different size (usually a smaller size) of the step bound. The algorithm stops when the NLP objective does not improve.

The SLP performance basically depends on the LP formulations and the point accepting mechanism. In this chapter, two LP formulations (LP-I & LP-II) are developed and three approach variants (SLP-I, SLP-II & SLP-III) are tested. The SLP-I and the SLP-II employ the formulations LP-I and LP-II respectively. The SLP-III is the hybrid form of the previous two. They all use the same point accepting mechanism, which is modified from Lasdon and Waren (1983).

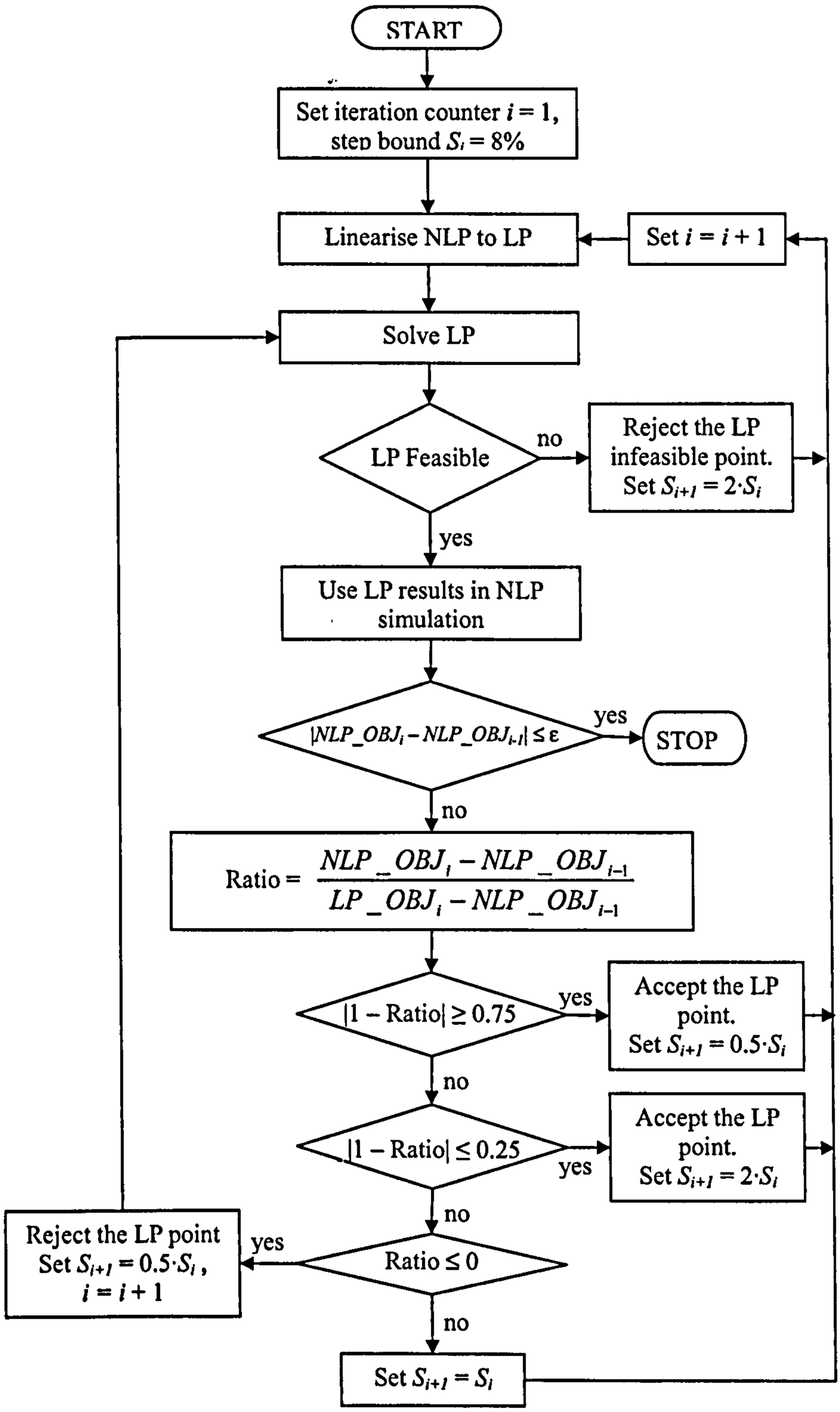

Figure 4.5: "Base + Delta" (SLP-I/SLP-II) Approach algorithm.

4.3.3.1 First "Base + Delta" Approach (SLP-I)

The heartland of the "Base + Delta" Approach is the linearisation of the NLP master problem. The nonlinear members of Eq. 4.2, $y_j = f_j(u_1, u_2, u_3, \ldots, u_I)$, can actually be approximated by their linear counterparts (Eq. 4.8). The coefficients in the linear equation, c_{ij}, are the gradients of the functions f_j at the base point $\left(u_i^{base}, y_j^{base}\right)$, or $c_{ij} = \left.\frac{\partial y_j}{\partial u_i}\right|_{u_i = u_i^{base}}$. The gradients can be either determined symbolically (e.g. using the LINEARISE function in gPROMS) or estimated by Eq. 4.10 with a very small δ. There is no need to linearise the objective function in the example problem, since the profit calculation is already linear. Based on the information above, the first LP formulation (LP-I) is derived and it is assigned in the SLP-I algorithm (Figure 4.5).

LP-I:

$$\max\left(P = \left(\sum_i \alpha_i^u \cdot u_i + \sum_j \alpha_j^y \cdot y_j\right) \cdot PD\right) \qquad \text{(Eq. 4.1)}$$

Subject to

$$y_j = \sum_i c_{ij}\left(u_i - u_i^{base}\right) + y_j^{base} \qquad \text{(Eq. 4.8)}$$

$$\max\left(u_i^{\min}, u_i^{\min} \cdot (1-\Delta)\right) \le u_i \le \min\left(u_i^{\max}, u_i^{\max} \cdot (1+\Delta)\right) \qquad \text{(Eq. 4.9)}$$

$$y_j^{\min} \le y_j \le y_j^{\max} \qquad \text{(Eq. 4.4)}$$

Approximated gradient of function f_j.

$$c_{ij} = \frac{f_j\left(u_i^{base} + \delta\right) - f_j\left(u_i^{base}\right)}{\delta} \qquad \text{(Eq. 4.10)}$$

where

c_{ij} = Approximated gradient of function f_j at the base point.

u_i^{base} = Value of base point input variable u_i.

y_j^{base} = Value of base point output variable y_j.

δ = Small perturbation from the base point.

Δ = Step bound in percentage of the base point.

4.3.3.2 Second "Base + Delta" Approach (SLP-II)

Maintaining a feasible solution is not straightforward for the "Base + Delta" Approach. The LP approximation is intrinsically less accurate than the original NLP model. A feasible solution suggested by the LP optimisation might turn out to be infeasible in the NLP simulation. The situation especially affects tight constraints, like the ethylene product purity in the example. The formulation LP-I is simple, but it does not take the solution feasibility into account. A modified formulation (LP-II) from the LP-I is therefore proposed. The LP-II includes variables to measure the magnitude of the violation of each constraint, called the infeasibility. The infeasibility variables will be multiplied by different weighting constants according to their magnitudes. Then the sum of the weighted constraint violations, namely total infeasibility, is included in the objective function as a penalty. The SLP-II approach adapts the LP-II formulation in the "Base + Delta" algorithm. The algorithms of the SLP-I and the SLP-II are basically the same, except for the LP formulation used.

LP-II:

$$\max\left(\left(\sum_i \alpha_i^u \cdot u_i + \sum_j \alpha_j^y \cdot y_j\right) \cdot PD - TY^{\inf}\right) \quad \text{(Eq. 4.11)}$$

Subject to

$$y_j = \sum_i c_{ij}\left(u_i - u_i^{base}\right) + y_j^{base} \quad \text{(Eq. 4.8)}$$

$$\max\left(u_i^{\min}, u_i^{\min} \cdot (1-\Delta)\right) \le u_i \le \min\left(u_i^{\max}, u_i^{\max} \cdot (1+\Delta)\right) \quad \text{(Eq. 4.9)}$$

$$y_j^{\inf} \ge y_j - y_j^{\max} \quad \text{(Eq. 4.12)}$$

$$y_j^{\inf} \ge y_j^{\min} - y_j \quad \text{(Eq. 4.13)}$$

$$y_j^{\inf} \ge 0 \quad \text{(Eq. 4.14)}$$

$$TY^{\inf} = \sum_j \omega_j y_j^{\inf} \quad \text{(Eq. 4.15)}$$

where

y_j^{inf} = Infeasibility of output variable y_j.

TY^{inf} = Total infeasibility.

ω_j = Weight constant of infeasibility y_j^{inf}.

4.3.3.3 Third "Base + Delta" Approach (SLP-III)

The third "Base + Delta" Approach (SLP-III) is a combination of the SLP-I and the SLP-II approaches. The SLP-I approach should be quick because of its simple LP-I formulations, but it does not favour a feasible solution. The SLP-II approach can minimise the infeasibility with the penalty term in the LP-II objective function.

Unfortunately, the penalty term also makes the SLP-II approach more difficult to accept a new point. It slows down the SLP-II approach and possibly traps the approach in a local optimum. Applying the two approaches in turn should theoretically eliminate their adverse effects. The SLP-III approach first uses the SLP-I approach. If the SLP-I solution is feasible, it stops. If not, the SLP-II approach starts from the SLP-I solution aiming to eliminate the infeasibility. As the SLP-I solution should be nearer to the optimum, the SLP-II approach should locate it in a shorter time (Figure 4.6).

4.3.4 Hybrid Approach of Simultaneous and "Base + Delta"

The Hybrid Approach is designed to combine the strength of the Simultaneous Approach and the "Base + Delta" Approach, and to overcome their shortcomings. The Simultaneous Approach tackles the NLP problem directly. Despite an accurate result, it takes a long computational time. The "Base + Delta" Approach does not guarantee the best solution, but it proceeds quickly.

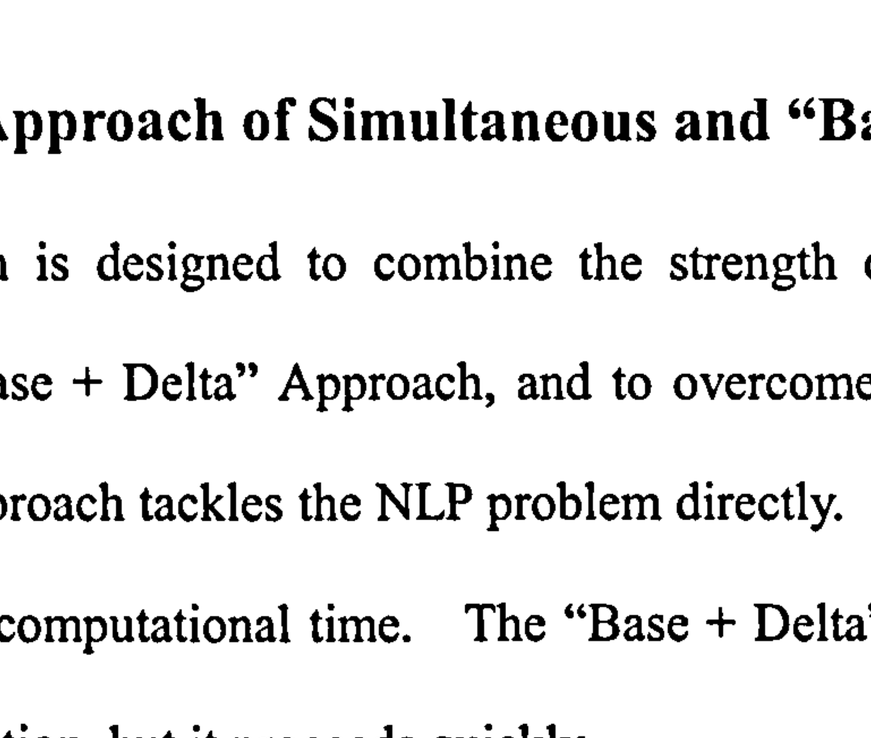

Figure 4.6: "Base + Delta" (SLP-III) Approach algorithm.

Like the "Base + Delta" SLP-III approach, the Hybrid Approach is divided into two phases. Firstly, the "Base + Delta" SLP-I approach is used to locate a near-optimal solution. The aim of the SLP-I approach here is to obtain a better initial point for the Simultaneous Approach as quickly as possible. Feasibility is not the main concern. Secondly, the Simultaneous Approach is initialised by the SLP-I solution and the NLP optimisation proceeds. As the SLP-I solution should be closer to the optimal solution than the initial point, the computational time of the Simultaneous Approach should be reduced.

Another idea to speed up the site-wide optimisation is applying sensitivity analysis. It is a technique to figure out how influential a variable is on a specific function in a mathematical model. Prior to the optimisation, a sensitivity analysis can determine which input variables are much less influential on the objective function. Those input variables are marked as low priority variables and fixed as constants during the optimisation. With fewer degrees of freedom in the problem, the optimisation should run faster. In addition, the fixing of the low priority variables should not affect the solution quality too much. Widely used sensitivity analysis methods include the Morris method (Morris, 1997) and Sobol's method (Saltelli *et al.*, 2005). A preliminary study of Morris method used on the ethylene process model has been carried out, but the result was not very promising. Hence, the application of the sensitivity analysis has been dropped out from the thesis.

4.4 Case Studies

Two case studies were examined in this section. They both rely on the 3-column ethylene process. The first one is the single-feed example. The only available raw

material in this example is ethane. The second one is somewhat more complicated, the multi-feed example. This process has two raw materials, ethane and propane. Not all approaches will be tested using the second example. Only those which showed potential in the first example would be considered. A Linux computer with CPU speed 1794 MHz was used to perform all the optimisations described below.

4.4.1 Single-Feed Example

The single-feed example process has the ethane feed as the only raw material. The feed contains 70% ethane, 15% propane and 15% 1,3-butadiene on a mass basis. The raw material passes through the 3-column process shown in Figure 4.1 to produce ethylene as the main product. The process has two more by-products, the fuel gas (hydrogen, methane) and the C3 chemicals. In the example, the process operation was considered under a steady state with a single time period. To generalise, the period duration was set to be 1 second. Special operability constraints were also placed on the distillation columns to keep their operation away from the flooding velocity and the weep point. The flooding velocity and the weep point were determined by correlations presented in (Sinnott, 2005). Based on the correlations, the feasible distillation regions were found for all the three columns (Figure 4.7). The boundaries of the regions were fitted as polynomial functions in terms of the reflux ratio and the boil-up ratio, and were included in the optimisation.

An initial base case was set up in order to have an unbiased comparison among the approaches. All the approaches had to start the optimisation from the base case. The objective was to maximise the process profit as well as to satisfy the constraints (bounds on input and output variables). Table 4.1 summarises the input and output

variables of the optimisation together with their base case values, their bounds, and their weights (prices/costs) in the objective function. Although the numbers of optimisation input and output variables are 9 and 20 respectively, the total number of model variables involved in the 3-column process is actually 26,250. It is also noted that the ethylene product purity in the base case (96.85 mole%) had not reached the lower bound (99.00 mole%).

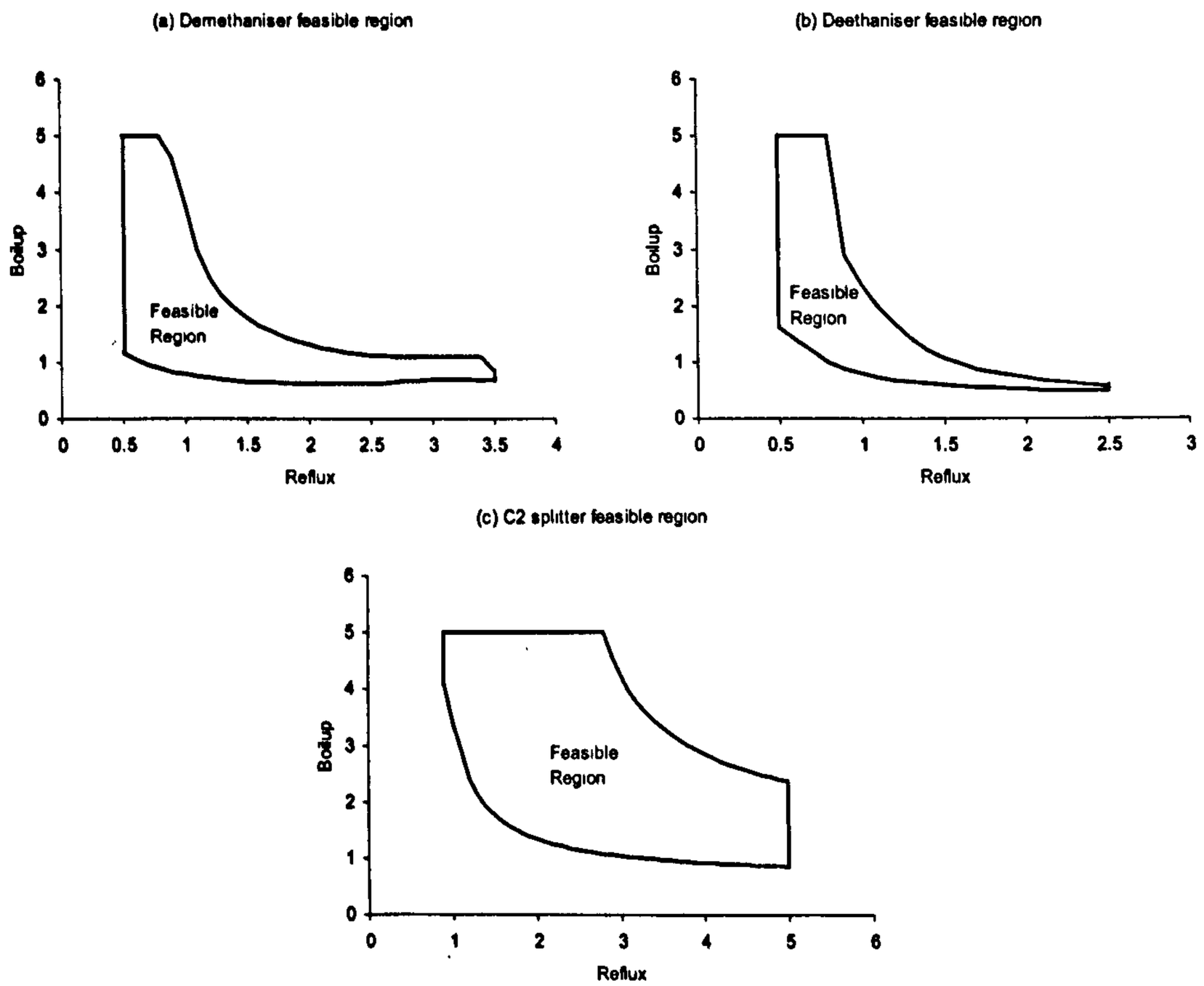

Figure 4.7: Distillation operation feasible regions.

Table 4.1: Single-feed optimisation example variables.

Input Variabies (u)	Base Value	Price/ Cost	Lower Bound	Upper Bound
Ethane feed flowrate (kg/s)	15.76	-0.260	1.00	20.00
Steam feed flowrate (kg/s)	8.00	-0.010	1.00	20.00
Reactor heat flux (J/m^2s)	40,000	-2.0E-7	35,000	45,000
Demethaniser boil-up, Bup1	0.71		0.67	5.00
Demethaniser reflux, R1	2.00		0.50	3.40
Deethaniser boil-up, Bup2	1.81		0.50	5.00
Deethaniser reflux, R2	0.50		0.50	2.50
C2 splitter boil-up, Bup3	3.73		1.00	5.00
C2 Splitter reflux, R3	1.80		0.90	5.00
Output Variables (y)	**Base Value**	**Price/ Cost**	**Lower Bound**	**Upper Bound**
Reactor steam dilution ratio	0.3995		0.35	0.45
Reactor outlet pressure (Pa)	219,407		150,000	
Reactor outlet temperature (K)	1,105			1,300
Demethaniser condenser duty, Qc1 (J)	9.1E6	-1.05E-8		
Demethaniser reboiler duty, Qr1 (J)	5.5E6	-1.26E-8		
Deethaniser condenser duty, Qc2 (J)	3.1E6	-1.05E-8		
Deethaniser reboiler duty, Qr2 (J)	2.9E6	-1.26E-8		
C2 Splitter condenser duty, Qc3 (J)	8.0E6	-1.05E-8		
C2 Splitter reboiler duty, Qr3 (J)	6.2E6	-1.26E-8		
Demethaniser feasible region upper bound function	0.4630		0.00	
Demethaniser feasible region lower bound function	0.3472		0.00	
Deethaniser feasible region upper bound function	6.3932		0.00	
Deethaniser feasible region lower bound function	0.2061		0.00	
C2 splitter feasible region upper bound function	6.6768		0.00	
C2 splitter feasible region lower bound function	2.3589		0.00	
Ethylene prcduct molar purity	0.9685		0.99	1.00
Ethylene production flowrate (kg/s)	8.98	0.587	2.80	9.80
C3+ stream ethylene molar composition	0.17		0.00	0.10
C3+ stream flowrate (kg/s)	4.30	0.200		
H_2/CH_4 stream flowrate (kg/s)	2.48	0.050		
Objective, Profit ($/s)	0.9597			
Period Duration (s)	1			

4.4.1.1 Simultaneous Approach Result

In the Simultaneous Approach, the gPROMS SQP solver took 2,268 CPU seconds and 23 major iterations to optimise the single-feed problem. The objective, profit, has been increased about 18% from the base case's 0.9597 $/s to 1.1339 $/s. The ethylene product purity has also been brought to the lower bound, 99.00 mole%, and so the solution is feasible with respect to all constraints.

4.4.1.2 Separate Approach Result

The Separate Approach decomposed the process into the Reaction System and the Distillation System. They were both optimised by the gPROMS SQP solver. Following the algorithm shown in Figure 4.4, the approach converged in four iterations and required a total of 4,020 CPU seconds (Table 4.2). The objective has been improved by 10% to 1.0558 $/s, but it is 7% less than the Simultaneous Approach.

Table 4.2: Separate approach iteration results.

Iteration	System	*RS* / *DS* (C_2H_4)	*RS* / *DS* (C_2H_6)	|*RS-DS*| (C_2H_4)	|*RS-DS*| (C_2H_6)	System Obj. ($/s)	CPU Time (s)
Start	React.	0.0000	0.8650	Tolerance = 0.001		1.1921	
	Dist.	0.0000	0.8650			0.9597	
1	React.	0.0000	0.8650			1.4235	25.74
	Dist.	0.0002	0.9178	0.0002	0.0528	1.0024	35.98
2	React.	0.0002	0.9178			1.4747	601.19
	Dist.	0.0002	0.9205	0.0000	0.0027	1.0509	31.89
3	React.	0.0002	0.9205			1.4782	1085.97
	Dist.	0.0003	0.9224	0.0001	0.0019	1.0525	31.19
4	React.	0.0003	0.9224			1.4800	2168.97
	Dist.	0.0004	0.9230	0.0001	0.0006	1.0539	38.78
Final Combined System							Total CPU:
		6.0E-5	0.9224			1.0558	4019.71

4.4.1.3 "Base + Delta" Approach Result

A computer subroutine has been developed for gPROMS to execute the "Base + Delta" Approach. The subroutine first asks gPROMS to simulate the model at a base point and linearises the NLP model. Then it captures the information to generate a LP model in GAMS format (Brooke *et al.*, 1992). The LP model is optimised by the solver CPLEX (ILOG, 2008). After that, the LP solution is sent back to gPROMS for further simulations and linearisations.

The measurement of the infeasibility takes an important part in the LP-II formulation. The weight constants (ω_j) of different output variables should be varied according to the variables' magnitudes (Table 4.3). This prevents some of the output variables dominating the infeasibility calculation. Although the LP-I formulation does not involve the infeasibility, the term of the total infeasibility (TY^{inf}) is also back-calculated by equations (Eq. 4.12 – 4.15) for the SLP-I approach. This helps in comparing the three "Base + Delta" approaches performance.

Table 4.3: Output variable weights (ω_j) in "Base + Delta" infeasibility calculations.

Output variable (y)	Weight (ω_j)
Reactor steam dilation ratio	10
Reactor outlet pressure (Pa)	0.1
Reactor outlet temperature (K)	0.0001
Demethaniser feasible region upper bound function	1000
Demethaniser feasible region lower bound function	1000
Deethaniser feasible region upper bound function	1000
Deethaniser feasible region lower bound function	1000
C2 splitter feasible region upper bound function	1000
C2 splitter feasible region lower bound function	1000
Ethylene product molar purity	100
Ethylene production flowrate (kg/s)	10
C3+ stream ethylene molar composition	10

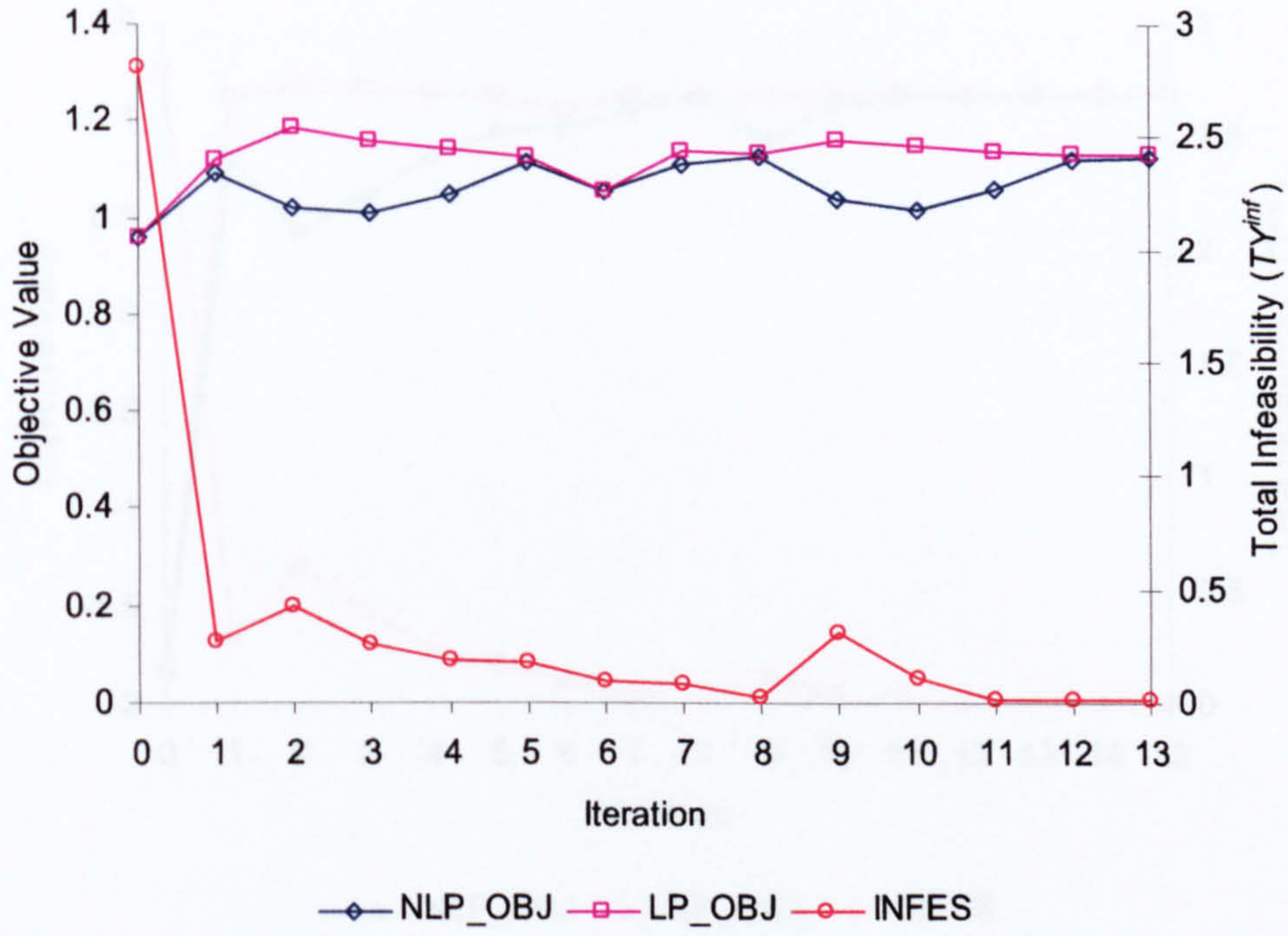

Figure 4.8: SLP-I approach single-feed example iteration results.

SLP-I

The SLP-I approach took 714 CPU seconds and 13 iterations to converge. It obtained an objective of 1.1251 \$/s. The value is 17% more than the base case profit, and is just 0.8% less than the Simultaneous Approach's. The back-calculated total infeasibility (TY^{inf}) is 0.0153. It mainly came from the small deviation of the ethylene product purity (98.98% vs. 99.00%). The solution may be considered to be practically feasible. The iteration results of the objective values (LP and NLP) and the total infeasibility are shown in Figure 4.8.

SLP-II

The SLP-II approach took longer to converge as it tried to reduce the infeasibility during the optimisation. It required 870 CPU seconds and 15 iterations. The

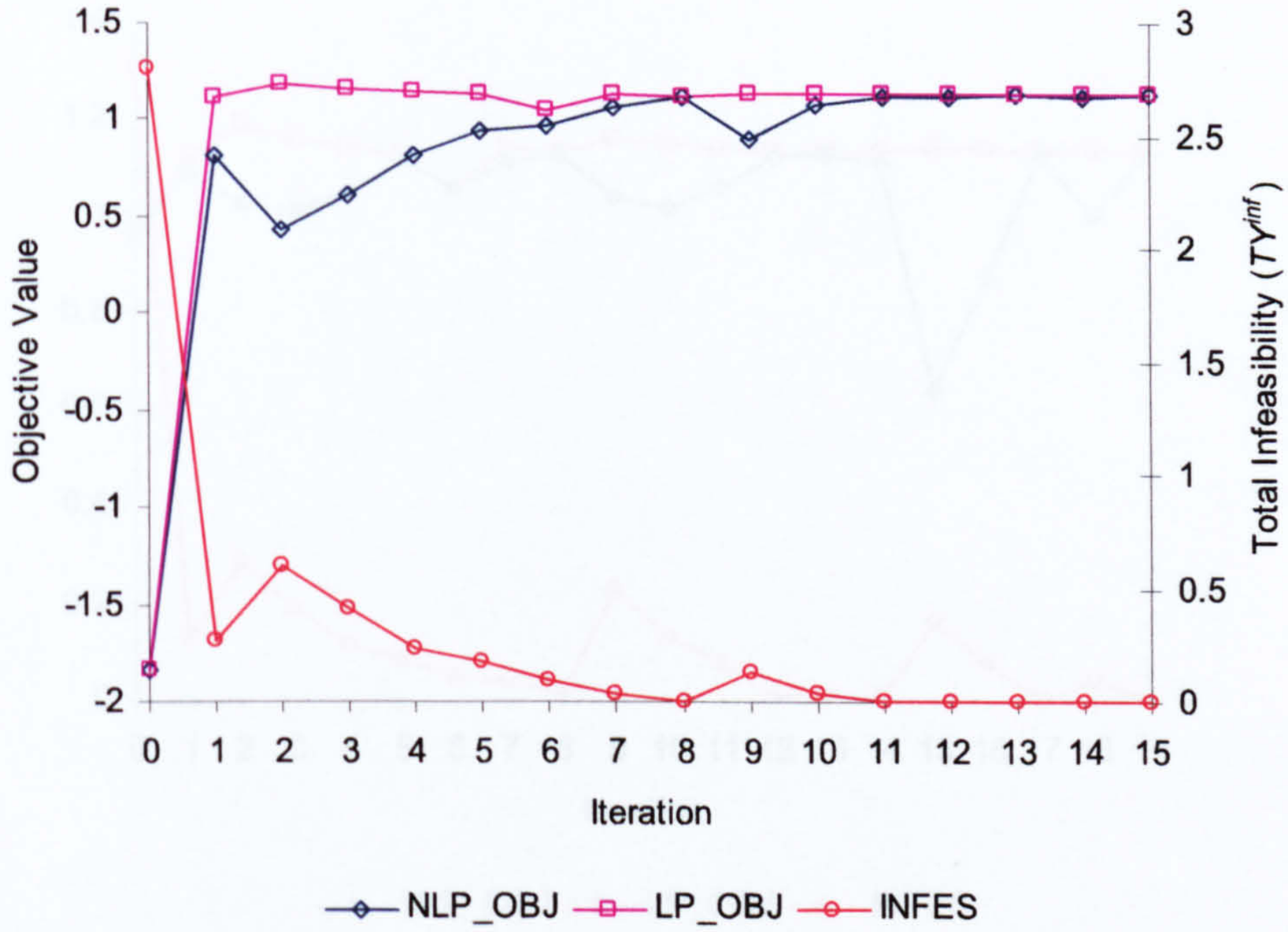

Figure 4.9: SLP-II approach single-feed example iteration results.

longer time spent, however, did not significantly improve the solution. Its solution objective is 1.1254 $/s with a total infeasibility of 0.0013 units (Figure 4.9) while the SLP-I approach attained an objective of 1.1251 $/s.

SLP-III

The SLP-III approach first captured the SLP-I result and then used the SLP-II approach to improve it. After the original 13 iterations of the SLP-I, the SLP-II approach needed 6 more iterations to obtain the optimal solution. The SLP-III approach used a total of 1,212 CPU seconds and 19 iterations. This raised the profit to 1.1309 $/s with a total infeasibility of 0.0152 (Figure 4.10). It obtained a solution close to that of the Simultaneous Approach in just about half of the solution time.

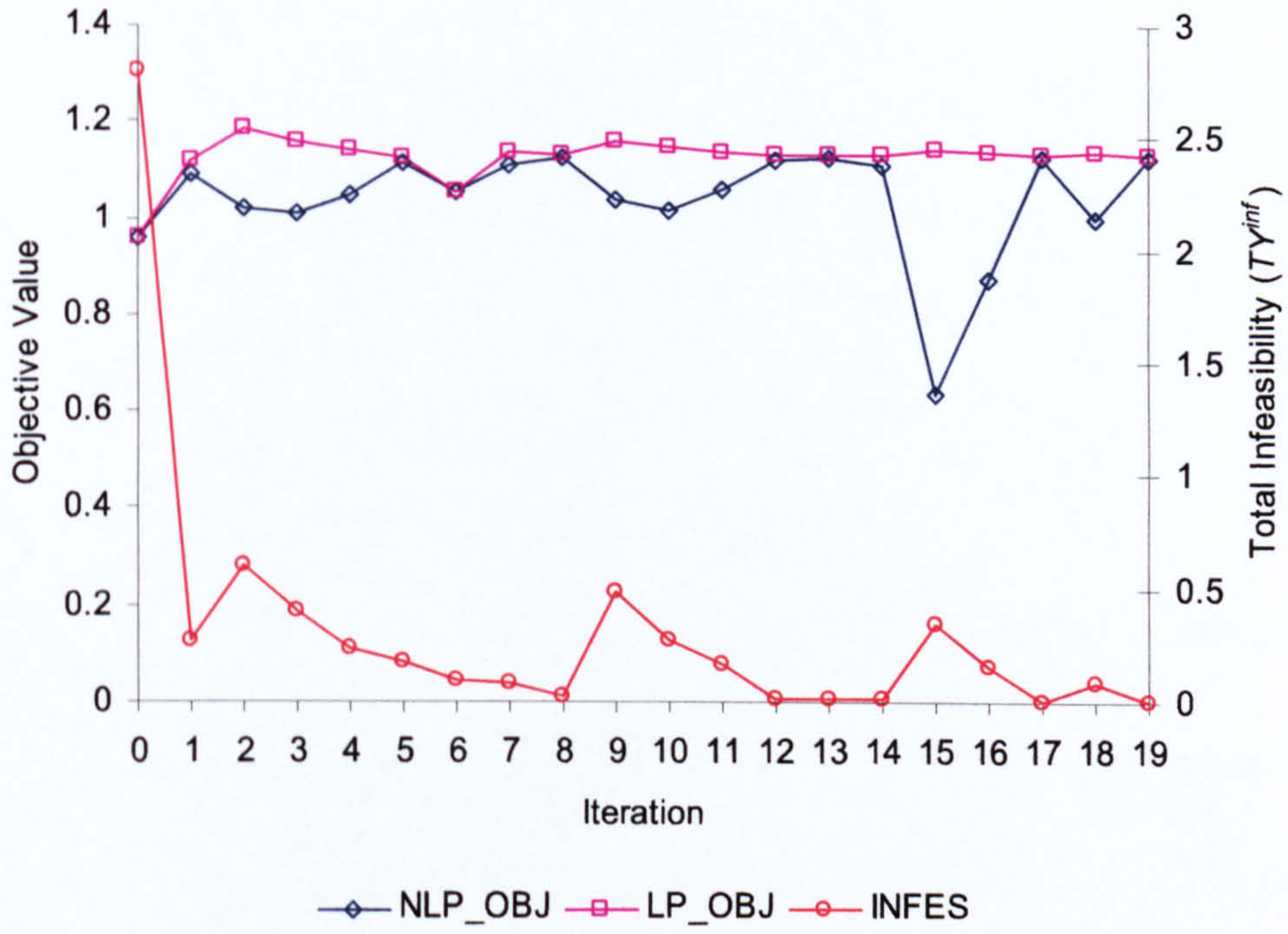

Figure 4.10: SLP-III approach single-feed example iteration results.

4.4.1.4 Hybrid Approach Result

The Hybrid Approach obtained the same result (Profit = 1.1335 \$/s) as the Simultaneous Approach. The SQP solver optimised the problem after the SLP-I solution in 683 CPU seconds and 15 major iterations. In total, the Hybrid Approach required 1,397 CPU seconds. That is a 40% reduction in the computational time. The results of all the approaches are summarized in Table 4.4. The problem dimensions, including the sub-problems solved in different approaches, and their corresponding optimisation tolerances are also reported in Table 4.5.

Table 4.4: Single-feed example selected result summary.

	Base Case	Simult. Approach	Separate Approach	Base + Delta (SLP-I)	Min.	Max.
Objective, Profit ($/s)	0.9597	1.1339	1.0558	1.1251		
Ethane feed (kg/s)	15.76	16.25	16.92	16.36	1	20
Reactor heat flux (J/m2-s)	40000	44523	45000	44343	33000	45000
Ethylene production (kg/s)	8.98	9.80	9.80	9.80	2.8	9.8
Ethylene product molar purity	0.9685	0.9900	0.9899	0.9898	0.99	1
CPU Time (sec)		2267.7	4019.7	714.5		
Total Infeasibility in Base + Delta				0.0153		

	Base + Delta (SLP-II)	Base + Delta (SLP-III)	Hybrid Approach	Min.	Max.
Objective, Profit ($/s)	1.1254	1.1309	1.1335		
Ethane feed (kg/s)	16.33	16.28	16.24	1	20
Reactor heat flux (J/m2-s)	44317	44287	44567	33000	45000
Ethylene production (kg/s)	9.80	9.80	9.80	2.8	9.8
Ethylene product molar purity	0.9900	0.9900	0.9900	0.99	1
CPU Time (sec)	870.8	1212.3	1397.6		
Total Infeasibility in Base + Delta	0.0013	0.0153			

Table 4.5: Problem dimensions and optimisation tolerances in single-feed example.

Approach	Total no. of variables involved	Degrees of freedom	No. of constraints	Optimisation tolerance
Simultaneous	26,250	9	12	0.001[1]
Separate				
Reaction Sys.	19,434	3	3	0.001[1]
Distillation Sys.	7,330	6	9	0.001[1]
Base + Delta				
SLP-I	255	9	12	LP[2]
SLP-II	268	9	12	LP[2]
SLP-III	(SLP-I + SLP-II)			
Hybrid				
SLP-I	268	9	12	LP[2]
Simultaneous	26,250	9	12	0.001[1]

Remarks:
1. gPROMS SRQPD solver, "OptimisationTolerance". Definition can be found in (PSE, 2004a).
2. Linear programming model, optimisation tolerance is not applicable.

4.4.1.5 Results Analysis

Four different approaches were tested in the single-feed example. Positively, they all improved the process profit from the base case and provided feasible solutions. The profit rise mainly stemmed from increasing the ethylene production. In the results of the approaches, all the ethylene production rates reached the allowable maximum, 9.80 kg/s. This is about a 9% increase from the base case value of 8.98 kg/s.

The Simultaneous Approach gave the best solution, and its objective was the highest. The Separate Approach, on the other hand, had the lowest objective. This could be explained by the decomposition in the approach. The Reaction System tried to maximise its own objective by increasing the reactor heat flux to the maximum of 45,000 J/m^2-s. Though the reactor yield increased significantly, the high heat flux also favoured the production of less profitable by-products. To reach the maximum ethylene production rate with high heat flux, the process required more feedstock. Consequently, the high revenue was compromised by the higher material and reactor cost. This proves that the decomposition approach could overlook the site-wide opportunity. This also reflects the importance of using "site-wide" methods when solving site-wide optimisation problems.

The Separate Approach also unexpectedly spent a longer computation time than the Simultaneous Approach. The smaller size in the decomposed sub-problems should give it a faster performance. Most of the time in the Separate Approach was spent on the Reaction System optimisation. This was because the recycle stream in the system complicated the optimisation. The Simultaneous Approach also involved the recycle stream, but it only underwent one optimisation. The Separate

Approach instead needed to solve the optimisation with the recycle stream repeatedly, four times in the example. Although every single Reaction System optimisation was faster than the Simultaneous Approach, the cumulative effect made the Separate Approach much slower overall.

The "Base + Delta" Approach was the fastest approach. In this single-feed example, the SLP-I approach was able to provide a feasible solution even without the measure of the infeasibility. The SLP-II approach included the infeasibility directly and only obtained a similar solution. The extra effort expended by the SLP-II approach was not clearly justified in this example. This might need a more complicated case to verify. By combining the previous two approaches, the SLP-III approach did very well indeed. It could get a solution close to the Simultaneous Approach in a much shorter time. The "Base + Delta" Approach is obviously worth further investigation.

The Hybrid Approach also successfully combined the strengths of the Simultaneous and the "Base + Delta" Approaches. Its accuracy was as good as the Simultaneous Approach, and its solution time was competitively short. This suggests the approach is also promising.

To summarise, the Simultaneous Approach, "Base + Delta" Approach and Hybrid Approach showed their potential in the single-feed example. In terms of the solution quality and computational time, they out-performed the Separate Approach. Therefore, they are considered further using the multi-feed example for additional studies.

Table 4.6: Multi-feed optimisation example variables.

Input Variables (u)	Base Value	Price/ Cost	Lower Bound	Upper Bound
Ethane feed flowrate (kg/s)	7.76	-0.26	5.00	20.00
Propane feed flowrate	8.00	-0.30	5.00	20.00
Steam feed flowrate (kg/s)	8.00	-0.01	1.00	20.00
Reactor heat flux (J/m^2s)	40,000	-2.0E-7	35,000	45,000
Demethaniser boil-up, Bup1	0.71		0.67	5.00
Demethaniser reflux, R1	2.00		0.50	3.40
Deethaniser boil-up, Bup2	1.81		0.50	5.00
Deethaniser reflux, R2	0.50		0.50	2.50
C2 splitter boil-up, Bup3	3.73		1.00	5.00
C2 Splitter reflux, R3	1.80		0.90	5.00

Output Variables (y)	Base Value	Price/ Cost	Lower Bound	Upper Bound
Reactor steam dilution ratio	0.4358		0.40	1.00
Reactor outlet pressure (Pa)	235,503		150,000	
Reactor outlet temperature (K)	1,277			1,300
Demethaniser condenser duty, Qc1 (J)	8.24E6	-1.05E-8		
Demethaniser reboiler duty, Qr1 (J)	3.97E6	-1.26E-8		
Deethaniser condenser duty, Qc2 (J)	2.59E6	-1.05E-8		
Deethaniser reboiler duty, Qr2 (J)	2.82E6	-1.26E-8		
C2 Splitter condenser duty, Qc3 (J)	6.06E6	-1.05E-8		
C2 Splitter reboiler duty, Qr3 (J)	4.64E6	-1.26E-8		
Demethaniser feasible region upper bound function	0.4630		0.00	
Demethaniser feasible region lower bound function	0.3472		0.00	
Deethaniser feasible region upper bound function	6.3932		0.00	
Deethaniser feasible region lower bound function	0.2061		0.00	
C2 splitter feasible region upper bound function	6.6768		0.00	
C2 splitter feasible region lower bound function	2.3589		0.00	
Ethylene product molar purity	0.9774		0.99	1.00
Ethylene production flowrate (kg/s)	6.86	0.587	2.80	9.80
C3+ stream ethylene molar composition	0.0001		0.00	0.10
C3+ stream flowrate (kg/s)	3.72	0.29		
H_2/CH_4 stream flowrate (kg/s)	5.19	0.05		
Objective, Profit ($/s)	-0.1767			
Period Duration (s)	1			

4.4.2 Multi-Feed Example

The multi-feed example is slightly more complicated than the single-feed example. It is used to examine the performance of the approaches with a more complex problem. The example is modified from the single-feed example. A propane feed is added as another raw material stream; this contains 70% propane, 15% *n*-butane and 15% *iso*-butane in mass. Besides maximising the objective, the optimisation also determines the optimal proportion between the ethane feed and the propane feed. The numbers of model equations, optimisation input variables and output variables in this example are 26,402, 10, and 20 respectively.

A base case was assigned to the multi-feed example. It was also based on the base case of the single-feed example, but some data were added or modified (Table 4.6). It is noted that the ethylene product purity was below the lower bound (97.74% vs. 99.00%), and the objective function was negative (-0.1767 $/s) in the base case.

4.4.2.1 Simultaneous Approach Result

The Simultaneous Approach optimised the multi-feed example to a feasible solution with the objective function at 1.0691 $/s. It was a significant improvement on the base case value. The SQP solver used 5,169 CPU seconds and 30 major SQP iterations.

4.4.2.2 "Base + Delta" Approach Result

SLP-I

The SLP-I approach could still converge very quickly. It completed in 12 iterations

within 868 CPU seconds. Unfortunately, the back-calculation showed the total infeasibility (TY^{inf}) was too high (1.2016). It was mainly caused by excess ethylene production (9.84 kg/s) and poor ethylene product purity (97.85%). Although the objective value is high (1.0731 \$/s), the SLP-I solution is effectively infeasible. The iteration objective values of the SLP-I approach are plotted in Figure 4.11.

SLP-II

The SLP-II approach could obtain a feasible solution for the multi-feed example. The total infeasibility (TY^{inf}) is 0.0042, but its objective is only 0.6031 \$/s. That is just about half of the Simultaneous Approach objective. The approach converged in 1,703 CPU seconds after 27 iterations (Figure 4.12).

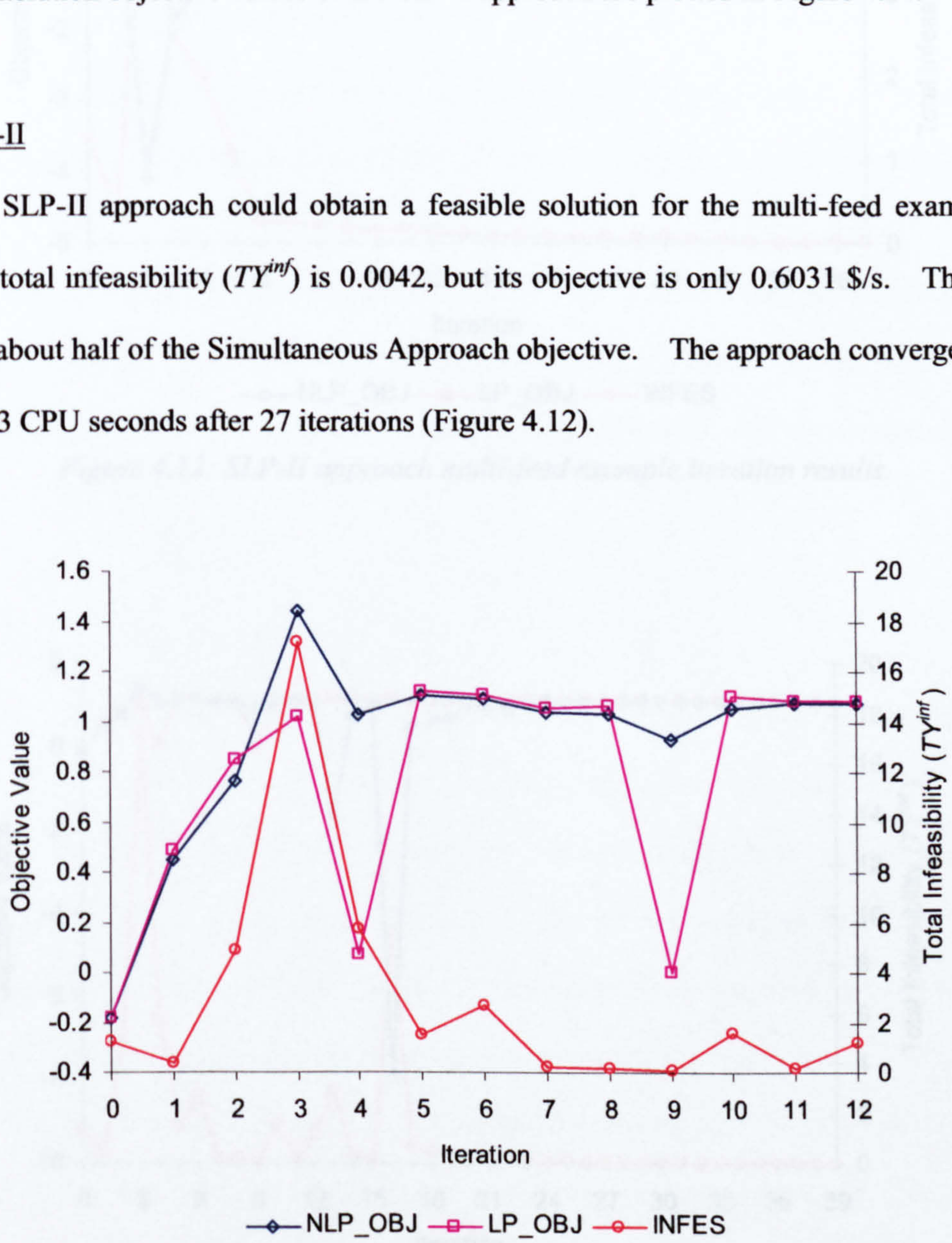

Figure 4.11: SLP-I approach multi-feed example iteration results.

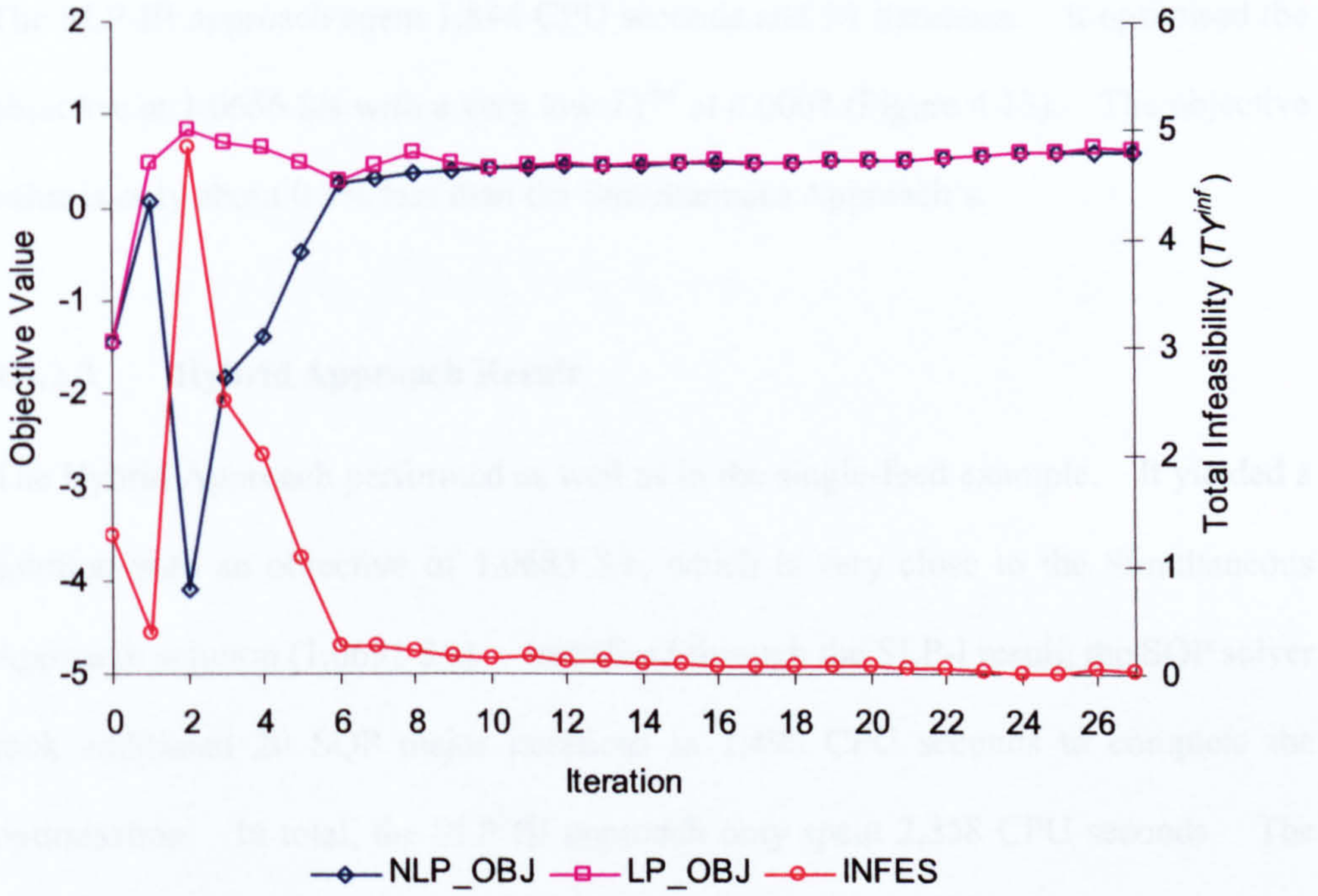

Figure 4.12: SLP-II approach multi-feed example iteration results.

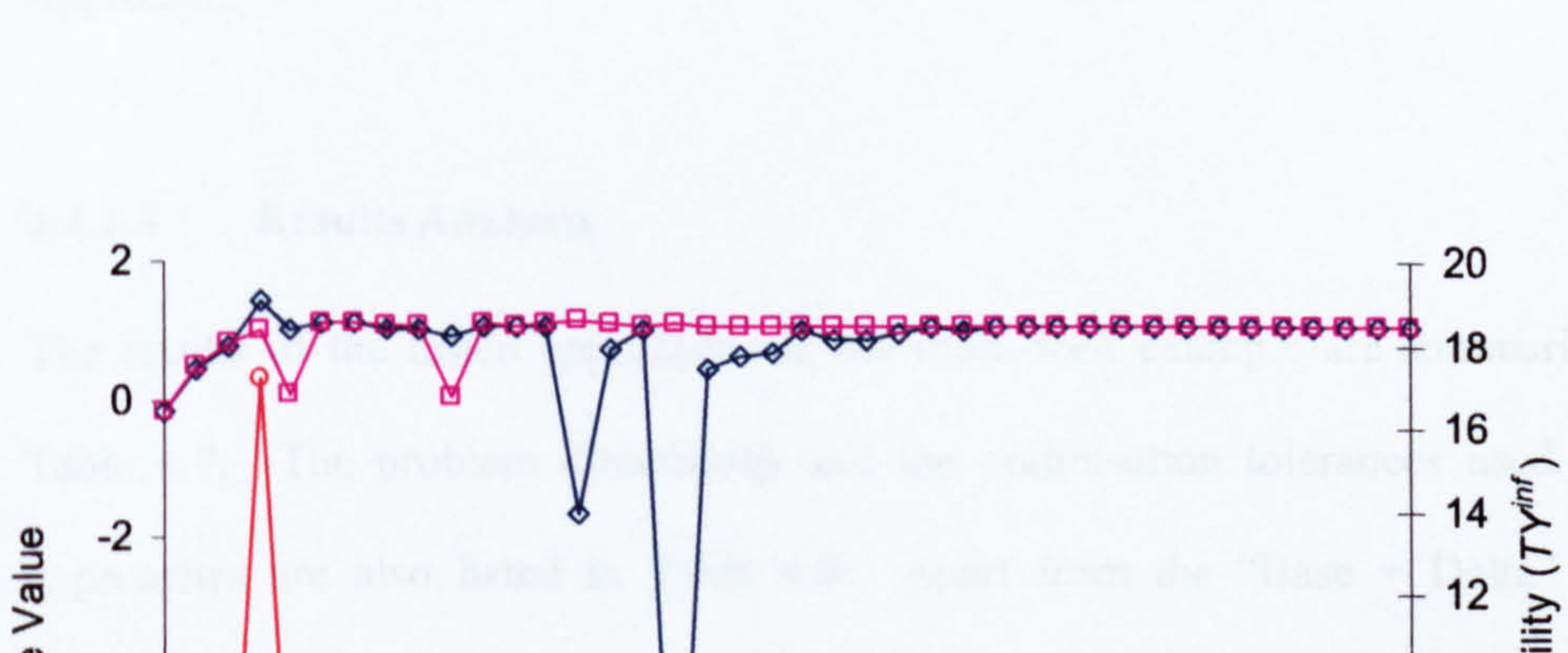

Figure 4.13: SLP-III approach multi-feed example iteration results.

SLP-III

The SLP-III approach spent 1,844 CPU seconds and 39 iterations. It optimised the objective at 1.0656 $/s with a very low TY^{inf} at 0.0007 (Figure 4.13). The objective value is only about 0.3% less than the Simultaneous Approach's.

4.4.2.3 Hybrid Approach Result

The Hybrid Approach performed as well as in the single-feed example. It yielded a solution with an objective of 1.0685 $/s, which is very close to the Simultaneous Approach solution (1.0691 $/s). Initialised through the SLP-I result, the SQP solver took additional 20 SQP major iterations in 1,490 CPU seconds to complete the optimisation. In total, the SLP-III approach only spent 2,358 CPU seconds. The solution time was reduced by more than half compared with the Simultaneous Approach.

4.4.2.4 Results Analysis

The results of the tested approaches in the multi-feed example are summarised in Table 4.7. The problem dimensions and the optimisation tolerances used in the approaches are also listed in Table 4.8. Apart from the "Base + Delta" SLP-I approach, other approaches could improve the process operation from deficit to profitable in the multi-feed example. That was basically achieved by maximising the ethylene production and avoiding the usage of the propane feed. Taking the Simultaneous Approach result as an example, the propane feed flowrate was reduced to the minimum 5 kg/s. The ethane feed flowrate instead was increased. Together with increased heat flux (45,000 J/m^2-s) applied to the reactor, ethylene production

reached the maximum (9.80 kg/s). This was because ethylene was the most profitable product. The heavy components in the propane feed however tended to produce heavier products like propylene in the reactor. Furthermore, the propane feed was more expensive than the ethane feed. The propane feed was hence economically unfavourable in the multi-feed process.

Table 4.7: Multi-feed example selected result summary.

	Base Case	Simultaneous App.	Base + Delta (SLP-I)	Min.	Max.
Objective, Profit ($/s)	-0.1767	1.0691	1.0731		
Ethane fed (kg/s)	7.76	13.71	13.77	5	20
Propane fed (kg/s)	8.00	5.00	5.00	5	20
Reactor heat flux (J/m2-s)	40000	45000	45000	35000	45000
Ethylene production (kg/s)	6.86	9.80	9.84	2.8	9.8
Ethylene product molar purity	0.9774	0.9900	0.9785	0.99	1
CPU Time (sec)		5169	868		
Total infeasibility in Base + Delta			1.2061		

	Base + Delta (SLP-II)	Base + Delta (SLP-III)	Hybrid Approach	Min.	Max.
Objective, Profit ($/s)	0.6031	1.0656	1.0685		
Ethane fed (kg/s)	9.65	13.72	13.71	5	20
Propane fed (kg/s)	6.29	5.00	5.00	5	20
Reactor heat flux (J/m2-s)	37619	45000	45000	35000	45000
Ethylene production (kg/s)	8.09	9.80	9.80	2.8	9.8
Ethylene product molar purity	0.9900	0.9900	0.9900	0.99	1
CPU Time (sec)	1703	1844	2358		
Total infeasibility in Base + Delta	0.0042	0.0007			

Table 4.8: Problem dimensions and optimisation tolerances in multi-feed example.

Approach	Total no. of variables involved	Degrees of Freedom	No. of constraints	Optimisation tolerance
Simultaneous	26,402	10	12	0.001[1]
Base + Delta				
SLP-I	256	10	12	LP[2]
SLP-II	269	10	12	LP[2]
SLP-III	(SLP-I + SLP-II)			
Hybrid				
SLP-I	256	10	12	LP[2]
Simultaneous	26,402	10	12	0.001[1]

Remarks:
1. gPROMS SRQPD solver, "OptimisationTolerance". Definition can be found in (PSE, 2004a).
2. Linear programming model, optimisation tolerance is not applicable.

Although the approaches had shown good potential in the single-feed example, their performance varied in the multi-feed example. The Simultaneous Approach still obtained the best solution, but the direct optimisation also required the longest solution time.

The "Base + Delta" Approach did not perform as well here. The SLP-I Approach could only obtain an infeasible solution despite a fast convergence. It indicates that the incapability of handling the infeasibility is a big shortcoming of the SLP-I Approach. The SLP-II Approach did not perform very well either. Its objective was far lower than the Simultaneous result, and it required double computational time. This could be explained by the penalty function in the LP-II formulation. The penalty function caused the approach to reject points with high infeasibility. In this example, the initial base case was infeasible. It incurred the point rejections in the early iterations. As the rejection made a smaller step bound for the next iteration, the early rejections trapped the algorithm in a local optimum. This resulted in a poor final solution for the SLP-II Approach. The SLP-III Approach was the only "Base + Delta" Approach which had a good performance. It

was because initially the SLP-I algorithm brought it closer to the optimum. Although the SLP-I solution was not feasible, it was close enough for the SLP-II algorithm to locate an optimal feasible solution. The SLP-III Approach finally converged to a near-optimal solution, and it was quicker than the Simultaneous Approach.

The Hybrid Approach matched the Simultaneous Approach's accuracy. The Hybrid Approach objective function was only 0.06% lower than that of the Simultaneous Approach. With the swift action of the first half SLP-I algorithm, the Hybrid Approach's computational time was also very competitive.

4.4.3 Concluding Remarks on Case Studies

Based on the results of the two examples, the Simultaneous Approach, "Base + Delta" SLP-III Approach and Hybrid Approach were better than the others. They all dealt with the site-wide optimisation problem as a whole. The Separate Approach, which tackled the problem via problem size reduction, did not perform well. It missed out the site-wide considerations. This proved that the site-wide optimisation ought to be solved in a site-wide fashion.

The Simultaneous Approach was the best in terms of solution quality. It obtained the best solutions in both examples, but it was also the slowest. In contrast, the SLP-III Approach was the fastest and its solution was the poorest among the potential three. The Hybrid Approach was in the middle. Its solution was considerably near to the Simultaneous Approach and its computational time was relatively short. It is straightforward to conclude that the Hybrid Approach is the

most effective solution approach for the single-site single-period optimisation problem.

The Hybrid Approach's fast solution is basically due to the first half SLP-I algorithm's good performance. The SLP-I Approach performance however has greatly deteriorated from the single-feed to the multi-feed example. It is reasonable to believe that the SLP-I result will worsen as the problem becomes more complicated. After this chapter, the thesis goes on to study multi-period and multi-site optimisations. The problem size and complexity increase severely. A quick and close-optimal solution from the SLP-I Approach is not guaranteed at that time. Without the SLP-I shortcut, the Hybrid Approach is likely to perform similarly to the Simultaneous Approach. Based on that argument, among all the approaches presented in this chapter, the Simultaneous Approach would be the most promising one for the complex site-wide optimisations in the following chapters. The Simultaneous Approach is hence the only recommended approach for the rest of the thesis.

4.5 Conclusions

A single-site single-period site-wide optimisation was carried out on a 3-column ethylene process model, which involved rigorous process unit representations. Two different examples were developed based on the 3-column process, the single-feed example and the multi-feed example. Four approaches had been proposed for the study, namely, the Simultaneous Approach, Separate Approach, "Base + Delta" Approach, and Hybrid Approach.

The approaches were first tested on the single-feed example. The Separate

Approach tried to reduce the problem size and to speed up the optimisation. Unfortunately, it could not achieve the targets and was screened out after the test. Only the remaining approaches, the Simultaneous Approach, the "Base + Delta" Approach and the Hybrid Approach, were applied to the multi-feed example. They all solve problems in a "site-wide" fashion. This strongly indicates the importance of applying site-wide methods for the site-wide optimisation.

The approach performance consistency was tested using the multi-feed example. The "Base + Delta" Approach could not maintain its standard very well. Only the SLP-III Approach out of the three variants could provide a relatively good solution. The Simultaneous Approach and the Hybrid Approach though performed consistently throughout the two examples. The Simultaneous Approach achieved the best solutions albeit with a long solution time. The Hybrid Approach obtained similar but slightly worse solutions relatively quickly.

According to the results in the two examples, the Hybrid Approach has been determined to be the most effective approach for the single-site single-period optimisation. Also based on the decline in the "Base + Delta" SLP-I solution quality, the Hybrid Approach speed is likely to slow down to the level of the Simultaneous Approach as the problem becomes more complicated. It implies that the Simultaneous Approach would be the only suitable approach to apply again in the more complicated multi-site/period studies in the following chapters.

5 Single-site Multi-period Problem

5.1 Introduction

The single-site multi-period problem is a supply chain problem, which, in addition to production optimisation, deals with inventory control in a single plant site. It is only meaningful to talk about inventory control over a planning time horizon. In order to handle the time horizon, a steady-state process model must be replicated several times to form a multi-period framework. In each period, the process operation is still at steady state but its operating conditions and price information can be different from other periods. The adjacent periods in the framework are linked by inventory variables (Figure 5.1).

Chapter 4 has concluded that the direct optimisation, Simultaneous Approach, is the most recommended approach for the site-wide problems so far. It also suggests that a rigorous process model can enhance the solution quality. Direct optimisation on the rigorous process model should be carried out whenever possible. Unfortunately, the model size that can be handled by a typical computer is physically limited by the computer's memory capacity. The limit will eventually be reached

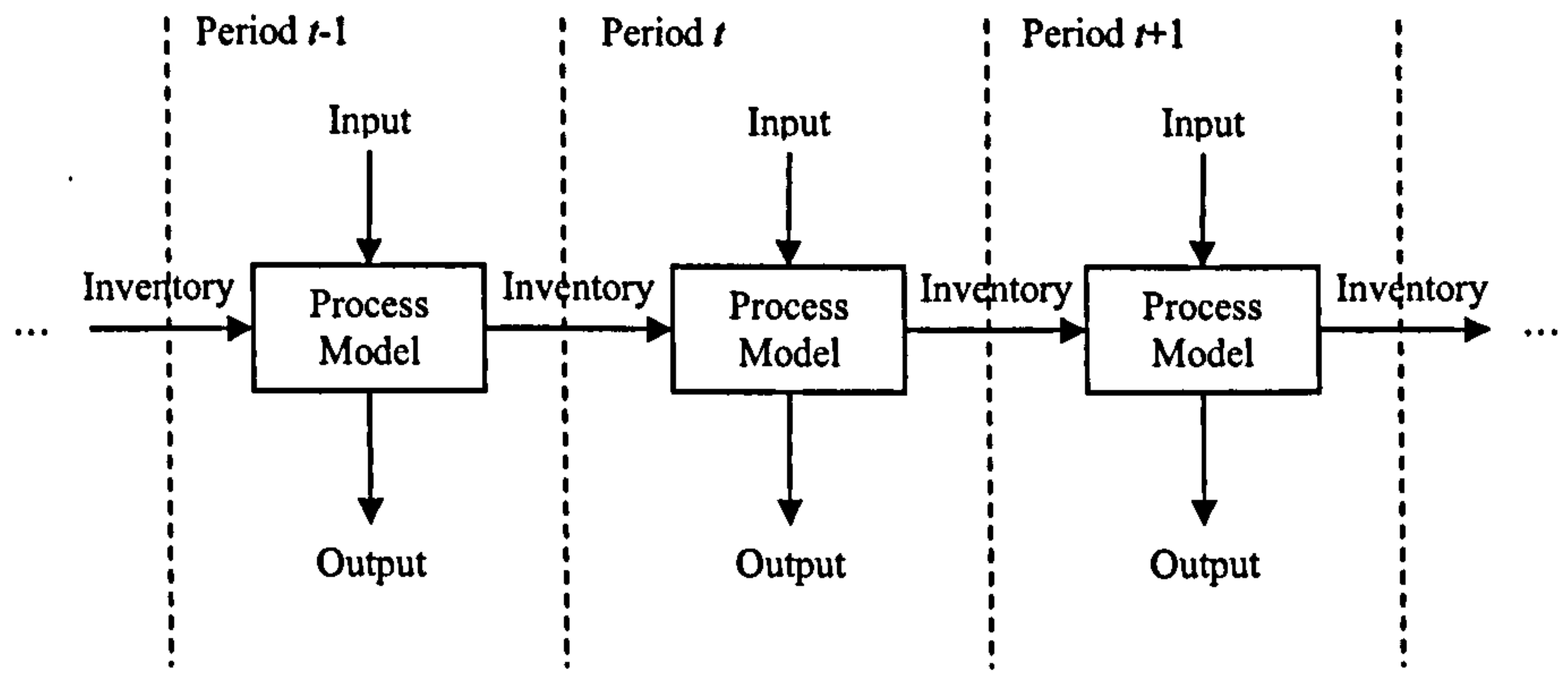

Figure 5.1: Schematic diagram of multi-period model.

when the number of periods keeps rising. A large-scale rigorous process model is especially vulnerable to this problem. It seems that solving the large-scale multi-period model using direct optimisation maybe impractical.

To make the multi-period problem solvable, decomposition of the multi-period model and simplification of the model formulation are two obvious solutions. On the other hand, Chapter 4 has indicated the importance of using site-wide optimisation techniques method for site-wide optimisation. This chapter's goal is then to investigate a decomposition method and a simplification method to solve the single-site multi-period problem while retaining as much of the site-wide information as possible. Nonetheless, a novel technique to allow direct optimisation to be applied to large-scale multi-period models is developed in Chapter 6.

This chapter is outlined as follows. First, it employs the 5-column ethylene process described in Chapter 3 as the basis. Second, the chapter proposes a decomposition method and a simplification method for the single-site multi-period problem and explains them. These are the Rolling Horizon Approach and Feasible Operation Table Approach respectively. Then the chapter develops two examples from the 5-column process. The first is a small example, the 3-period example, which is small enough for the Simultaneous Approach to perform. The two proposed approaches as well as the Simultaneous Approach are used to solve the example. Their results are compared to the Simultaneous Approach result. The second example is the 4-period example. Its size is just too large for the Simultaneous Approach. This example is only solved by the two new approaches. Their performance consistency is examined this time. Finally, conclusions about the studies are made.

5.2 Problem Statement

The problem attempted in this chapter is the single-site multi-period optimisation problem. The 5-column ethylene process described in Chapter 3 represents the single plant site in the problem (Figure 5.2). It includes a flexible multi-tube steam cracking reactor and five distillation columns. The process accepts three types of raw materials, ethane, propane and butane, and produces three types of products, ethylene, propylene and C4 chemicals. The process units are modelled according to the explanations in Chapter 3.

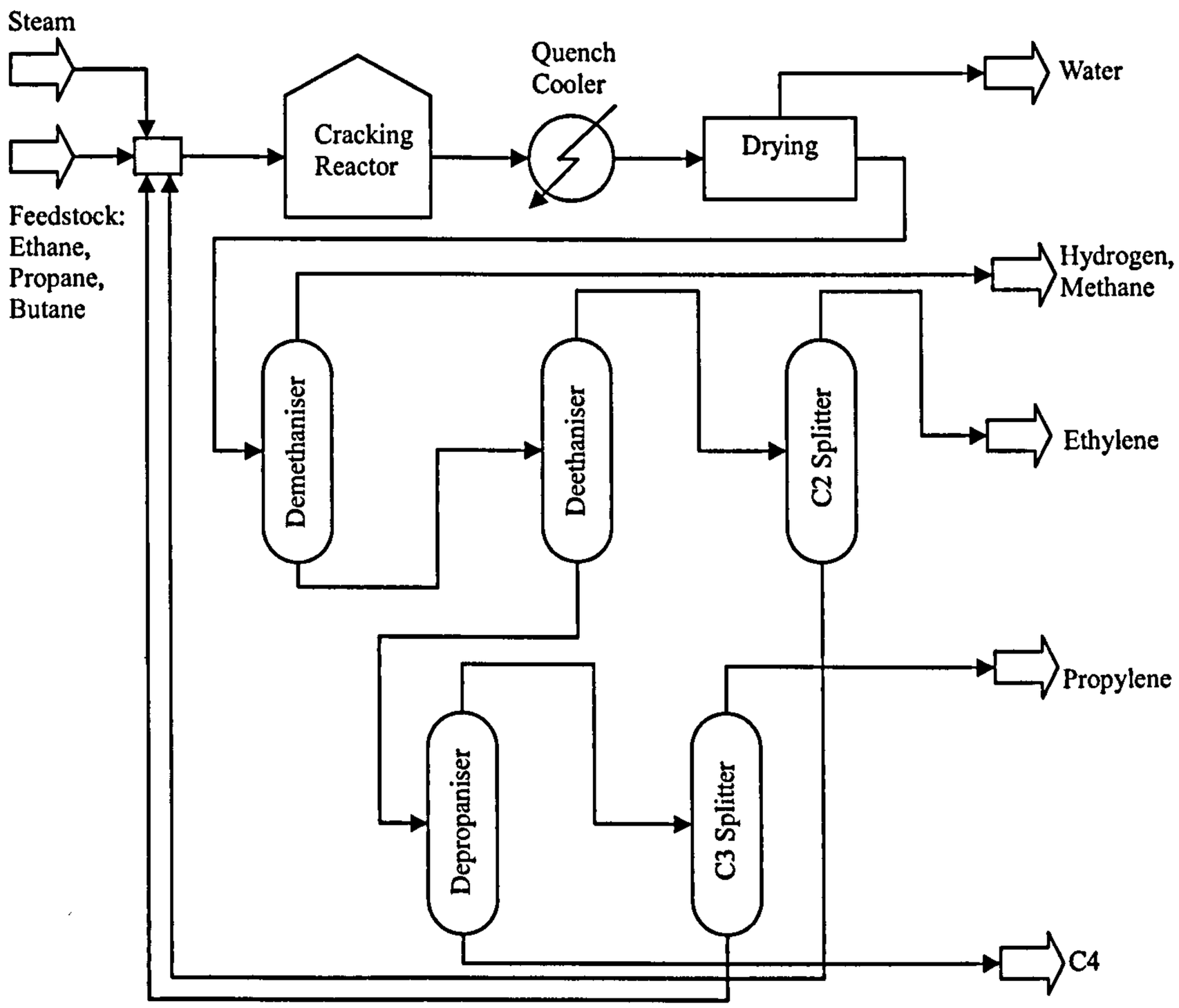

Figure 5.2: 5-Column ethylene process.

The multi-period framework is constructed to optimise production and control the inventory of the plant site. The plant site configurations are identical in all the periods, but the operating conditions, such as variable bounds, material prices and period durations, can be varied. The process operation in a period is independent from that of other periods. The periods are only connected by the raw material and product inventories.

In general, the multi-period model can be divided into three parts, the process, model, the raw material inventory balance and the product inventory balance (Figure 5.3). The process model can be represented using the same terminology in Chapter 4 with the input variables (u), the output variables (y) and their relations $y = f(u)$. The raw material inventory balance and the product inventory balance, however, need some new variables. The raw material consumption (mu) and the product production (my) are specially extracted from the sets of the input variables (u)

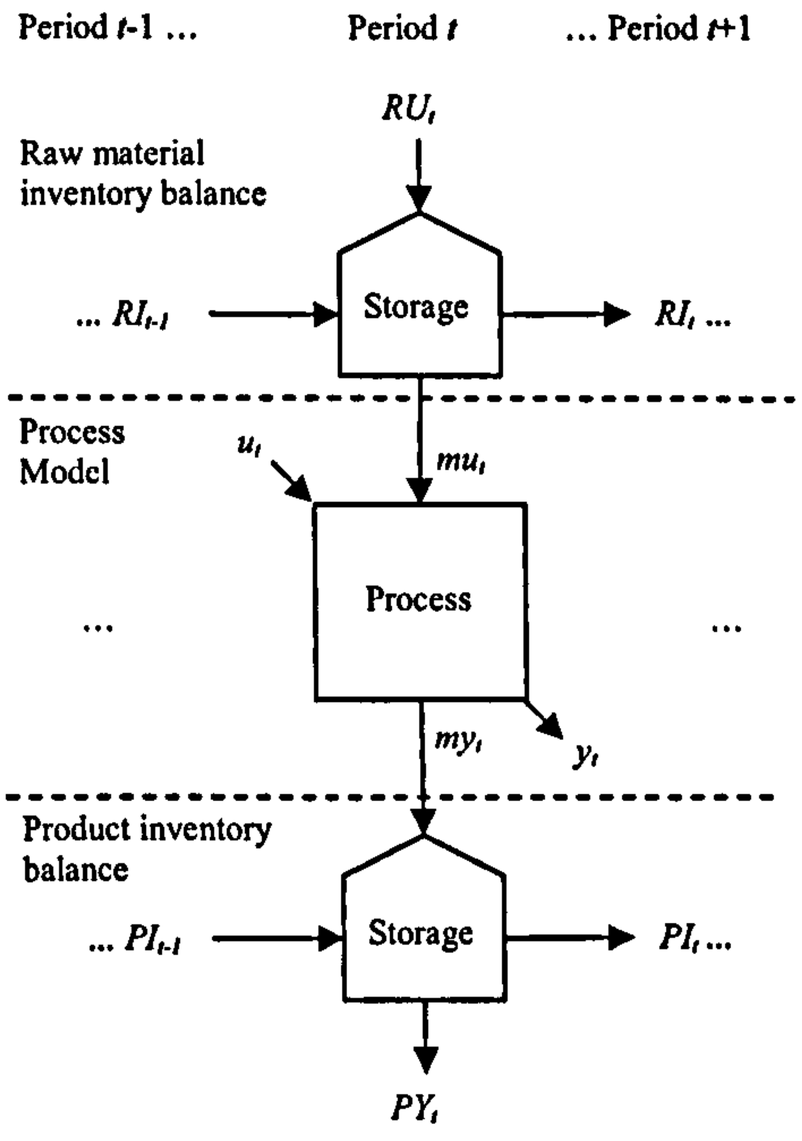

Figure 5.3: Generalised divisions of the multi-period model.

and the output variables (y) respectively. They can formulate the two inventory balances together with the raw material fresh feed (RU), the raw material inventory (RI), the product sale (PY) and the product inventory (PI). The objective of the multi-period model can be solely calculated by these variables, u, y, RU, RI, PY and PI.

The objective of the single-site multi-period optimisation is to maximise the overall profit for the time horizon by varying the process operating variables (u, mu & RU) and the inventory levels (RI & PI) in each period. Additionally, the final solution has to satisfy all the variable bounds. The mathematical representation of the problem is described below.

Indices:

i	Process model input variable index.
j	Process model output variable index.
k	Raw material specie index, $k \in i$.
l	Product specie index, $l \in j$.
t	Time period index.

Variables:

$u_{i,t}$	Process model input variable i at time period t.
$mu_{k,t}$	Raw material k consumption rate at time period t, $mu_{k,t} \in u_{i,t}$
$y_{j,t}$	Process model output variable j at time period t.
$my_{l,t}$	Product l production rate at time period t, $my_{l,t} \in y_{j,t}$.
$RU_{k,t}$	Fresh feed flowrate of raw material k at time period t.

$RI_{k,t}$	Inventory of raw material k at the end of time period t.
$PY_{l,t}$	Sale of product l at time period t.
$PI_{l,t}$	Inventory of product l at the end of time period t.
P_t	Profit at time period t.
TP	Total profit of the time horizon.

Parameters:

$\alpha_{i,t}^{u}$	Price/cost associated with variable $u_{i,t}$.
$\alpha_{j,t}^{y}$	Price/cost associated with variable $y_{j,t}$.
$\beta_{k,t}^{RU}$	Purchase cost of raw material k at time period t.
$\beta_{l,t}^{PY}$	Sale price of product l at time period t.
$\gamma_{k,t}^{RI}$	Inventory cost of raw material k at time period t.
$\gamma_{l,t}^{PI}$	Inventory cost of product l at time period t.
$u_{i,t}^{\min}$, $u_{i,t}^{\max}$	Lower and upper bounds of input variable $u_{i,t}$ respectively.
$y_{j,t}^{\min}$, $y_{j,t}^{\max}$	Lower and upper bounds of output variable $y_{j,t}$ respectively.
$RU_{k,t}^{\min}, RU_{k,t}^{\max}$	Lower and upper bounds of raw material feedstock $RU_{k,t}$ respectively.
$RI_{k,t}^{\min}, RI_{k,t}^{\max}$	Lower and upper bounds of raw material inventory $RI_{k,t}$ respectively.
$PY_{l,t}^{\min}, PY_{l,t}^{\max}$	Lower and upper bounds of product sale $PY_{l,t}$ respectively.
$PI_{l,t}^{\min}, PI_{l,t}^{\max}$	Lower and upper bounds of product inventory $PI_{l,t}$ respectively.
I	The total number of the input variables u_i.
J	The total number of the output variables y_j.

PD_t Duration of the time period t.

Equations:

$f_{j,t}$ Mathematical relations of y_j in terms of $\forall u_i$, both linear and nonlinear, at time period t.

Process Model:

$$y_{j,t} = f_{j,t}\left(u_{1,t}, u_{2,t}, u_{3,t}, \cdots, u_{I,t}\right) \quad \text{(Eq. 5.1)}$$

$$u_{i,t}^{\min} \le u_{i,t} \le u_{i,t}^{\max} \quad \text{(Eq. 5.2)}$$

$$y_{j,t}^{\min} \le y_{j,t} \le y_{j,t}^{\max} \quad \text{(Eq. 5.3)}$$

Raw material inventory balance:

$$RI_{k,t} = RI_{k,t-1} + RU_{k,t} - mu_{k,t} \cdot PD_t \quad \text{(Eq. 5.4)}$$

$$RI_{k,t}^{\min} \le RI_{k,t} \le RI_{k,t}^{\max} \quad \text{(Eq. 5.5)}$$

$$RU_{k,t}^{\min} \le RU_{k,t} \le RU_{k,t}^{\max} \quad \text{(Eq. 5.6)}$$

Product inventory balance:

$$PI_{l,t} = PI_{l,t-1} + my_{l,t} \cdot PD_t - PY_{l,t} \quad \text{(Eq. 5.7)}$$

$$PI_{l,t}^{\min} \le PI_{l,t} \le PI_{l,t}^{\max} \quad \text{(Eq. 5.8)}$$

$$PY_{l,t}^{\min} \le PY_{l,t} \le PY_{l,t}^{\max} \quad \text{(Eq. 5.9)}$$

Profit of time period t:

$$P_t = \left[\sum_i \alpha^u_{i,t} \cdot u_{i,t} + \sum_j \alpha^y_{j,t} \cdot y_{j,t} - \sum_k \beta^{RU}_{k,t} \cdot RU_{k,t} + \sum_l \beta^{PY}_{l,t} \cdot PY_{l,t} \right. \\ \left. - \sum_k \gamma^{RI}_{k,t} \cdot \tfrac{1}{2}\left(RI_{k,t} + RI_{k,t-1}\right) - \sum_l \gamma^{PI}_{l,t} \cdot \tfrac{1}{2}\left(PI_{l,t} + PI_{l,t-1}\right) \right] \cdot PD_t \qquad \text{(Eq. 5.10)}$$

At $t = 1$, $RI_{k,t-1}$ and $PI_{k,t-1}$ are the initial inventory levels and their values are given as constants in the optimisation.

Objective -- Total profit: $$\max\left(TP = \sum_t P_t \right) \qquad \text{(Eq. 5.11)}$$

5.3 Solution Approaches

This section introduces two new solution approaches to attempt to solve the single-site multi-period problem. They are the Rolling Horizon Approach with four variants and the Feasible Operation Table Approach. The approaches focus on decomposing or simplifying the problem. The Simultaneous Approach, a direct optimisation method, proposed in Chapter 4 however would be used for the case studies if possible.

5.3.1 Simultaneous Approach

The Simultaneous Approach would be tested so long as the computer is capable to handle the large-scale optimisation. The approach does not have any specific solution strategy. It only applies the gPROMS SQP solver to execute a direct optimisation for the multi-period problem. It should result in a solution with good quality but a long computational time.

5.3.2 Rolling Horizon Approach

"Rolling Horizon" is a decomposition technique for multi-period problems (Shah, 1992; Dimitriadis *et al.*, 1997). The time horizon in the multi-period problem is evidently a collection of individual time periods. The periods are only connected to their neighbours by some "linking" variables. It is straightforward to separate the time horizon into separate time intervals through the "linking" variables. In the case of this chapter, the "linking" variables are raw material and product inventories only. This transforms the attempted multi-period problem into a set of time interval problems together with an inventory allocation problem.

The Rolling Horizon Approach is proposed to settle the inventory allocation when the disconnected time interval problems can be solved in a site-wide fashion and independently. In the Rolling Horizon Approach, the interval problems will be optimised either in the forward order or the reverse order of time. The former is called forward rolling and the latter is called backward rolling. The time intervals can contain more than one period providing the periods are adjacent to each other. The interval profit is maximised. The optimised inventory levels of the interval are transferred to the next interval by fixing the corresponding variables. The next interval is then optimised. After the whole time horizon is solved, all the interval results are integrated to obtain the overall solution of the original problem. The main advantage of the Rolling Horizon Approach is the possibility to solve problems with any number of time periods.

Four variants of the Rolling Horizon Approach are studied here, (1) Forward Rolling, One-at-a-time (FR-1); (2) Backward Rolling, One-at-a-time (BR-1); (3) Backward Rolling, Two-at-a-time (BR-2); and (4) Backward Rolling, Hybrid 2/1

(BR-HB). They are classified according to their time rolling directions and their time interval lengths.

5.3.2.1 Forward Rolling, One-at-a-time (FR-1)

The FR-1 Approach is a basic form of the forward rolling approach. Each disconnected time interval contains a single time period only, and the solution procedure starts from the beginning of the time horizon. The inventory levels at the end of each period ($RI_{k,t}$ & $PI_{k,t}$) are determined during each period's optimisation. Their values are passed on to the next period. The approach moves a period forwards every time the period optimisation finishes, until the end of the time horizon (Figure 5.4).

The overall solution quality of the approach depends greatly on the inventory levels estimated in the individual period optimisations. The period inventory levels cannot be changed once they have been determined. Hence, each period must be able to estimate how valuable its inventory is to the whole problem. To achieve this,

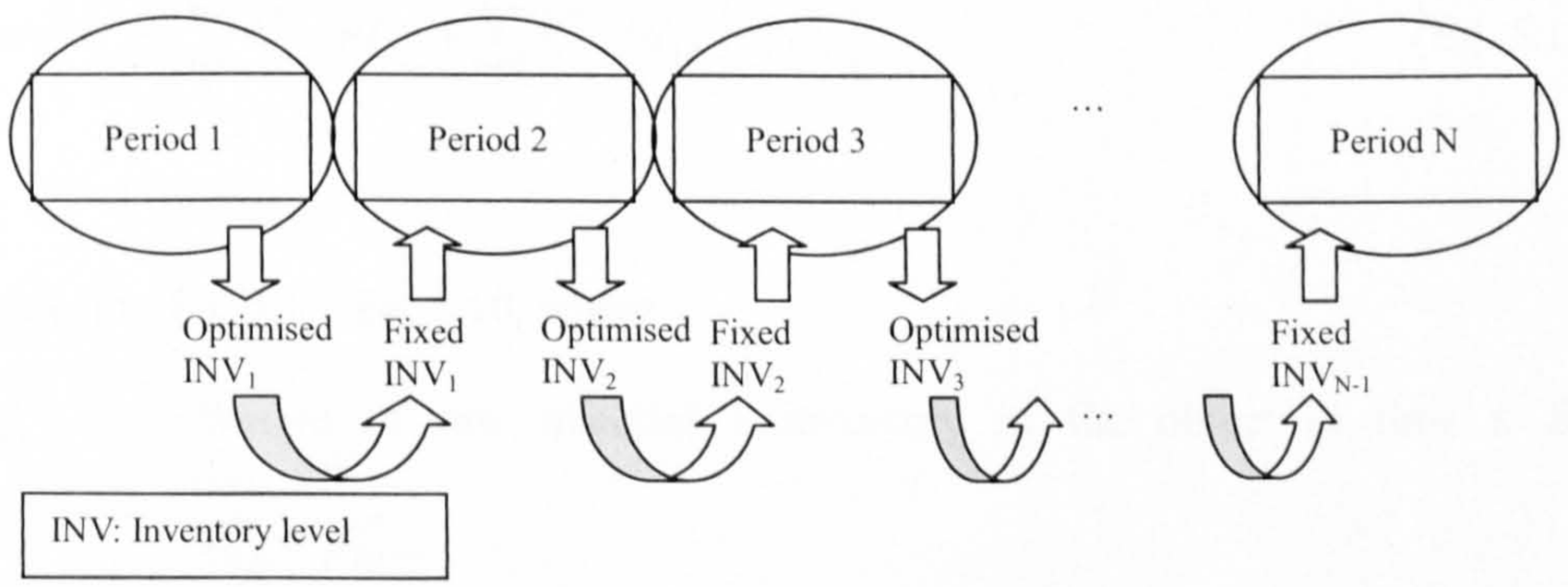

Figure 5.4: FR-1 approach schematic diagram.

inventory terms with user-defined weights have to be added to the optimisation objective.

Suitable weights of the inventory terms are vital for obtaining a good overall solution. The inventory carried over to the next period can be thought of "selling to the next period". Then the inventory terms should appear with a positive sign in the objective function. The inventory should only be passed on if it is profitable. The material price difference between periods is an important factor in deciding whether keeping inventory is profitable or not. It is usually worth building up inventory when the material price is higher in the future. Therefore, the subsequent period's material price is a sensible value for the weight of the inventory term.

The FR-1 Approach forms its sub-problem with equations from Eq. 5.1 to Eq. 5.10 and a modified objective Eq. 5.12. The solution of the original problem can be obtained by combining the results of all periods, and the overall objective value can be calculated via Eq. 5.11. The FR-1 Approach is summarised in Figure 5.5.

FR-1 sub-problem (FR-1-SP):

$$\max\left(P_t + \left(\sum_k \lambda_{k,t}^{RI} \cdot RI_{k,t} + \sum_l \lambda_{l,t}^{PI} \cdot PI_{l,t}\right) \cdot PD_t\right) \qquad \text{(Eq. 5.12)}$$

Subject to Eq. 5.1 – Eq. 5.10, where

$\lambda_{k,t}^{RI}$ Weight of raw material k inventory in the object at time t. Set $\lambda_{k,t}^{RI} = \beta_{k,t+1}^{RI}$.

$\lambda_{l,t}^{PI}$ Weight of product l inventory in the objective at time t. Set $\lambda_{l,t}^{PI} = \beta_{l,t+1}^{PI}$.

(1) Set $t = 1$.
(2) Optimise sub-problem FR-1-SP for Period t.
(3) Obtain inventory variables $RI_{k,t}$ & $PI_{l,t}$ from (2).
(4) If $t <$ N (total number of periods), then set $t = t + 1$ and go to (5). Else STOP.
(5) Fix $RI_{k,t-1}$ & $PI_{l,t-1}$ with the values in (3) and go to (2).

Figure 5.5: FR-1 approach.

5.3.2.2 Backward Rolling, One-at-a-time (BR-1)

The BR-1 Approach is the counterpart of the FR-1 Approach in the form of backward rolling. The BR-1 Approach also decomposes the horizon period-by-period, but it starts the optimisation from the end of the horizon. The period optimisation will determine the inventory levels at the beginning of the period ($RI_{k,t-1}$ & $PI_{k,t-1}$). These values are then sent to the next optimisation, which is the previous period. After each optimisation, the BR-1 Approach moves back a period until the start of the time horizon (Figure 5.6).

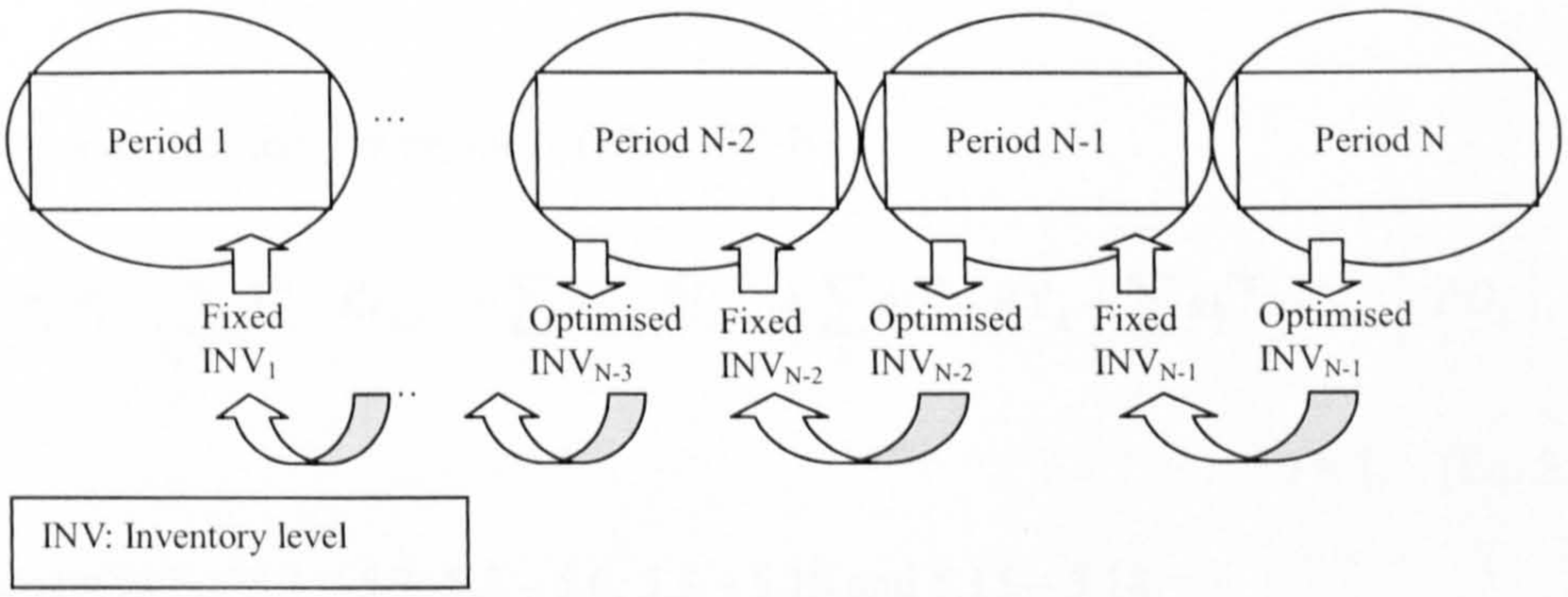

Figure 5.6: BR-1 approach schematic diagram.

Bringing forward the inventories from the pervious period can be considered as "purchasing the inventory". Therefore, the period optimisation objective should include penalty terms of the "purchased inventories". The material prices in the preceding period could be reasonable values for the penalty weights.

The estimation of the opening inventory in the period, however, does not guarantee the availability of the material. If there is not enough production or inventory in previous periods, the backlog of the material is continuously accumulated to the first period. Infeasibility occurs when the production and the initial inventory in the first period cannot provide the entire backlog. To remove the infeasibility from the overall solution, another group of penalty variables with relatively high penalty weights is introduced to the optimisation of the first period. Hence the BR-1 Approach involves two sub-problems.

BR-1 sub-problem for period 2 and onwards (BR-1-SP-A):

$$\max\left(P_t - \left(\sum_k \lambda_{k,t}^{RI} \cdot RI_{k,t-1} + \sum_l \lambda_{l,t}^{PI} \cdot PI_{l,t-1} \right) \cdot PD_t \right), t = 2, 3, 4, \ldots \quad \text{(Eq. 5.13)}$$

Subject to Eq. 5.1 – 5.10.

BR-1 sub-problem for period 1 (BR-1-SP-B):

$$\max\left(P_t - \left(\sum_k \lambda_{k,t}^{RI} \cdot RI_{k,t-1} + \sum_l \lambda_{l,t}^{PI} \cdot PI_{l,t-1} + \sum_k \omega_k^{RX} \cdot RX_k + \sum_l \omega_l^{PX} \cdot PX_l \right) \cdot PD_t \right),$$

$t = 1$. (Eq. 5.14)

Subject to Eq. 5.1 – 5.3, 5.5 – 5.6, 5.8 – 5.10 and 5.15 – 5.18.

Raw material inventory balance in period 1

$$RI_{k,t} = RI_{k,t-1} + RU_{k,t} - mu_{k,t} \cdot PD_t + RX_k, t = 1. \quad \text{(Eq. 5.15)}$$

$$0 \le RX_k \quad \text{(Eq. 5.16)}$$

Product inventory balance in period 1

$$PI_{l,t} = PI_{l,t-1} + my_{l,t} \cdot PD_t - PY_{l,t} + PX_l, t = 1. \quad \text{(Eq. 5.17)}$$

$$0 \le PX_l \quad \text{(Eq. 5.18)}$$

where

RX_k Penalty variable for raw material k inventory.

PX_l Penalty variable for product l inventory.

$\lambda_{k,t}^{RI}$ Weight of raw material k inventory in the objective at time t. Set $\lambda_{k,t}^{RI} = \beta_{k,t-1}^{RI}$.

$\lambda_{l,t}^{PI}$ Weight of product l inventory in the objective at time t. Set $\lambda_{l,t}^{PI} = \beta_{l,t-1}^{PI}$.

ω_k^{RX} Weight of raw material k inventory penalty.

ω_l^{PX} Weight of product l inventory penalty.

The BR-1 Approach firstly uses the BR-1-SP-A sub-problem to obtain results from the last period to the second period. It then changes to the BR-1-SP-B sub-problem to complete the first period (Figure 5.7). If the penalty variables (RX_k & PX_l) have positive values in the first period result, their magnitudes reflect the amounts of the unavailable inventories. They should be removed from the inventory levels. This can be accomplished by fixing RX_k and PX_l to zero and resetting the inventory levels for all periods by Eq. 5.19 and Eq. 5.20. After the

(1) Set t = N (total number of periods).
(2) Optimise sub-problem BR-1-SP-A for period t.
(3) Obtain inventory variables $RI_{k,t-1}$ & $PI_{l,t-1}$ from (2).
(4) Set $t = t - 1$ & fix $RI_{k,t}$ & $PI_{l,t}$ with the values in (3).
(5) If $t > 1$, go to (2). Else go to (6).
(6) Solve sub-problem BR-1-SP-B and obtain penalty variables RX_k, PX_l.
(7) If $RX_k > 0$, apply Equ. (5.8) for periods t = 1 to N.
(8) If $PX_l > 0$, apply Equ. (5.9) for periods t = 1 to N.
(9) STOP

Figure 5.7: BR-1 approach.

removal of the unavailable inventory, the individual period results are combined to form the solution of the original problem. Eq. 5.11 is then used to back calculate the overall objective.

$$RI_{k,t} = \max\left(RI_{k,t} - RX_k, RI_{k,t}^{\min}\right), t = 1, 2, 3, \ldots \quad \text{(Eq. 5.19)}$$

$$PI_{l,t} = \max\left(PI_{l,t} - PX_l, PI_{l,t}^{\min}\right), t = 1, 2, 3, \ldots \quad \text{(Eq. 5.20)}$$

5.3.2.3 Backward Rolling, Two-at-a-time (BR-2)

The BR-2 Approach is a modified version of the BR-1 Approach. It employs the same mechanism as the BR-1 Approach, except two periods are grouped in a time interval. This strategy intends to capture the interactions between two adjacent periods directly, and hence to produce a better inventory level estimation. The approach starts from optimising the last two periods together and determines the inventory levels at the beginning of the second last period. The approach then rolls back two periods for the next optimisation. The rolling proceeds until the first

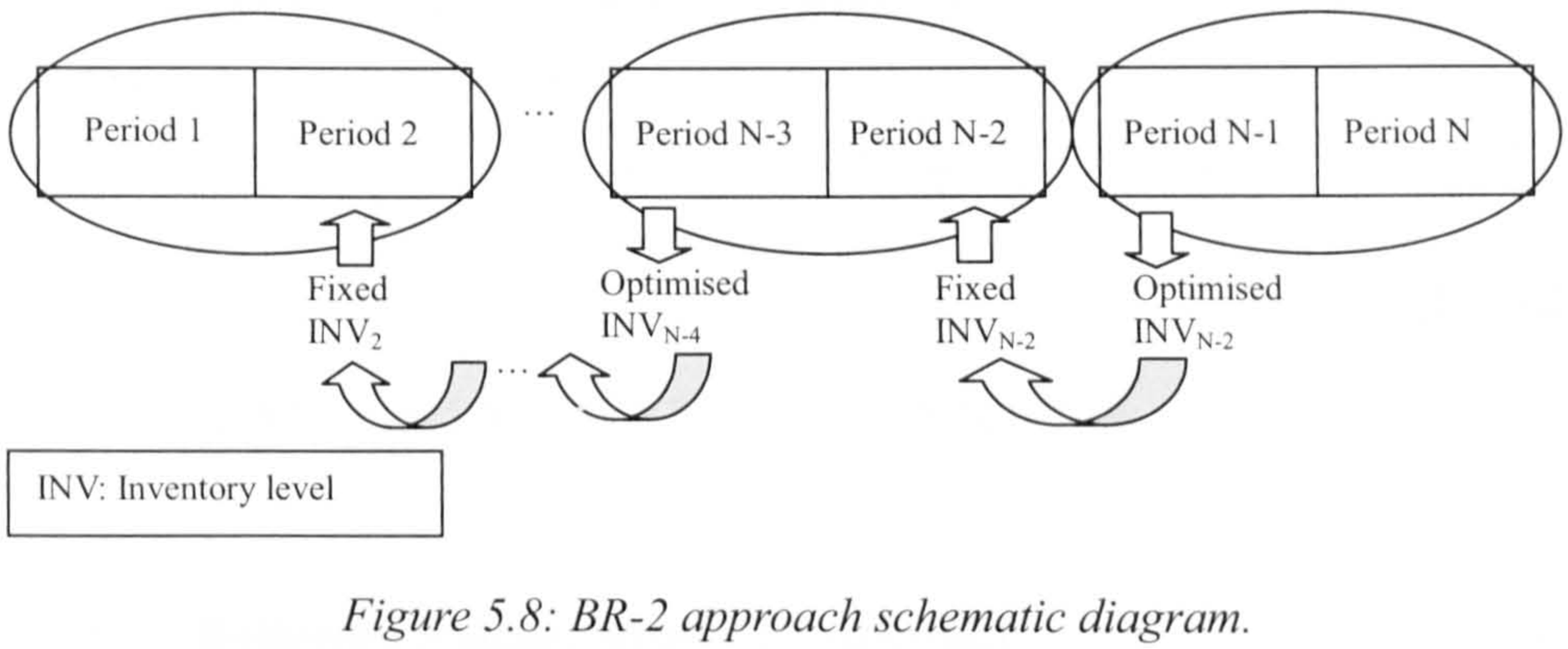

Figure 5.8: BR-2 approach schematic diagram.

(1) Set t = N (total number of periods).
(2) Optimise sub-problem BR-2-SP-A for periods t & $t-1$.
(3) Obtain inventory variables $RI_{k,t-2}$ & $PI_{l,t-2}$ from (2).
(4) Set $t = t-2$ & fix $RI_{k,t}$ & $PI_{l,t}$ with the values in (3).
(5) If $t > 2$, go to (2). Else go to (6).
(6) Solve sub-problem BR-2-SP-B and obtain penalty variables RX_k, PX_l.
(7) If $RX_k > 0$, apply Equ. (5.8) for periods t = 1 to N.
(8) If $PX_l > 0$, apply Equ. (5.9) for periods t = 1 to N.
(9) STOP

Figure 5.9: BR-2 approach.

period is reached (Figure 5.8). After the whole time horizon is optimised, the infeasibility removal procedures are carried out as in the BR-1 Approach (Figure 5.9). For convenience, the BR-2 Approach is only applied on problems with an even number of periods. The BR-2 sub-models are reported below.

BR-2 sub-problem for period 3 and onwards (BR-2-SP-A):

$$\max\left(P_t + P_{t-1} - \left(\sum_k \lambda^{RI}_{k,t-1} \cdot RI_{k,t-2} + \sum_l \lambda^{PI}_{l,t-1} \cdot PI_{l,t-2} \right) \cdot PD_{t-1} \right), t \geq 3. \qquad \text{(Eq. 5.21)}$$

Subject to Eq. 5.1 – 5.10.

BR-2 sub-problem for periods 1 and 2 (BR-2-SP-B):

$$\max\left(P_t + P_{t-1} - \left(\sum_k \lambda_{k,t-1}^{RI} \cdot RI_{k,t-2} + \sum_l \lambda_{l,t-1}^{PI} \cdot PI_{l,t-2} + \sum_k \omega_k^{RX} \cdot RX_k + \sum_l \omega_l^{PX} \cdot PX_l \right) \cdot PD_{t-1} \right)$$

$t = 2.$ (Eq. 5.22)

Subject to Eq. 5.1 – 5.3, 5.5 – 5.6, 5.8 – 5.10 and 5.15 – 5.18.

5.3.2.4 Backward Rolling, Hybrid 2/1 (BR-HB)

Hybrid 2/1 (BR-HB) is the final backward rolling strategy tested in this chapter. It adopts two time periods in one disconnected interval, but it only moves back a period in every optimisation (Figure 5.10). The inventory levels in between two periods obtained in the optimisation are transferred to the next round. As the intermediate inventory levels are directly optimised without adding any weight on the objective function, the results are expected to be more reliable. Using these results in the subsequent optimisation should be able to enhance the approach accuracy. The sub-models of the BR-HB Approach are the same as the BR-2 Approach. It also applies the identical infeasibility removal procedures as well (Figure 5.11).

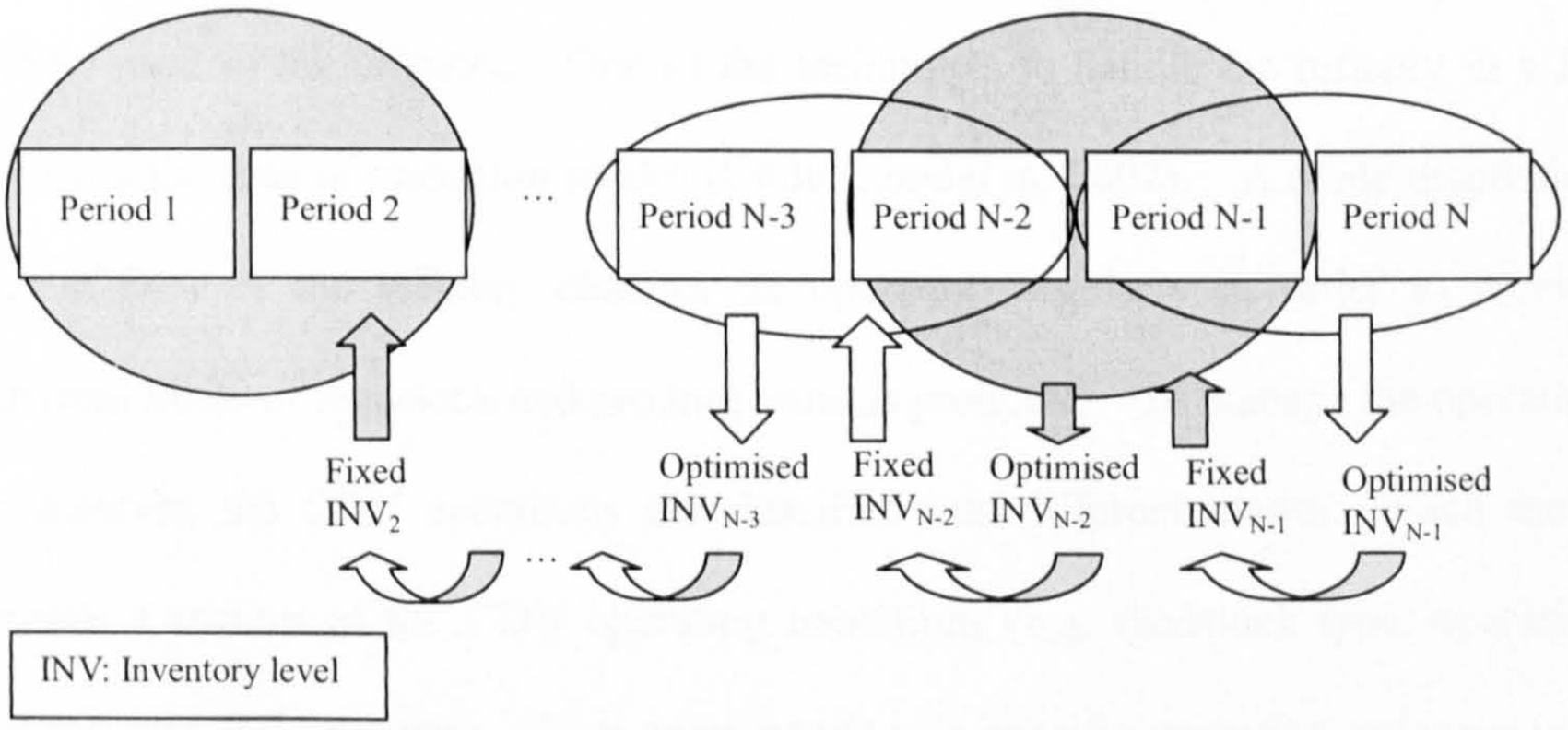

Figure 5.10: BR-HB approach schematic diagram.

(1) Set t = N (total number of periods).
(2) Optimise sub-problem BR-2-SP-A for periods t & $t-1$.
(3) Obtain inventory variables $RI_{k,t-1}$ & $PI_{l,t-1}$ from (2).
(4) Set $t = t-1$ & fix $RI_{k,t}$ & $PI_{l,t}$ with the values in (3).
(5) If $t > 1$, go to (2). Else go to (6).
(6) Solve sub-problem BR-2-SP-B and obtain penalty variables RX_k, PX_l.
(7) If $RX_k > 0$, apply Equ. (5.8) for periods t = 1 to N.
(8) If $PX_l > 0$, apply Equ. (5.9) for periods t = 1 to N.
(9) STOP

Figure 5.11: BR-HB approach.

5.3.3 Feasible Operation Table Approach (FOT)

The FOT Approach simplifies the multi-period problem into a mixed integer linear programming (MILP) problem, and solves it for the whole time horizon at once. Using linear programming (LP) for supply chain management is a common practice in petroleum refining industry (Sahdev *et al.*, ca. 1999). Several commercial software packages, including PIMS from Aspen Technology (AspenTech, 2007), RPMS from Honeywell (Honeywell, 2007; Mostovoi & Khokhlov, 2007) and GRTMPS from Haverly Systems, Inc. (Haverly, 2003), have been developed and widely used in the industry. One of the techniques to handle the refinery in a LP model is the idea of operation modes (Göthe-Lundgren, 2002). A crude distillation unit (CDU) in the refinery changes its operation regularly in order to receive different kinds of feedstock and produce various products. To manage the operation changeover, the CDU operations are classified into different modes. Each mode records a pattern of the CDU operating conditions (e.g. feedstock type, operating temperature and pressure), which corresponds to a specific operation outcome (e.g. product type, product quality and production yield). Therefore, the LP model can

solve the refinery supply chain problem via selecting suitable operation modes. The FOT Approach attempts to use the same idea in the ethylene process.

The first step of the FOT Approach is to construct a feasible operation table for the ethylene process. In the feasible operation table, the operation modes should be designed for different operation cases, such as, a high ethylene production case with mainly ethane feedstock or a high ethylene production case with mainly propane feedstock. To ensure the operation modes are accurate, feasible and effective, optimisations are executed on the rigorous ethylene process model (single-site single-period model) with the objective including the designed operation cases. After the optimisations, the process model's input variables (u_i) and output variables (y_j) are listed in the feasible operation table.

Once the process operation is simplified as a set of alternative operation modes, the FOT model is only required to choose a suitable mode for the plant for each time period and allocate inventories across the time horizon. The mode selection can be accomplished by using linear formulations and integer variables. The inventory allocation and the objective calculation also only involve linear equations. A multi-period mixed integer linear programming (MILP) model is hence sufficient for the FOT Approach. To express the idea, new elements are required.

New indices:

md	Operation mode index.

New binary variables:

$z_{md,t}$	Status of the operation mode *md* in period *t*. 1 is on and 0 is off.

New parameters:

$UO_{i,md}$ Value of input variable u_i in operation mode *md*.

$YO_{j,md}$ Value of output variable y_j in operation mode *md*.

$MUO_{k,md}$ Value of raw material consumption rate mu_k in operation mode *md*.

$MYO_{l,md}$ Value of product production rate my_l in operation mode *md*.

New equations for process operations:

$$u_{i,t} = \sum_{md} \left(UO_{i,md} \times z_{md,t} \right) \quad \text{(Eq. 5.23)}$$

$$y_{j,t} = \sum_{md} \left(YO_{j,md} \times z_{md,t} \right) \quad \text{(Eq. 5.24)}$$

$$mu_{k,t} = \sum_{md} \left(MUO_{k,md} \times z_{md,t} \right) \quad \text{(Eq. 5.25)}$$

$$my_{l,t} = \sum_{md} \left(MYO_{l,md} \times z_{md,t} \right) \quad \text{(Eq. 5.26)}$$

$$\sum_{md} z_{md,t} = 1, \; z_{md,t} = 0 \text{ or } 1. \quad \text{(Eq. 5.27)}$$

The new equations (Eq. 5.23 – Eq. 5.27) represent the selection of the operation modes over the periods. They replace the process model equations (Eq. 5.1 – 5.3). They join other existing equations of the raw material inventory balance, the product inventory balance and the profit calculation (Eq. 5.4 – Eq. 5.10) to form the FOT MILP model. The model objective is still to maximise the total profit, which has already been described by Eq. 5.11.

All advantages of the FOT Approach stem from the feasible operation table. The table skips all the process operation details in the approach. This makes the FOT MILP model fairly small. Although the model has already included all time

periods, the FOT approach is still expected to be very fast. Also, because a complete time horizon is considered in the model, it should give a good inventory allocation result. In addition, the feasible modes in the table ensure that the approach result is operationally feasible. The only possible drawback is that the pre-designed operational modes might not fit the problem very well and lead to a poor overall result.

5.4 Case Studies

The two examples studied in this section are based on the 5-column ethylene process. The first one is the 3-period example, and the second one is the 4-period example. The approaches used to solve the example were all implemented on a Linux machine with CPU speed 1794 MHz.

5.4.1 3-Period Example

The 3-period example involves three time periods, each of which lasts for 604,800 seconds (7 days). The process in the three periods is the 5-column ethylene process. It accepts three kinds of feedstock, ethane, propane and butane. The process produces ethylene as the main product and propylene and C4 chemicals as by-products. The objective of the example is to maximise the total profit over the 3-period horizon by varying the process input variables and allocating material inventories.

The final solution of the example also has to comply with the constraints set in the problem. The original polynomial constraints concerning the flooding velocity and the weep point of the distillation column in Chapter 3 have been replaced by the

ratio of the boil-up to reflux. The ratio is bounded in a selected range to approximate the feasible operation region. This helps to relieve some of the complexity in the multi-period model. The constraints could in principle have different values in different periods though they do not vary in the example. The material and utility prices are the only parameters to vary across the periods. Tables 5.1, 5.2 and 5.3 report the input, output and inventory variables respectively, together with their constraints and prices/costs. A base case with the objective $\$0.2814\times10^6$ was set as the starting point of the approaches.

Table 5.1: Input variables of 3-period example.

			Price/Cost in Period		
Input Variables	Min.	Max.	1	2	3
Ethane fresh feed (kg/s)	2.5	15.0	-0.26	-0.40	-0.30
(Ethane feed mass compositions: C_2H_6: 70%, C_3H_8: 15%, C_4H_6: 15%					
Propane fresh feed (kg/s)	2.5	15.0	-0.30	-0.30	-0.35
(Propane feed mass compositions: C_3H_8: 70 %, n-C_4H_{10}: 15 %, iso-C_4H_{10}: 15 %)					
Butane fresh feed (kg/s)	2.5	15.0	-0.43	-0.30	-0.40
(Butane feed mass compositions: n-C_4H_{10}: 50 %, iso-C_4H_{10}: 50 %)					
Ethane consumption (kg/s)	1.0	15.0			
Propane consumption (kg/s)	1.0	15.0			
Butane consumption (kg/s)	1.0	15.0			
Steam feed (kg/s)	1.0	20.0	-0.01	-0.01	-0.01
Reactor heat flux (kJ/m^{2}s)	30.0	45.0	-2E-4	-2E-4	-2E-4
Demethaniser boil-up, Bup1	0.5	3.0			
Demethaniser reflux, R1	0.5	3.0			
Deethaniser boil-up, Bup2	0.5	3.0			
Deethaniser reflux, R2	0.5	3.0			
C2 splitter boil-up, Bup3	0.5	5.0			
C2 splitter reflux, R3	0.5	5.0			
Depropaniser boil-up, Bup4	0.5	4.0			
Depropaniser reflux, R4	0.5	4.0			
C3 splitter boil-up, Bup5	0.5	5.0			
C3 splitter reflux, R5	0.5	5.0			
			Period 1	Period 2	Period 3
Period Duràtion (s)			604,800	604,800	604,800

N.B. Shaded area indicates variations across periods.

Table 5.2: Output variables of 3-period example.

Output Variables	Min.	Max.	Price/Cost in Period 1	2	3
Reactor steam dilution ratio	0.4	1.0			
Reactor inlet flowrate (kg/s)	0.0	32.4			
Reactor outlet pressure (kPa)	150.0				
Reactor outlet temperature (K)	0	1,200			
Demethaniser condenser duty, Qc1 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5
Demethaniser reboiler duty, Qr1 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5
Deethaniser condenser duty, Qc2 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5
Deethaniser reboiler duty, Qr2 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5
C2 splitter condenser duty, Qc3 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5
C2 splitter reboiler duty, Qr3 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5
Depropaniser condenser duty, Qc4 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5
Depropaniser reboiler duty, Qr4 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5
C3 splitter condenser duty, Qc5 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5
C3 splitter reboiler duty, Qr5 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5
Demethaniser ratio boilup:reflux	0.3333	3.0000			
Deethaniser ratio boilup:reflux	0.3333	3.0000			
C2 splitter ratio boilup:reflux	0.3333	3.0000			
Depropaniser ratio boilup:reflux	0.3333	3.0000			
C3 splitter ratio boilup:reflux	0.3333	3.0000			
Ethylene product molar purity	0.99	1.00			
Ethylene production rate (kg/s)	2.0	10.0			
Propylene product molar purity	0.90	1.00			
Propylene production rate (kg/s)	1.0	10.0			
C4 stream propylene composition	0.0	0.1			
C4 production rate (kg/s)	0.0				
H_2/CH_4 stream flowrate	0.0		0.05	0.05	0.05
Ethylene sales (kg/s)	1.0	15.0	0.587	0.650	0.550
Propylene sales (kg/s)	1.0	15.0	0.610	0.610	0.650
C4 sales (kg/s)	1.0	15.0	0.650	0.650	0.600

Table 5.3: Inventory variables in 3-period example.

Inventory Variables	Min.	Max.	Initial.	Inventory Cost
Ethane inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Propane inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Butane inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Ethylene inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Propylene inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
C4 inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3

5.4.1.1 Simultaneous Approach Result

The 3-period problem studied here involves total 101,554 equations. The numbers of input and constraint variables related to the optimisation are 63 and 60 respectively. The Simultaneous Approach used the gPROMS SQP solver to optimise all 3 periods at once. It took 40,717 CPU seconds (~ 11 hours) to reach the objective $\$3.4161\times10^{6}$, a more than 11 times increase in profit from the base case objective.

From the result, it is observed that the inventory level decisions were based not only on the price variations, but also on other site-wide factors. Taking ethane and ethylene as the examples, both had the lowest price in the first period and the highest price in the second. There were two possibilities for the optimisation. One was keeping ethane inventory in period 1 and making ethylene in period 2. Another was producing excess ethylene in period 1 and selling it in period 2. To make an appropriate decision, ethane, ethylene and all other material prices would have to be taken into account. Raw material butane had the cheapest price in period 2, which favours the production of C4 chemicals. Also, C4 chemicals were more expensive than propylene in period 2. This made the production of C4 chemicals economically viable in period 2. The Simultaneous Approach therefore chose to manufacture more ethylene in period 1 and keep some in storage to sell in period 2. This boosted both the sales of ethylene and C4 chemicals and the overall profit as the result. The unused ethane purchased in period 1 was used in period 3, since the ethane price that time was still higher than at period 1. In addition, some cheap propane was stocked in period 2 for the use in the last period. At the end of the horizon, all the inventory levels fell to their minimum bounds because no profit

contribution was considered there. Selected results of the Simultaneous Approach are plotted in Figure 5.12.

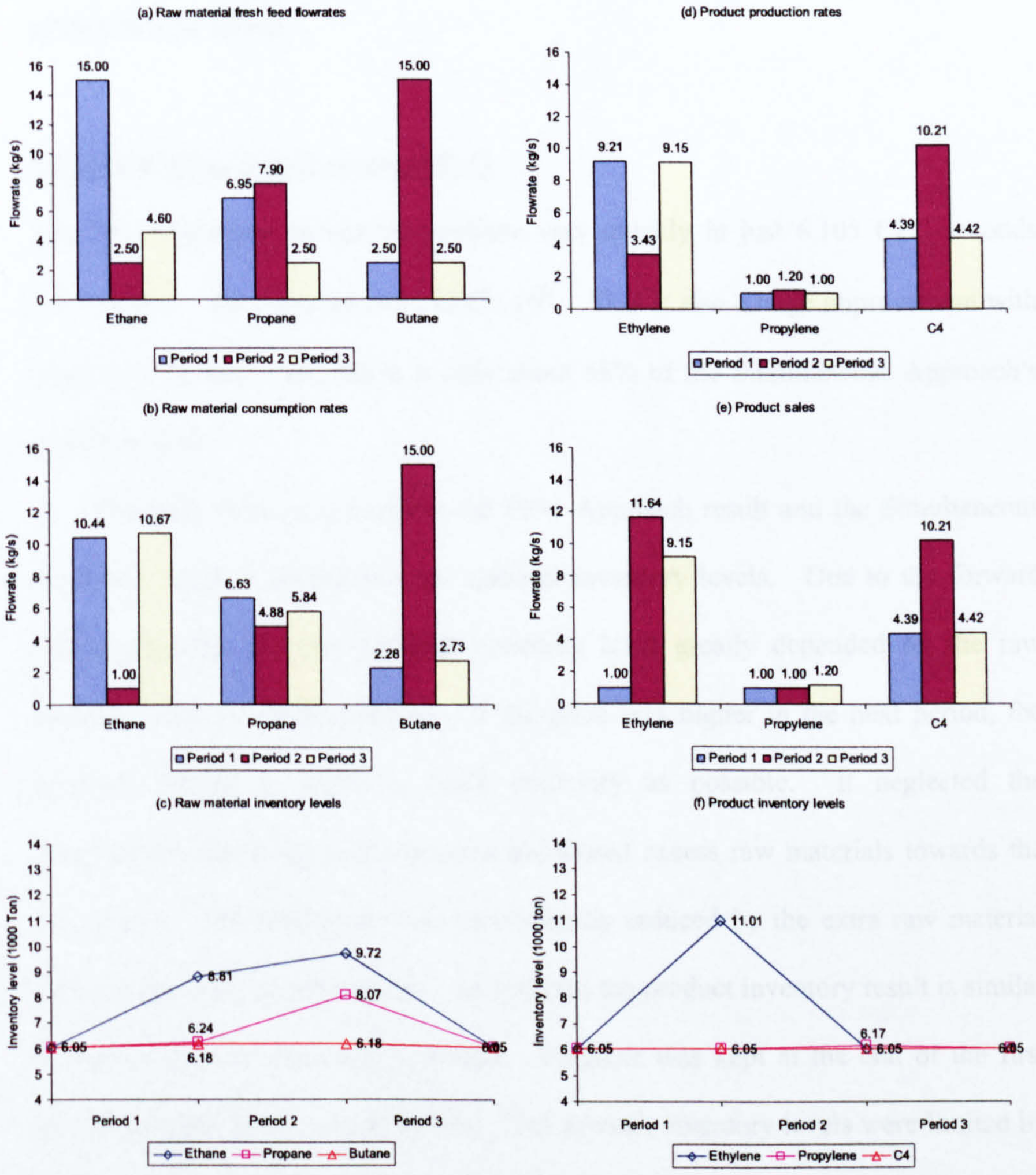

Figure 5.12: Simultaneous Approach selected results of 3-period example.

5.4.1.2 Rolling Horizon Approach Result

The basic forms of the forward rolling (FR-1) and the backward rolling (BR-1) were tested first to obtain some insights on the differences between these approaches. The individual optimisations in the Rolling Horizon Approach were performed by the gPROMS SQP solver.

Forward Rolling, One-at-a-time (FR-1)

The FR-1 Approach solved the problem very quickly in just 6,105 CPU seconds (~1.7 hours). Its objective is \$1.4222× 10^6. That is also a large improvement with respect to the base case, but it is only about 58% of the Simultaneous Approach's objective value.

The main difference between the FR-1 Approach result and the Simultaneous Approach result is around the raw material inventory levels. Due to the forward rolling property, the raw material inventory level greatly depended on the raw material price in the next period. If the price was higher in the next period, the approach tended to keep as much inventory as possible. It neglected the consumption capability of the process and stored excess raw materials towards the last period. The total profit was consequently reduced by the extra raw material cost and the extra inventory cost. In contrast, the product inventory result is similar to that of the Simultaneous Approach. Ethylene was kept at the end of the first period and sold in the second period. The product inventory levels were limited by the production capacity. Also, the product inventory would have to be sold for revenue. These prevented excess product inventory remaining at the end of the horizon (Figure 5.13).

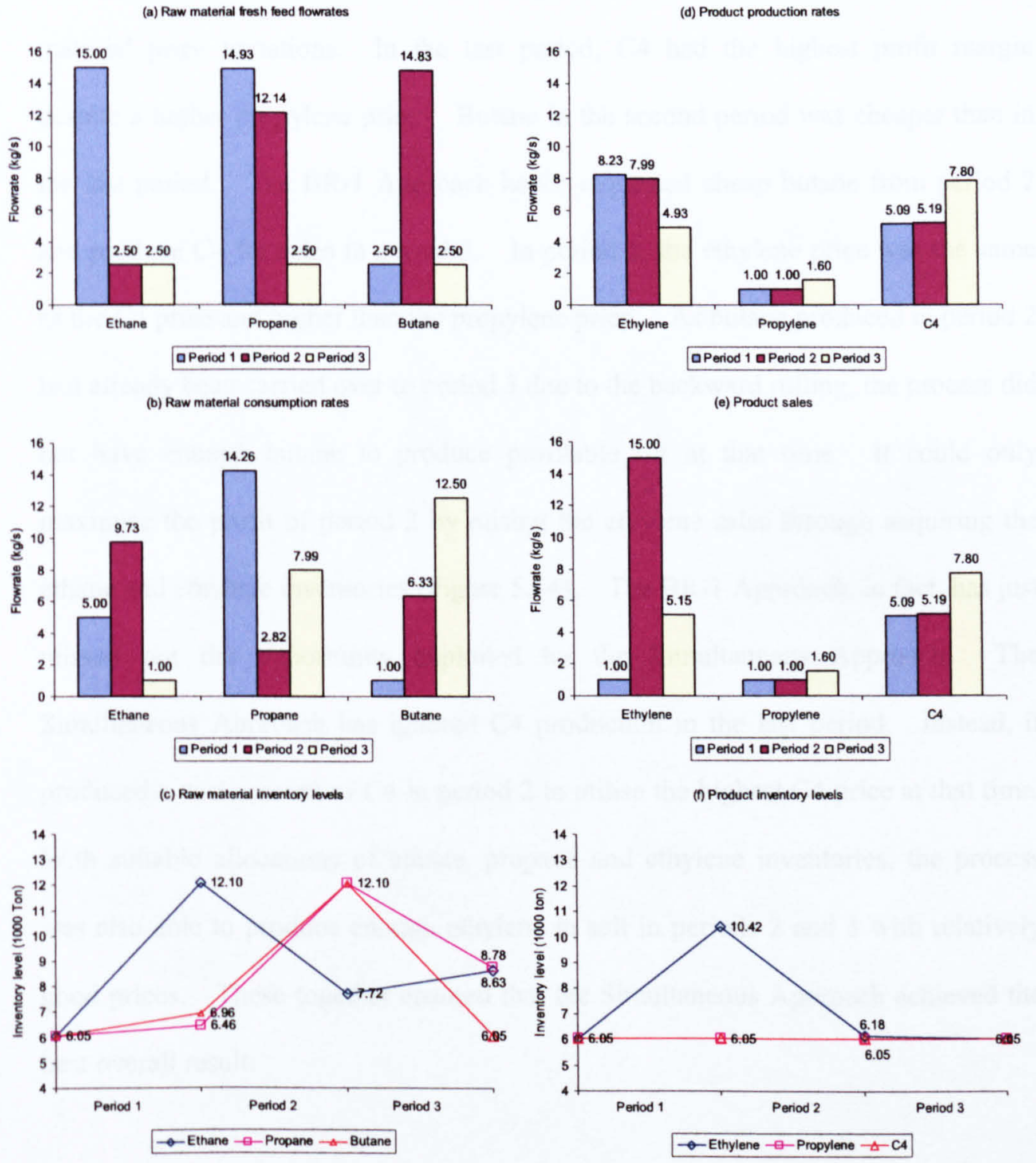

Figure 5.13: FR-1 Approach selected results of 3-period example.

Backward Rolling, One-at-a-time (BR-1)

The BR-1 Approach obtained an optimised total profit of \$3.2291× 10^6 in 17,239 CPU seconds (~4.8 hours). The objective value is about 5.5% less than that of the Simultaneous Approach, but the approach saved 57% of computational time. The backward rolling mechanism ensured that the inventory would be consumed by the following periods. It avoided the situation of excess inventory.

In the BR-1 Approach, the resulting inventory levels also depended on the material price variations. In the last period, C4 had the highest profit margin despite a higher propylene price. Butane in the second period was cheaper than in the last period. The BR-1 Approach hence requested cheap butane from period 2 and produce C4 for sales in period 3. In period 2, the ethylene price was the same as the C4 price and higher than the propylene price. As butane produced in period 2 had already been carried over to period 3 due to the backward rolling, the process did not have enough butane to produce profitable C4 at that time. It could only maximise the profit of period 2 by raising the ethylene sales through acquiring the ethane and ethylene inventories (Figure 5.14). The BR-1 Approach, in fact, has just missed out the opportunity exploited by the Simultaneous Approach. The Simultaneous Approach has ignored C4 production in the last period. Instead, it produced a vast amount of C4 in period 2 to utilise the highest C4 price at that time. With suitable allocations of ethane, propane and ethylene inventories, the process was also able to produce enough ethylene to sell in periods 2 and 3 with relatively good prices. These together ensured that the Simultaneous Approach achieved the best overall result.

Backward Rolling, Hybrid 2/1 (BR-HB)

The BR-1 Approach performed better than the FR-1 Approach in the 3-period example. This suggests that the backward rolling methods might be more powerful than the forward rolling methods. The BR-HB Approach was therefore tested to compare different backward rolling varieties.

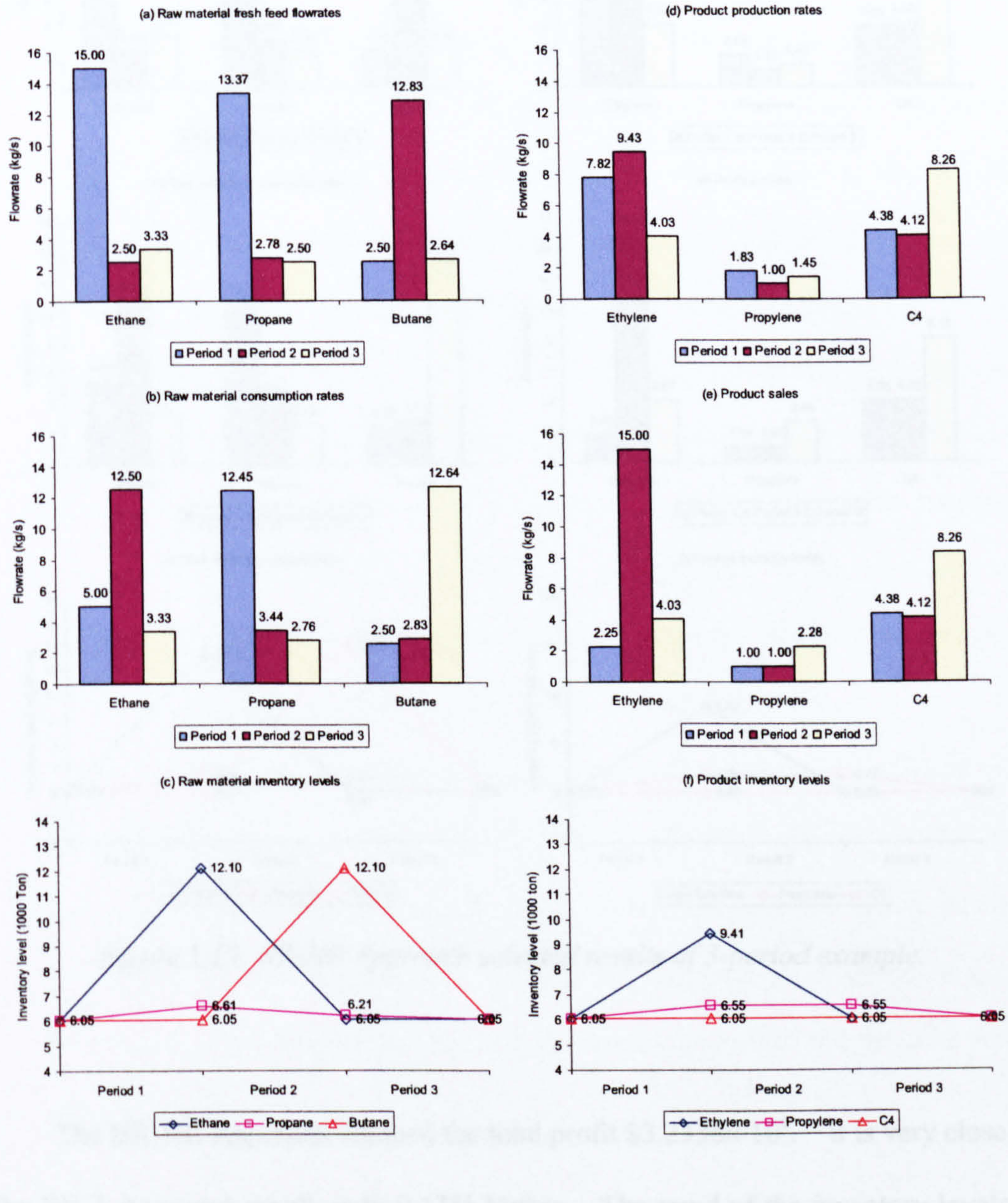

Figure 5.14: BR-1 Approach selected results of 3-period example.

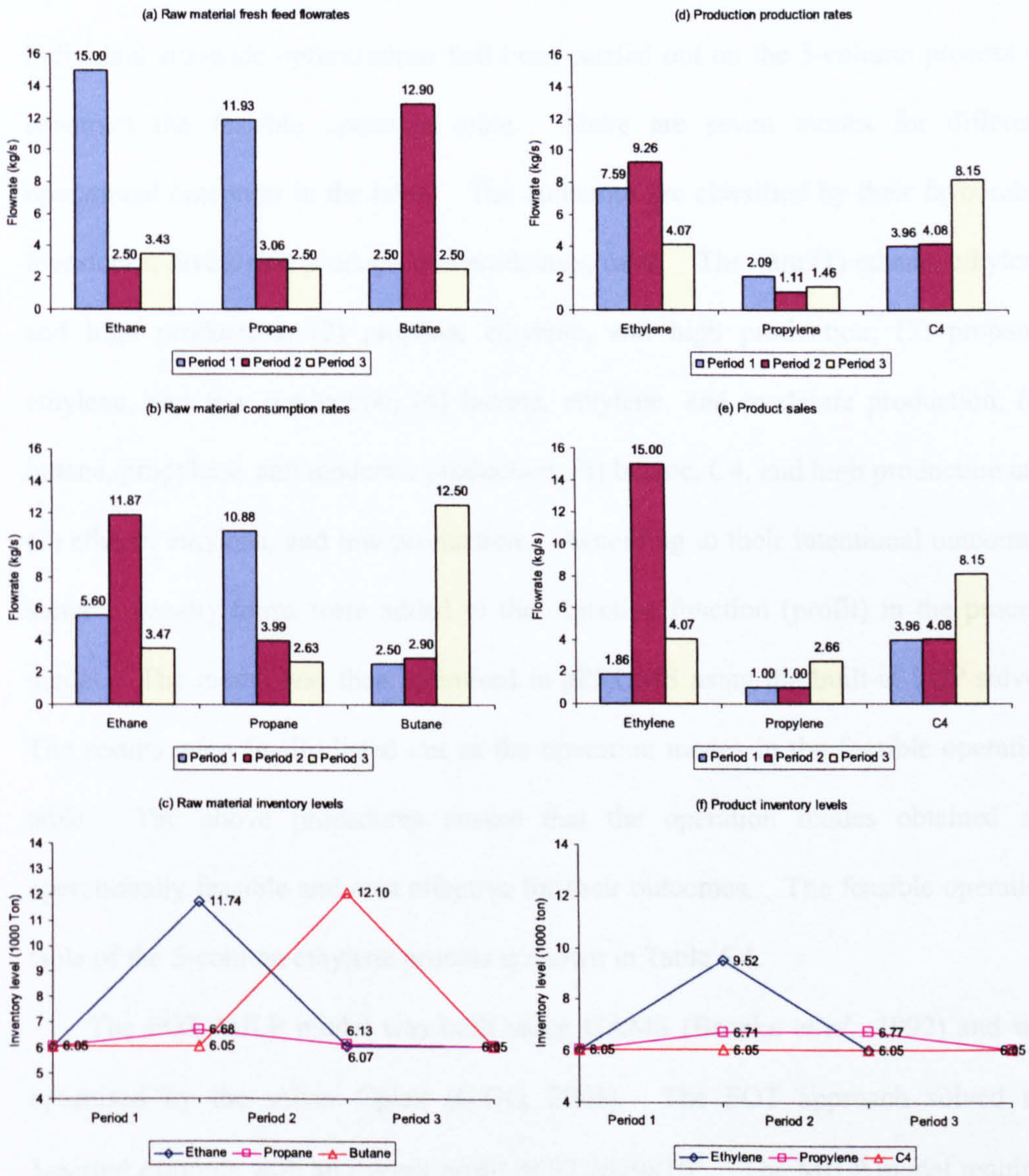

Figure 5.15: BR-HB Approach selected results of 3-period example.

The BR-HB Approach attained the total profit \$3.2336× 10^6. It is very close to the BR-1 Approach result, only 0.13% higher. The trend of the inventory levels is basically the same as the BR-1 Approach (Figure 5.15). The solution time is 26,508 CPU seconds (~7.3 hours). It is faster than the Simultaneous Approach, but takes 53% longer than the BR-1 Approach.

5.4.1.3 Feasible Operation Table Approach Result

Individual site-wide optimisations had been carried out on the 5-column process to construct the feasible operation table. There are seven modes for different operational outcomes in the table. The outcomes are classified by their favourable feedstocks, favourable products and production rates. They are (1) ethane, ethylene, and high production; (2) propane, ethylene, and high production; (3) propane, ethylene, and low production; (4) butane, ethylene, and moderate production, (5) butane, propylene, and moderate production, (6) butane, C4, and high production and (7) ethane, ethylene, and low production. According to their intentional outcomes, suitable penalty terms were added to the objective function (profit) in the process model. The model was then optimised in gPROMS using the built-in SQP solver. The results were finally listed out as the operation modes in the feasible operation table. The above procedures ensure that the operation modes obtained are operationally feasible and cost effective for their outcomes. The feasible operation table of the 5-column ethylene process is shown in Table 5.4.

The FOT MILP model was built using GAMS (Brooke *et al.*, 1992) and was optimised by the solver Cplex (ILOG, 2008). The FOT approach solved the 3-period example with an overall profit of $\$3.2679\times10^{6}$. The MILP model required only 3 CPU seconds to optimise. The computational time of the operation mode optimisations was not recorded, since the procedures are one-off and the table could be used repeatedly.

Table 5.4: Feasible operation table of 5-column ethylene process.

	Operation Mode						
Raw material consumptions (*mu*)	1	2	3	4	5	6	7
Ethane consumption (kg/s)	12.50	3.04	2.50	2.50	2.50	2.50	5.83
Propane consumption (kg/s)	2.95	15.00	15.00	2.50	2.50	2.50	4.91
Butane consumption (kg/s)	2.50	2.50	2.50	15.00	14.49	14.67	2.50
Process input variables (*u*)	1	2	3	4	5	6	7
Steam feed (kg/s)	9.12	9.26	9.26	9.26	9.26	9.26	9.30
Reactor heat flux (kJ/m^{2}s)	44.31	39.94	38.49	35.36	30.92	30.00	30.12
Demethaniser boil-up, Bup1	0.96	1.15	3.00	1.28	2.04	1.20	1.00
Demethaniser reflux, R1	2.81	2.52	2.24	2.08	3.00	2.42	2.99
Deethaniser boil-up, Bup2	3.00	2.02	1.80	1.84	3.00	2.60	2.54
Deethaniser reflux, R2	1.12	0.90	1.12	0.61	2.73	2.12	0.85
C2 splitter boil-up, Bup3	4.44	3.69	3.88	5.00	2.92	4.22	0.77
C2 splitter reflux, R3	1.48	1.23	1.29	1.67	1.79	2.76	2.31
Depropaniser boil-up, Bup4	2.02	0.62	2.70	1.86	3.11	0.50	1.05
Depropaniser reflux, R4	1.43	0.52	1.23	4.00	1.97	1.50	0.81
C3 splitter boil-up, Bup5	2.72	5.00	5.00	2.50	5.00	5.00	5.00
C3 splitter reflux, R5	5.00	3.66	4.45	3.21	1.67	2.84	5.00
Process output variables (*y*)	1	2	3	4	5	6	7
Reactor steam dilution ratio	0.40	0.40	0.40	0.40	0.40	0.40	0.45
Reactor inlet flowrate (kg/s)	31.91	32.40	32.40	32.40	32.40	32.40	30.02
Reactor outlet pressure (kPa)	150.00	164.26	173.05	181.40	197.85	200.58	204.91
Reactor outlet temperature (K)	1131.81	1147.68	1138.97	1161.91	1092.71	1082.56	1104.96
Demethaniser condenser duty, Qc1 (kJ)	11534	11504	17320	10225	14589	9039	9982
Demethaniser reboiler duty, Qr1 (kJ)	7726	8054	16586	7730	14118	8764	7487
Deethaniser condenser duty, Qc2 (kJ)	6599	4285	3165	2797	8073	6567	4766
Deethaniser reboiler duty, Qr2 (kJ)	7543	5303	5323	5601	11492	10133	5283
C2 splitter condenser duty, Qc3 (kJ)	6694	4505	2720	4478	3303	4988	5633
C2 splitter reboiler duty, Qr3 (kJ)	5428	3471	2150	4760	2914	5017	2433
Depropaniser condenser duty, Qc4 (kJ)	1659	326	2125	3190	4067	828	590
Depropaniser reboiler duty, Qr4 (kJ)	3122	1297	4178	4646	6497	1695	1550
C3 splitter condenser duty, Qc5 (kJ)	1854	1360	4217	1216	2710	1081	1863
C3 splitter reboiler duty, Qr5 (kJ)	1936	1104	3425	931	2100	852	1523
Demethaniser ratio boilup:reflux	0.34	0.46	1.34	0.62	0.68	0.49	0.33
Deethaniser ratio boilup:reflux	2.69	2.26	1.61	3.00	1.10	1.23	3.00
C2 splitter ratio boilup:reflux	3.00	3.00	3.00	3.00	1.64	1.53	0.33
Depropaniser ratio boilup:reflux	1.41	1.20	2.20	0.47	1.58	0.33	1.30
C3 splitter ratio boilup:reflux	0.54	1.37	1.12	0.78	3.00	1.76	1.00
Ethylene product molar purity	0.99	0.99	0.99	0.99	0.99	0.99	0.99
Propylene product molar purity	1.00	1.00	2.56	1.00	4.35	1.01	1.00
C4 stream propylene composition	0.04	0.10	0.06	0.01	0.04	0.07	0.10
H_2/CH_4 stream flowrate	3.92	6.40	9.35	7.66	6.15	5.53	3.40
Product production (*my*)	1	2	3	4	5	6	7
Ethylene production rate (kg/s)	9.27	7.50	4.32	5.50	3.80	3.70	5.00
Propylene production rate (kg/s)	1.00	1.00	2.56	1.00	4.35	1.01	1.00
C4 production rate (kg/s)	3.76	5.64	3.76	5.83	5.19	9.44	3.84

The FOT Approach offered a significant improvement to the objective value. It is only about 4% less than the Simultaneous Approach objective, and it is better than all rolling horizon varieties tested in this example. The FOT Approach solution time also out-performed the others.

In the FOT Approach result, the MILP model chose mode 1 in period 1, mode 6 in period 2 and mode 1 in period 3. Mode 1 favours ethane feedstock and high ethylene production. Mode 6 in contrast wants butane feedstock and high C4 production. The mode arrangement made the overall operation very similar to the Simultaneous Approach result. They both produced ethylene in period 1 and kept it to sell in period 2. In period 2, they also produced C4 chemicals and sold them immediately. Finally, they both stored ethane and propane from periods 1 and 2, and used them to manufacture ethylene cheaply in period 3 (Figure 5.16).

5.4.1.4 Results Analysis

The Simultaneous, FR-1, BR-1, BR-HB and FOT approaches had been examined in the 3-period example. They all improved the overall profit from the base case, but their computational times exhibit a wide range. The approaches' objective values and their CPU time are summarised in Table 5.5, and the optimisation dimensions and tolerance settings are also listed in Table 5.6.

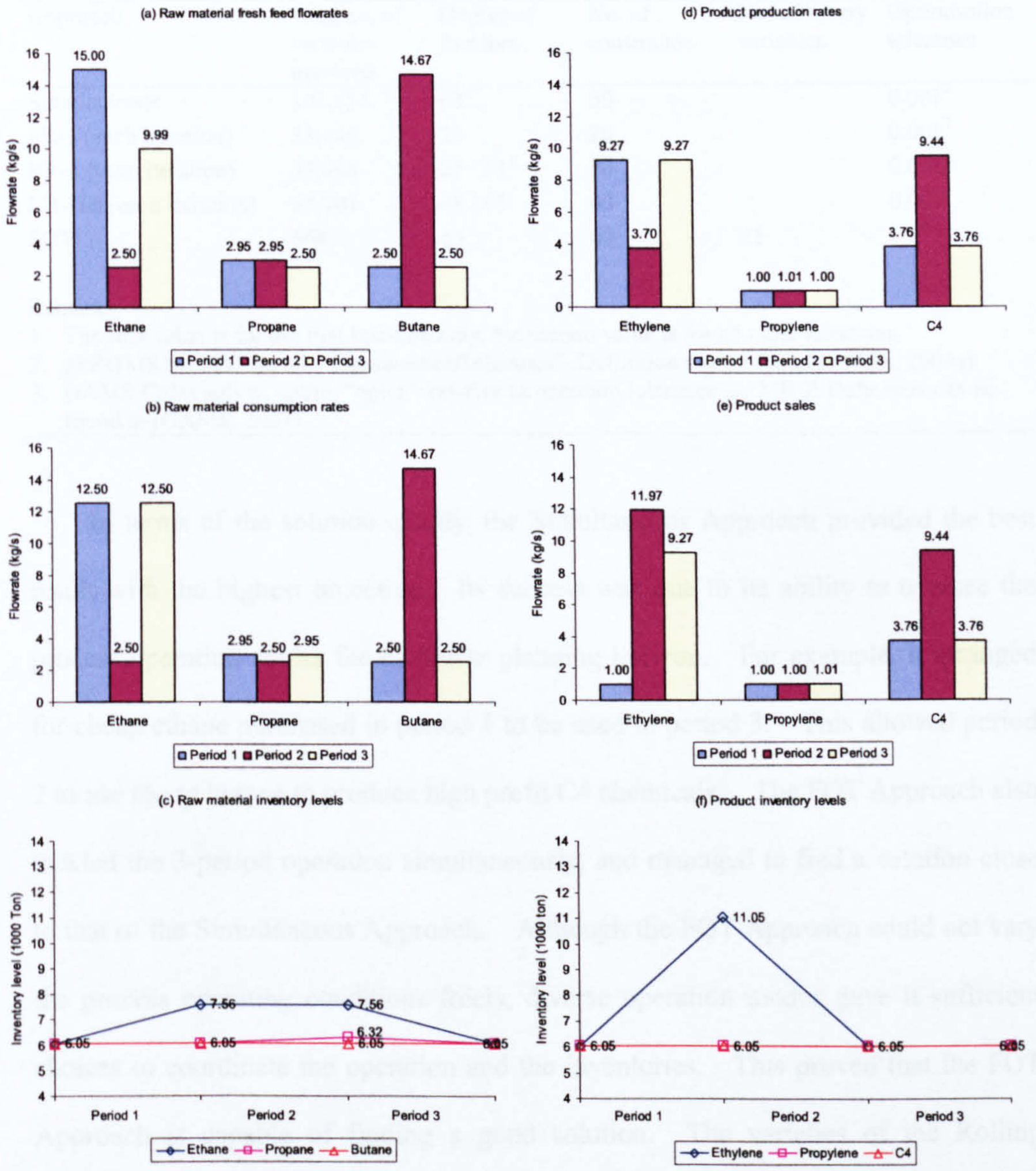

Figure 5.16: FOT Approach selected results of 3-period example.

Table 5.5: Approach objectives and model statistics in 3-period example.

	Base Case	Simult. Approach	FR-1 Approach	BR-1 Approach	BR-HB Approach	FOT Approach
Obj. Profit (10^6\$)	0.2814	3.4164	1.4222	3.2291	3.2336	3.2679
CPU Time (s)		40,717	6,104	17,238	26,507	3

Table 5.6: Problem dimensions and optimisation tolerance in 3-period example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	No. of binary variables	Optimisation tolerance
Simultaneous	101,554	63	60		0.001[2]
FR-1 (each iteration)	33,846	21	20		0.001[2]
BR-1 (each iteration)	33,846	27 / 21[1]	20		0.001[2]
BR-HB (each iteration)	67,701	48 / 42[1]	40		0.001[2]
FOT	568	63	60	21	0.0[3]

Remarks:
1. The first value is for the first iteration only, the second value is for all other iterations.
2. gPROMS SRQPD solver, "OptimisationTolerance". Definition can be found in (PSE, 2004a).
3. GAMS Cplex solver, option "optcr": relative termination tolerance for MILP. Definition can be found in (GAMS, 2007).

In terms of the solution quality, the Simultaneous Approach provided the best result with the highest objective. Its success was due to its ability to oversee the process operation across the complete planning horizon. For example, it arranged for cheap ethane purchased in period 1 to be used in period 3. This allowed period 2 to use cheap butane to produce high profit C4 chemicals. The FOT Approach also tackled the 3-period operation simultaneously, and managed to find a solution close to that of the Simultaneous Approach. Although the FOT Approach could not vary the process operating conditions freely, diverse operation modes gave it sufficient choices to coordinate the operation and the inventories. This proved that the FOT Approach is capable of finding a good solution. The varieties of the Rolling Horizon Approach however only focused on maximising individual periods' profits. They easily overlooked opportunities in other periods, and mistakenly allocated inventory for the process, such as keeping excess inventories in the FR-1 Approach, and placing butane inventory in period 2 for later use in the BR-1 Approach. As the result, they lost opportunities for better solutions.

In terms of the computational time, the FOT Approach performed very well.

This is because the FOT Approach employed a linear model to handle the problem. A linear model is much easier to solve than a nonlinear model. Furthermore, the feasible operation table simplified the entire 3-period problem to a MILP model, which only included 532 equations. Compared to the number of equations (101,554) involved in the full optimisation of the Simultaneous Approach, the MILP model is tiny, and linear.

The varieties of the Rolling Horizon Approach were relatively fast with respect to the Simultaneous Approach. In theory, the solution time of a model increases exponentially even the model size only increases linearly (Varvarezos *et al.*, 1992). The Rolling Horizon Approaches solved a smaller problem in each individual optimisation; this should be faster than the Simultaneous Approach. The FR-1 and BR-1 approaches were faster among other varieties as their individual problems were only single-period problems. The BR-HB Approach had a longer solution time, because it included 2-period problems in its individual optimisations. Even though it carried out one optimisation fewer than in the BR-1 and FR-1 approaches, the BR-HB approach still required a longer solution time in total according to the exponential increase theory.

5.4.2 4-Period Example

The 4-period example is based on the 3-period example with a new period attached at the end. Each period still lasts for 604,800 seconds (7days). The prices/costs are the only parameters that vary across the periods. The objective of the example is to maximise the total profit over the horizon. A base case with the objective value $\$0.0713\times10^6$ was assigned to the example. Solution approaches should start

the optimisation process from the base case. The input, output and inventory variables in the example are shown in Tables 5.7, 5.8 & 5.9.

The Simultaneous Approach was not examined in this example, because the 4-period model is too large to solve this way. The 3-period example result suggests that the backward rolling mechanism is more reliable than the forward rolling one. In this example, all three backward rolling approaches (BR-1, BR-2, BR-HB) are tested to explore the best backward rolling variety. However, the FR-1 Approach is still executed for comparison. The FOT Approach performed very well in the previous example and it is used in this example again.

Table 5.7: Input variables of 4-period example.

			Price/Cost in Period			
Input Variables	Min.	Max.	1	2	3	4
Ethane fresh feed (kg/s)	2.5	15.0	-0.26	-0.40	-0.30	-0.30
Propane fresh feed (kg/s)	2.5	15.0	-0.30	-0.30	-0.35	-0.29
Butane fresh feed (kg/s)	2.5	15.0	-0.43	-0.30	-0.40	-0.40
Ethane consumption (kg/s)	1.0	15.0				
Propane consumption (kg/s)	1.0	15.0				
Butane consumption (kg/s)	1.0	15.0				
Steam feed (kg/s)	1.0	20.0	-0.01	-0.01	-0.01	-0.01
Reactor heat flux (kJ/m^2s)	30.0	45.0	-2E-4	-2E-4	-2E-4	-2E-4
Demethaniser boil-up, Bup1	0.5	3.0				
Demethaniser reflux, R1	0.5	3.0				
Deethaniser boil-up, Bup2	0.5	3.0				
Deethaniser reflux, R2	0.5	3.0				
C2 splitter boil-up, Bup3	0.5	5.0				
C2 splitter reflux, R3	0.5	5.0				
Depropaniser boil-up, Bup4	0.5	4.0				
Depropaniser reflux, R4	0.5	4.0				
C3 splitter boil-up, Bup5	0.5	5.0				
C3 splitter reflux, R5	0.5	5.0				
			Period 1	Period 2	Period 3	Period 4
Period Duration (s)			604,800	604,800	604,800	604,800

N.B. Shaded area indicates variations across periods.

Table 5.8: Inventory variables of 4-period example.

Inventory Variables	Min.	Max.	Initial.	Inventory Cost
Ethane inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Propane inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Butane inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Ethylene inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
Propylene inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3
C4 inventory (1000 Ton)	6.048	12.096	6.048	-1.6534E-3

Table 5.9: Output variables of 4-period example.

			Price/Cost in Period			
Output Variables	Min.	Max.	1	2	3	4
Reactor steam dilution ratio	0.4	1.0				
Reactor inlet flowrate (kg/s)	0.0	32.4				
Reactor outlet pressure (kPa)	150.0					
Reactor outlet temperature (K)	0	1,200				
Demethaniser condenser duty, Qc1 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5	-1.05E-5
Demethaniser reboiler duty, Qr1 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5	-1.26E-5
Deethaniser condenser duty, Qc2 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5	-1.05E-5
Deethaniser reboiler duty, Qr2 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5	-1.26E-5
C2 splitter condenser duty, Qc3 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5	-1.05E-5
C2 splitter reboiler duty, Qr3 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5	-1.26E-5
Depropaniser condenser duty, Qc4 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5	-1.05E-5
Depropaniser reboiler duty, Qr4 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5	-1.26E-5
C3 splitter condenser duty, Qc5 (kJ)			-1.05E-5	-1.05E-5	-1.05E-5	-1.05E-5
C3 splitter reboiler duty, Qr5 (kJ)			-1.26E-5	-1.26E-5	-1.26E-5	-1.26E-5
Demethaniser ratio boilup:reflux	0.3333	3.0000				
Deethaniser ratio boilup:reflux	0.3333	3.0000				
C2 splitter ratio boilup:reflux	0.3333	3.0000				
Depropaniser ratio boilup:reflux	0.3333	3.0000				
C3 splitter ratio boilup:reflux	0.3333	3.0000				
Ethylene product molar purity	0.99	1.00				
Ethylene production rate (kg/s)	2.0	10.0				
Propylene product molar purity	0.90	1.00				
Propylene production rate (kg/s)	1.0	10.0				
C4 stream propylene composition	0.0	0.1				
C4 production rate (kg/s)	0.0					
H_2/CH_4 stream flowrate	0.0		0.05	0.05	0.05	0.05
Ethylene sales (kg/s)	1.0	15.0	0.587	0.650	0.550	0.550
Propylene sales (kg/s)	1.0	15.0	0.610	0.610	0.650	0.600
C4 sales (kg/s)	1.0	15.0	0.650	0.650	0.600	0.620

N.B. Shaded area indicates variations across periods.

5.4.2.1 Rolling Horizon Approach Result

Forward Rolling, One-at-a-time (FR-1)

The FR-1 Approach solved the 4-period example in 10,681 seconds (~3 hours), and the total profit is $\$2.0840\times10^6$. Unfortunately, the problem of excess raw material inventory in the last period still occurred (Figure 5.17).

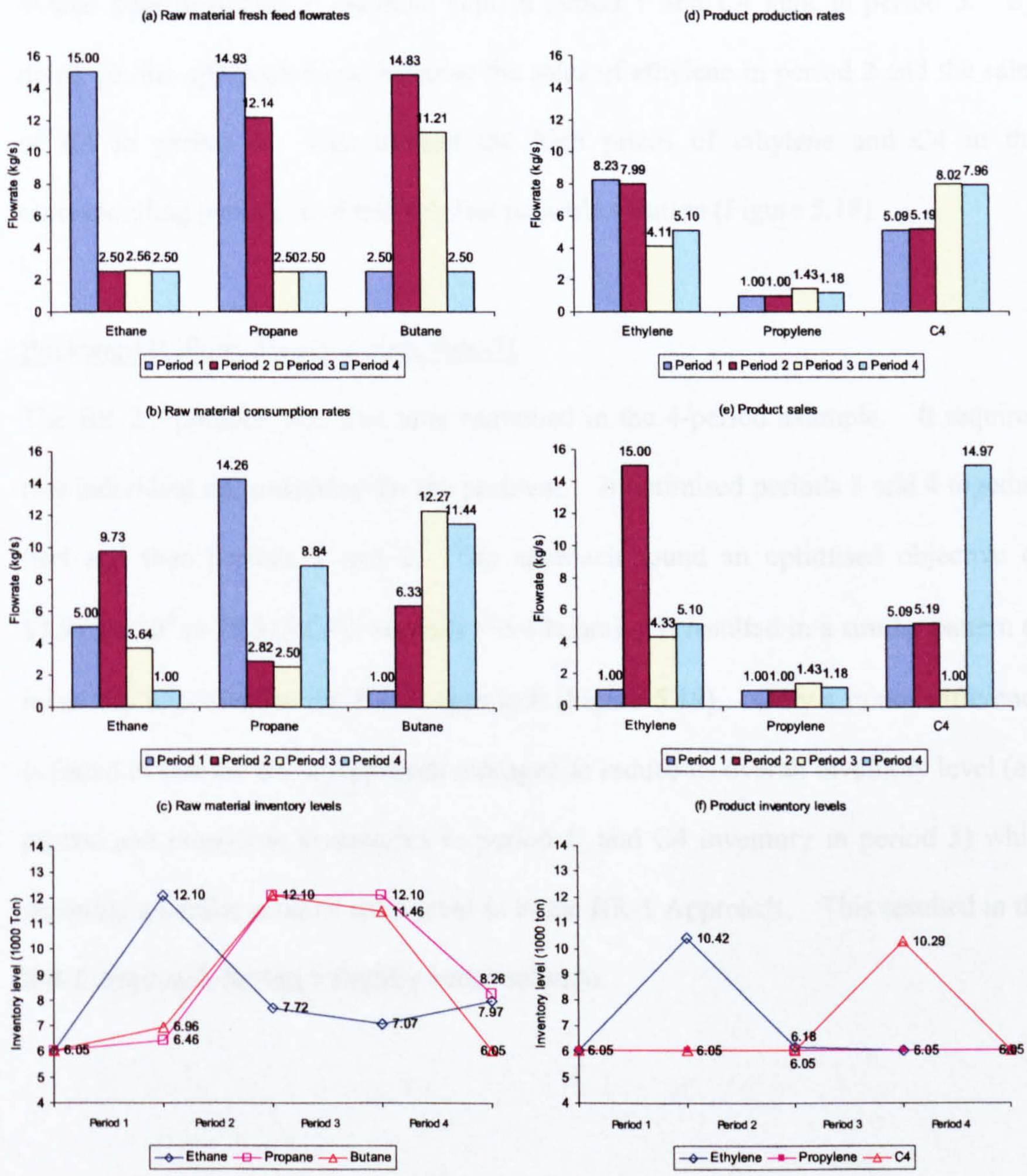

Figure 5.17: FR-1 Approach selected results of 4-period example.

Backward Rolling, One-at-a-time (BR-1)

The BR-1 Approach provided a better solution than the FR-1 Approach. Its optimised objective value is $\$3.9753\times10^6$, but it required a longer computational time of 16,305 seconds (~4.5 hours). The inventory level trends basically followed the material price variations. A larger amount of inventory would be kept if the next period price was higher. This could be observed from ethane kept in period 1, butane kept in period 2, ethylene kept in period 1 and C4 kept in period 3. By doing so, the approach could increase the sales of ethylene in period 2 and the sales of C4 in period 4. This utilised the high prices of ethylene and C4 in the corresponding periods to obtain the best possible solution (Figure 5.18).

Backward Rolling, Two-at-a-time (BR-2)

The BR-2 Approach was first time examined in the 4-period example. It required two individual optimisations for the problem. It optimised periods 3 and 4 together first and then periods 1 and 2. The approach found an optimised objective of $\$3.9787\times10^6$ in 19,355 CPU seconds (~5.4 hours). It resulted in a similar pattern of inventory allocation to the BR-1 Approach (Figure 5.19). Only a minor difference is found in that the BR-2 Approach managed to reduce its overall inventory level (e.g. ethane and propylene inventories in period 1, and C4 inventory in period 3) while retaining a similar product sales level as in the BR-1 Approach. This resulted in the BR-2 Approach having a slightly better solution.

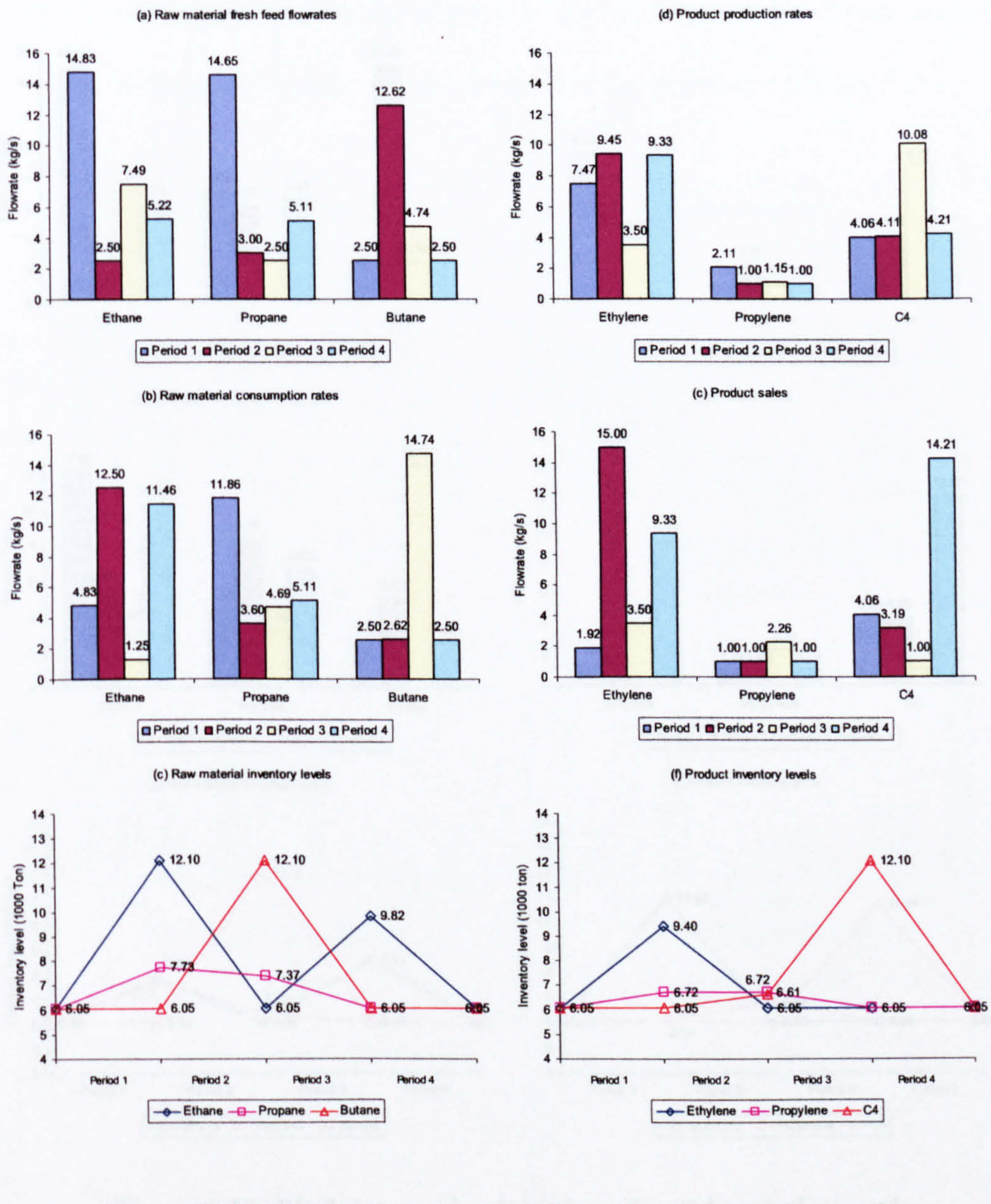

Figure 5.18: BR-1 Approach selected results of 4-period example.

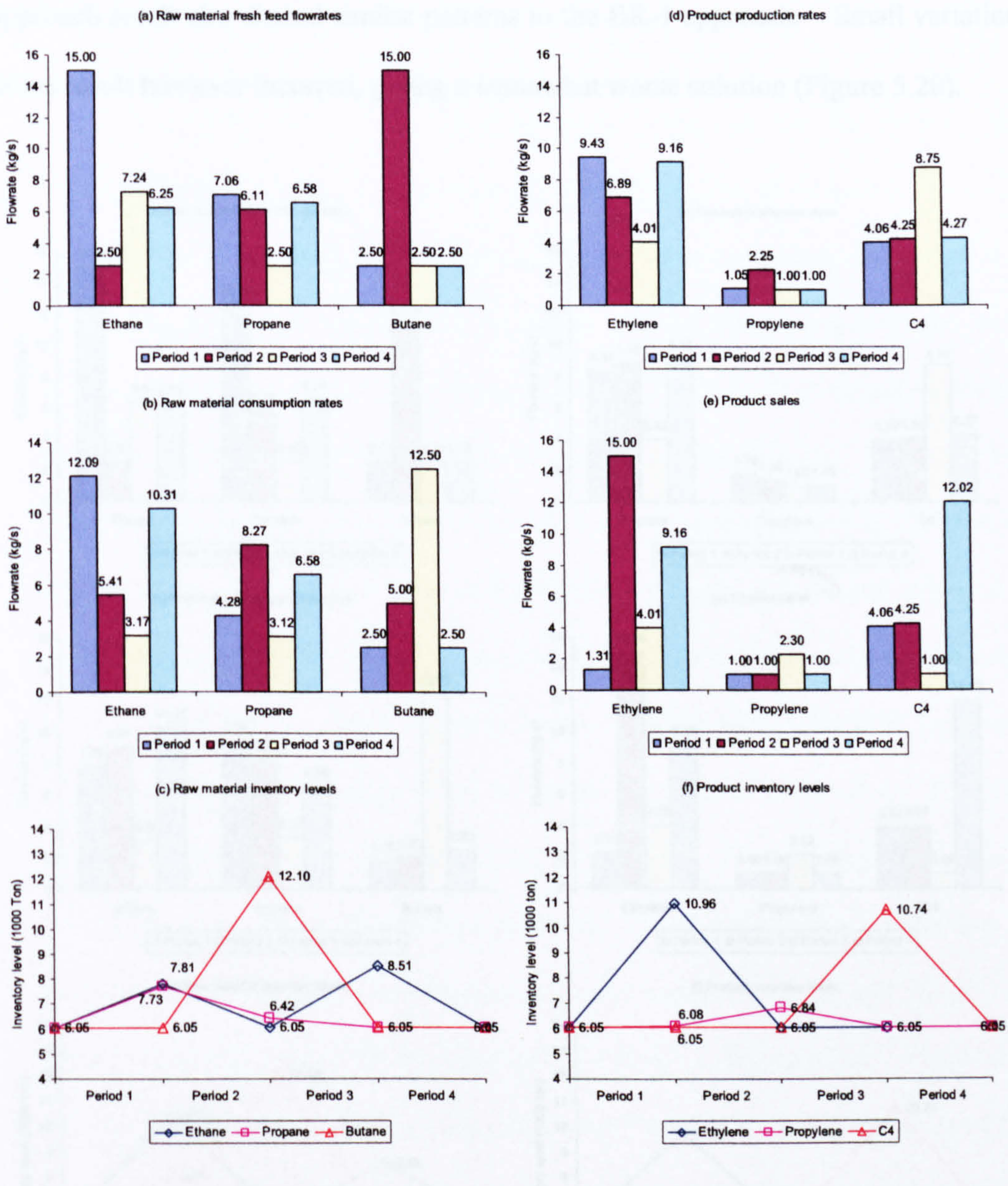

Figure 5.19: BR-2 Approach selected results of 4-period example.

Backward Rolling, Hybrid 2/1 (BR-HB)

The BR-HB Approach solved the example in 38,099 CPU seconds (~10.5 hours) with a total profit of $\$3.9473\times10^6$. The inventory levels and flowrates in the approach result also shared similar patterns to the BR-1 approach. Small variations in the result however incurred, giving a somewhat worse solution (Figure 5.20).

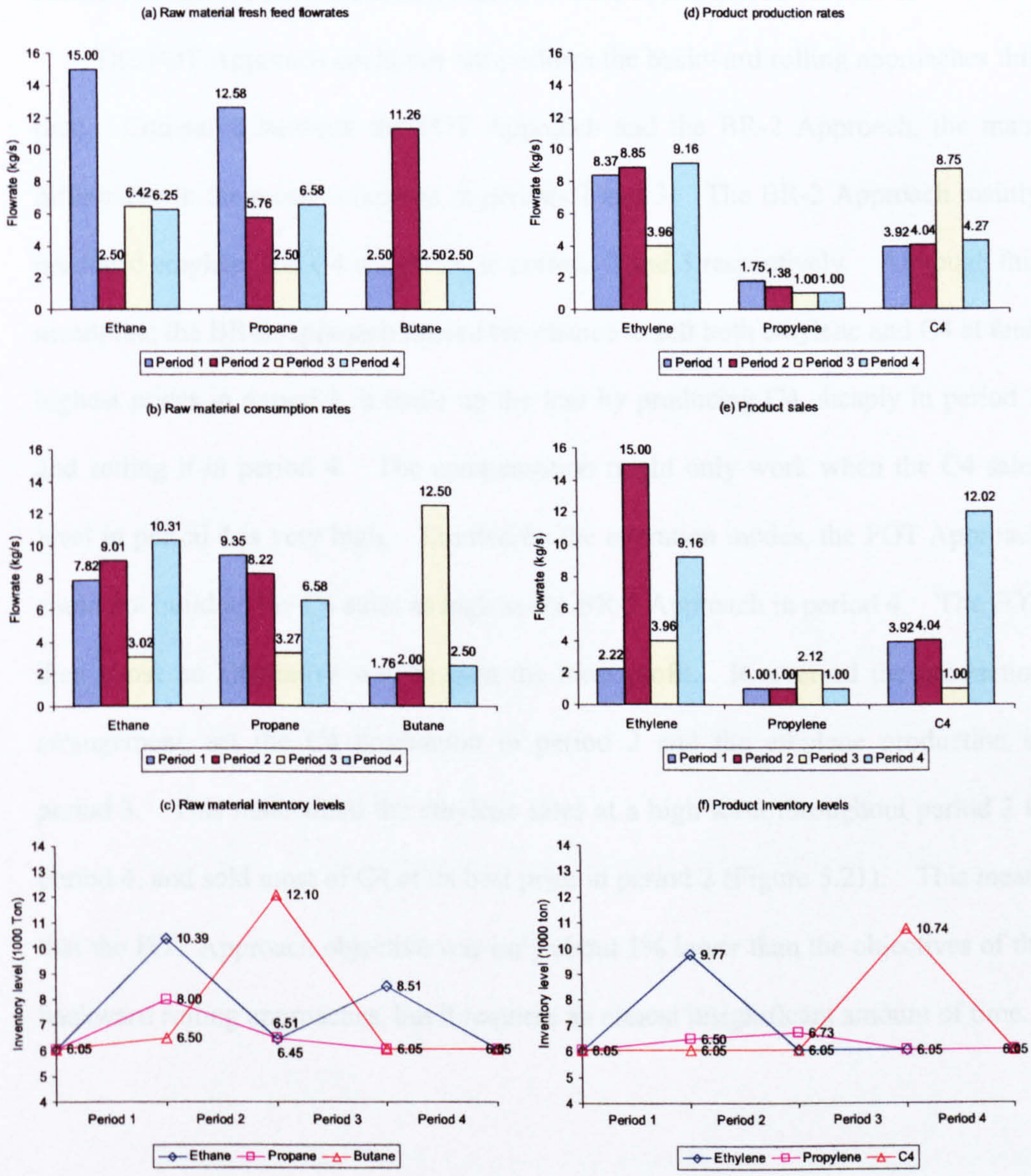

Figure 5.20: BR-HB Approach selected results of 4-period example.

5.4.2.2 Feasible Operation Table Approach Result

The FOT Approach employed the operation table presented in Table 5.4 to solve the 4-period example. Although an extra period was appended to the MILP model, the model size change was insignificant in affecting the computational time. The MILP model could still complete the optimisation in 3 CPU seconds. The optimised total profit is $\$3.9338\times10^6$. The operation modes selected for the periods are Period 1:Mode 1, Period 2:Mode6, Period 3:Mode 1, and Period 4:Mode 1.

The FOT Approach could not out-perform the backward rolling approaches this time. Compared between the FOT Approach and the BR-2 Approach, the main differences in the results occurred in periods 2 and 3. The BR-2 Approach mainly produced ethylene and C4 chemicals in periods 2 and 3 respectively. Although this meant that the BR-2 Approach missed the chance to sell both ethylene and C4 at their highest prices in period 2, it made up the loss by producing C4 cheaply in period 3 and selling it in period 4. The compensation might only work when the C4 sales level in period 4 is very high. Limited by the operation modes, the FOT Approach could not build up the C4 sales as high as the BR-2 Approach in period 4. The FOT then chose an alternative way to gain the most profit. It reversed the production arrangement, set the C4 production in period 2 and the ethylene production in period 3. This maintained the ethylene sales at a high level throughout period 2 to period 4, and sold most of C4 at its best price in period 2 (Figure 5.21). This meant that the FOT Approach objective was only about 1% lower than the objectives of the backward rolling approaches, but it requires an almost insignificant amount of time.

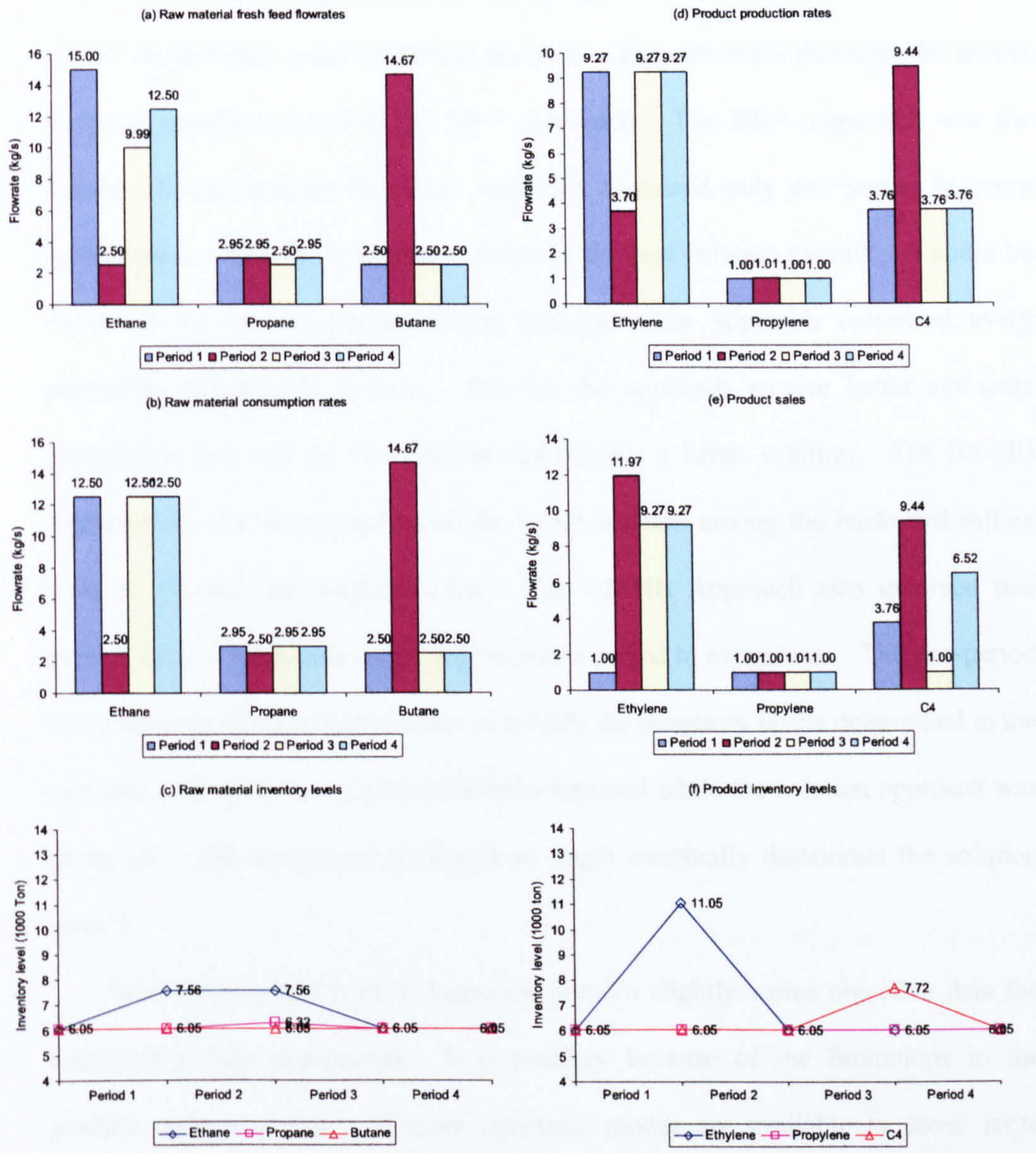

Figure 5.21: FOT Approach selected results of 4-period example.

5.4.2.3 Results Analysis

The objectives and model dimensions of the approaches tested in the 4-period example are listed in Table 5.10 and Table 5.11 respectively. The FR-1 Approach obtained the poorest solution. It was again hampered by keeping too much raw

material inventory. The backward rolling approaches, BR-1, BR-2 and BR-HB, located much better solutions for the example. They all could eliminate the excess inventory problem found in the FR-1 Approach. The BR-1 Approach was the fastest. It was because the BR-1 Approach contained only one period in every optimisation. The BR-2 Approach achieved the best solution overall. It could be explained by the two-period rolling strategy. The approach optimised every alternative two-periods in turn. This let the approach receive better site-wide information between the two periods and provide a better solution. The BR-HB Approach on the other hand found the worst solution among the backward rolling variants, though only slightly worse. The BR-HB Approach also involved two periods in its optimisation and it only moved a period in every turn. The one-period move allowed the later optimisation to modify the inventory levels determined in the pervious optimisation. The modification repeated while the solution approach was going on. The continuous modification might eventually deteriorate the solution quality.

In this example, the FOT Approach found a slightly worse objective than the backward rolling approaches. It is possibly because of the limitations in the feasible operation table. If more operation modes are available to cover more operation outcomes, the result could be improved. Nonetheless, the result obtained is the best for the current operation table, and its quick performance is also undeniable.

Table 5.10: Approach objectives and model statistics in 4-period example.

	Base Case	FR-1 Approach	BR-1 Approach	BR-2 Approach	BR-HB Approach	FOT Approach
Obj., Profit (10^6\$)	0.0714	2.0840	3.9753	3.9787	3.9473	3.9338
CPU Time (s)		10,681	16,303	19,355	38,099	3

Table 5.11: Problem dimensions and optimisation tolerance in 4-period example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	No. of binary variables	Optimisation tolerance
FR-I (each iteration)	33,846	21	20		0.001[2]
BR-1 (each iteration)	33,846	27 / 21[1]	20		0.001[2]
BR-2 (each iteration)	67,701	48 / 42[1]	40		0.001[2]
BR-HB (each iteration)	67,701	48 / 42[1]	40		0.001[2]
FOT	757	84	80	28	0.0[3]

Remarks:
1. The first value is for the first iteration only, the second value is for all other iterations.
2. gPROMS SRQPD solver, "OptimisationTolerance". Definition can be found in (PSE, 2004a).
3. GAMS Cplex solver, option "optcr": relative termination tolerance for MILP. Definition can be found in (GAMS, 2007).

5.4.3 Concluding Remarks on Case Studies

The decomposition method (Rolling Horizon Approach) and the simplification method (FOT Approach) have been examined using both 3-period and 4-period examples. They performed consistently throughout the two examples. The FR-1 Approach has clearly shown its weakness of handling raw material inventory. The backward rolling varieties could eliminate that problem and achieved fairly good solutions in both examples. The varieties' solutions were also very close to each other despite their different rolling strategies. This indicates that the rolling strategy employed in the backward rolling approach is not critical to the approach accuracy. The decisive metric then falls on the solution time. In terms of that, the BR-1 Approach is the best Rolling Horizon Approach variety.

The FOT Approach has also proved itself as an effective solution method. The current 7-mode table has already provided reasonably high accuracy. Keeping the entire time horizon in a holistic model also contributed to the FOT Approach's good results. It enables the FOT Approach to out-perform the decomposition methods. With its remarkably short solution time, the FOT Approach should be recommended prior to the Rolling Horizon Approach as a tool to obtain a lower bound solution rapidly.

Besides the Rolling Horizon and FOT Approaches, the Simultaneous Approach was also investigated in the 3-period example. It demonstrated that direct optimisation could improve the total profit by 4 to 5% from the decomposition or simplification methods. Although the direct optimisation required a very long time, the 4 to 5% improvement could be critical to an industry with a slim profit margin, such as ethylene production. This has enhanced our belief on solving the site-wide optimisation in a site-wide fashion. In the sense of multi-period/site problem, the idea can be interpreted as: a direct optimisation for a holistic multi-period/site model is always desirable. The obstacle of applying direct optimisation in large-scale multi-period/site models should be overcome, and the next chapter will explore a technique to achieve that.

5.5 Conclusions

An investigation of single-site multi-period optimisation methods was executed in this chapter. A 5-column ethylene process model with rigorous model formulations was used to develop two examples for the study, the 3-period example and the 4-period example. The chapter mainly focuses on using a decomposition method

and a simplification method to attempt the examples. The former is the Rolling Horizon Approach. It contains four different varieties, which are categorised by their rolling mechanism. They are the FR-1, BR-1, BR-2 and BR-HB approaches. The simplification method is called the Feasible Operation Table Approach. It simplifies the process operation into various operation modes, and it assigns a mode to each period.

The 3-period example was first used to examine the solution approaches. The Simultaneous Approach described in Chapter 4 was also tested in addition to the Rolling Horizon and FOT approaches. This aimed to compare the decomposition and simplification results to the direct optimisation result. The Simultaneous Approach obtained the best solution among all. The FR-1 Approach performed poorly as it failed to handle the raw material inventory well. The backward rolling varieties (BR-1 & BR-HB) managed to find relatively good solutions. The FOT Approach unexpectedly improved upon the Rolling Horizon Approach to have a solution close to the Simultaneous Approach. It also exhibited a quick computational time.

The 4-period example excluded the Simultaneous Approach, as the problem size is too large for the approach. Other approaches were then tested for their performance consistency. The FR-1 Approach again was the worst. The BR-2 Approach had the best solution in the example. However, the other backward rolling approaches (BR-1, BR-HB) also attained similar solutions. Based on the solution time, the BR-1 Approach should be recommended among the Rolling Horizon varieties. The FOT solution time in the 4-period example was still very short, and its solution was significantly close to the BR-2 Approach. Hence, the

FOT Approach is determined to be more effective than the Rolling Horizon Approach.

In spite of good results from the FOT and BR-1 approaches, the Simultaneous Approach remains unbeaten so far. This hints at an opportunity to apply direct optimisation for a holistic multi-period/site model. To achieve this, a novel technique to solve extremely large size models should be developed. An investigation on this aspect is discussed in the next chapter.

6 gBA Approach for Site-wide Supply Chain Optimisation

6.1 Introduction

Direct optimisation promises to be the most accurate method for the site-wide supply chain optimisation problem in Chapters 4 and 5. It could provide a few more percent of profit improvement over other approaches. This small improvement is vital for a slim profit margin industry like petrochemical manufacturing. Although the direct optimisation technique requires a very long computational time, it is still worth investing the time effort in the expected benefit.

The major difficulty to execute direct optimisation for the site-wide supply chain problems is that the holistic model size might be too large for a computer to handle. For example, it might exceed the memory capacity of the computer, as in the 4-period example in Chapter 5. This chapter hence aims to develop a technique to overcome the difficulty. The proposed technique is called the gBA (gPROMS-based application) Approach. It tackles the task by combining the strengths of the gPROMS simulation platform and an optimiser in the NAG numerical library. The approach comes with two variants. The first one, gBA-I, is basically used to test the possibility of the gBA Approach. The second one, gBA-II, is an advanced version to actually solve the memory problem for the direct optimisation.

Following this section, the chapter explains the idea of the gBA Approach. Then it examines the approach using a single-site single-period problem and two single-site multi-period problems. The problem results are studied, and a conclusion is made on the promise of the gBA Approach finally.

6.2 gBA Approach

A site-wide optimisation model can be generalised as a set of nonlinear equations $y = f(u)$ between optimisation input variables (u) and optimisation output variables (y). The optimisation objective function only depends on u and y. As the output variables y also depend on the input variables u, the objective can be further simplified as a function of u only, $OBJ = g(u)$. There are a lot of different nonlinear optimisation algorithms. They usually optimise a problem through iteration. In brief, they first start from an initial set of the input variables (u) and request different model information based on that particular set of u. The values of the output variables (y), the gradients of y ($\partial y/\partial u$), the objective value (OBJ) and the objective gradients ($\partial OBJ/\partial u$) are the most common types of information required by the algorithms. Then the algorithms perform some calculations according to the model information, in order to decide whether the current set of u is optimal or not. If not, a new set of u is generated. A new set of model information is also determined for the optimality checking. The procedures are repeated until an optimum is found.

In the 4-period example of Chapter 5, the optimisation problem had 84 input variables (u) and 80 output variables (y). In the sense of optimisation, the problem size was not particularly large. The gPROMS SQP solver however failed to solve it due to the memory capacity being exceeded. The SQP procedure did not require much memory, but the 4-period holistic process model had 135,407 variables in total. gPROMS had to involve all these variables to simulate the information required by the SQP procedure. This complex calculation eventually used up the memory in the computer, and the optimisation was abruptly terminated.

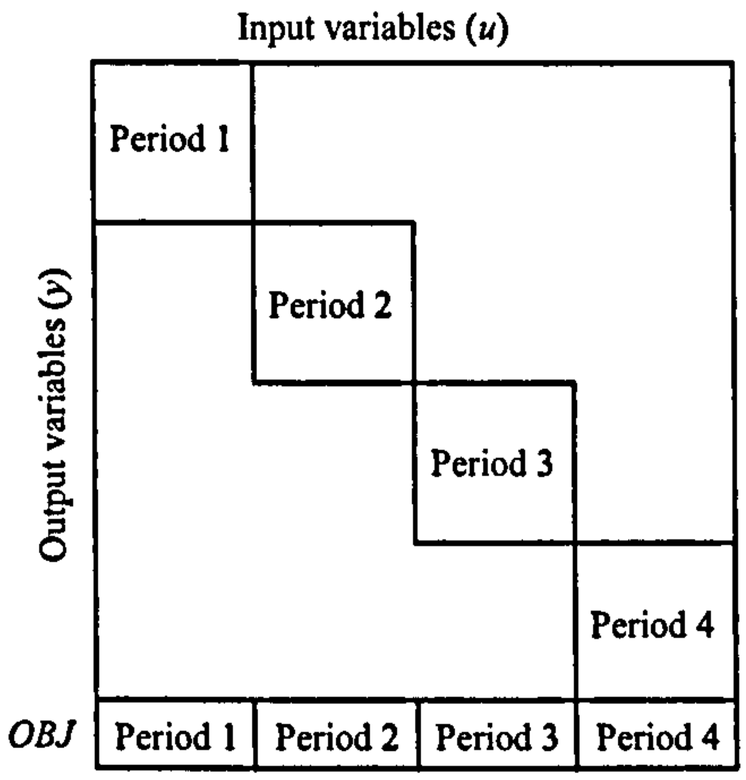

Figure 6.1: General block diagonal structure of a 4-period model.

A key issue to overcome the memory shortage in the direct site-wide optimisation is to reduce the simulation model size during the optimisation process. According to Chapter 5, a multi-period model is a collection of single-site models with material inventory linkages. The objective of the model is the sum of the individual period profits. The input variables in a period do not affect the output variables and the profits in other periods. It means that the output variables, profit and variable gradients of the individual periods can be calculated independently (Figure 6.1). In addition, the only cross-period equations, inventory balances, are linear. Their gradients are constant; so, their gradient values can be pre-determined and reported to the optimiser in advance. Combining the facts above, it suggests that the information required by the multi-period optimisation procedure can actually be obtained from separate simulations of the individual period models. Instead of the 4-period holistic simulation, four smaller, separate period simulations make direct optimisation possible.

A gBA program (PSE, 2004b) has been developed to make use of the idea for the direct site-wide optimisation of the multi-period problem. The gBA program is

similar in spirit to the simultaneous modular approach for the flowsheet optimisation (Chen & Stadtherr, 1985; Kisala *et al.*, 1987; Biegler *et al.*, 1997). The approach exploits the fact that some variables (state variables) in the flowsheet do not involve in the optimisation. Hence, it can reduce the optimisation problem size by only providing the information about the optimisation-related variables to the optimiser. They are the degrees of freedom (input variables), the constraint variables (output variables), and the connecting streams of the flowsheet units (modules).

Based on the principle, the gBA program connects the gPROMS simulations to an external optimiser. The program performs the gPROMS simulations associated with different periods in the multi-period model one-by-one, and then only sends the optimisation-required information to the external optimiser. Via the user input, the program also provides the optimiser the pre-defined cross-period information (i.e. the gradients of the inventory balances). By doing so, the optimiser skips all other details in the multi-period model and literally solves an optimisation problem only in the space of the input variables (u) and output variables (y).

The successive quadratic programming (SQP) routine E04UGA in the NAG Fortran Library (NAG, 2002) is employed as the optimiser in the gBA program. The SQP technique is believed to be very effective on solving the reduced optimisation problems (Locke *et al.*, 1983; Biegler, 1988). The routine is chosen also because it is designed for large-scale sparse nonlinear problems. That matches the characteristics of our site-wide optimisation problems. Once the initial set of input variables (u) and the bounds of input and output variables are specified in the beginning, the routine only requires the values of the output variables, the objective values, and their corresponding first derivatives to finish the optimisation. The

gPROMS simulations can determine all those values directly. The routine hence can be incorporated into the gBA program without any modification.

A trial program of the gBA Approach (gBA-I) has been developed first. The gBA-I program stores the process operations of all the periods in a single model, so that it still simulates the multi-period operations in a holistic way. It is used to test the feasibility of separating the simulator from the optimiser, rather than completely removing the direct optimisation difficulty. A simplified flowchart of the gBA-I procedure is presented in Figure 6.2.

In addition to the gBA-I program, an advanced version (gBA-II) is also developed. The gBA-II program separates the period operations into individual models. Whenever the optimiser requires the model information, the gBA-II program asks gPROMS to simulate the separate period models sequentially. This should dramatically reduce the size of the computer memory needed. The procedures of the gBA-II program are briefly illustrated in Figure 6.3.

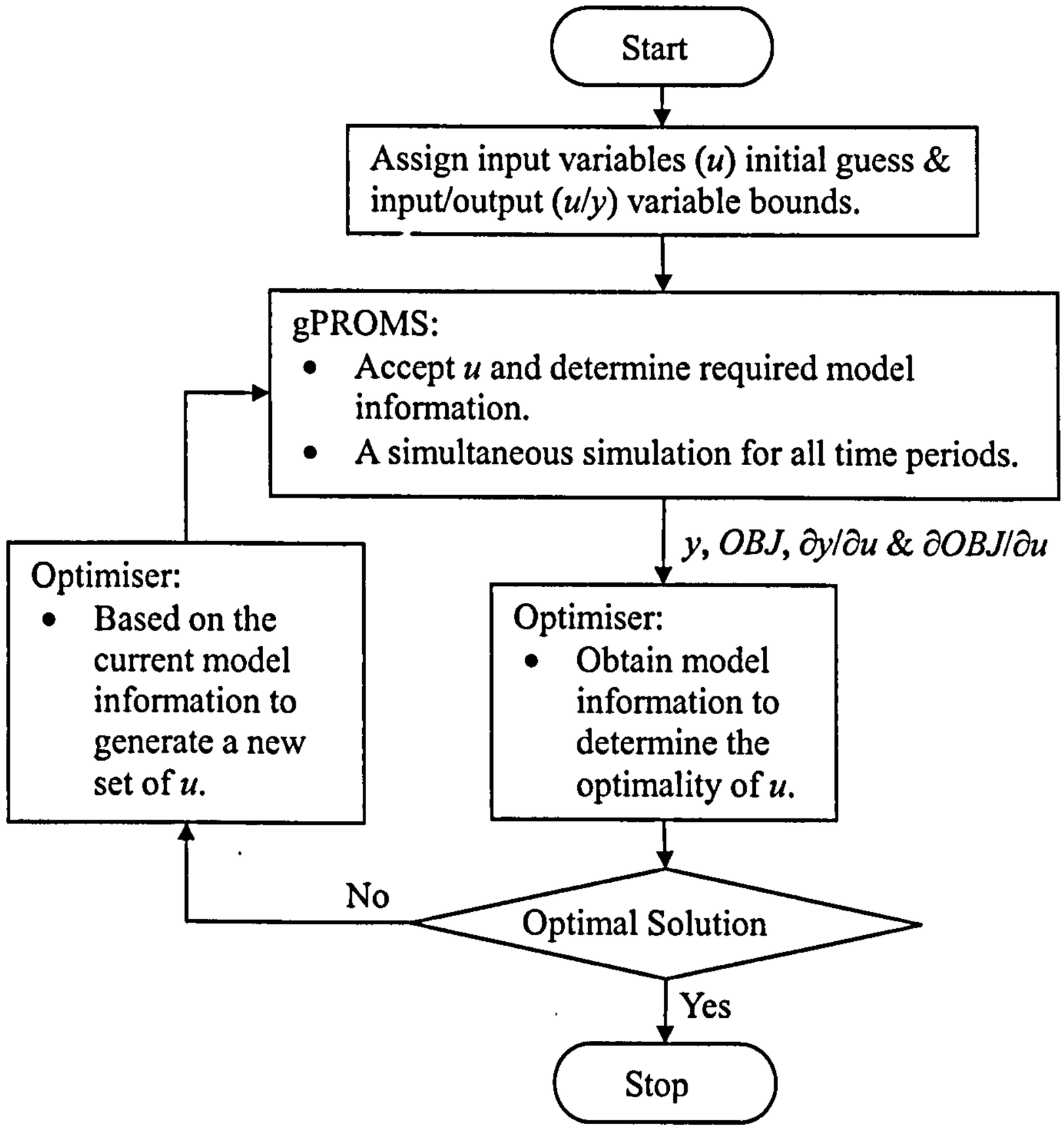

Figure 6.2: Simplified gBA-I Approach procedures flowchart.

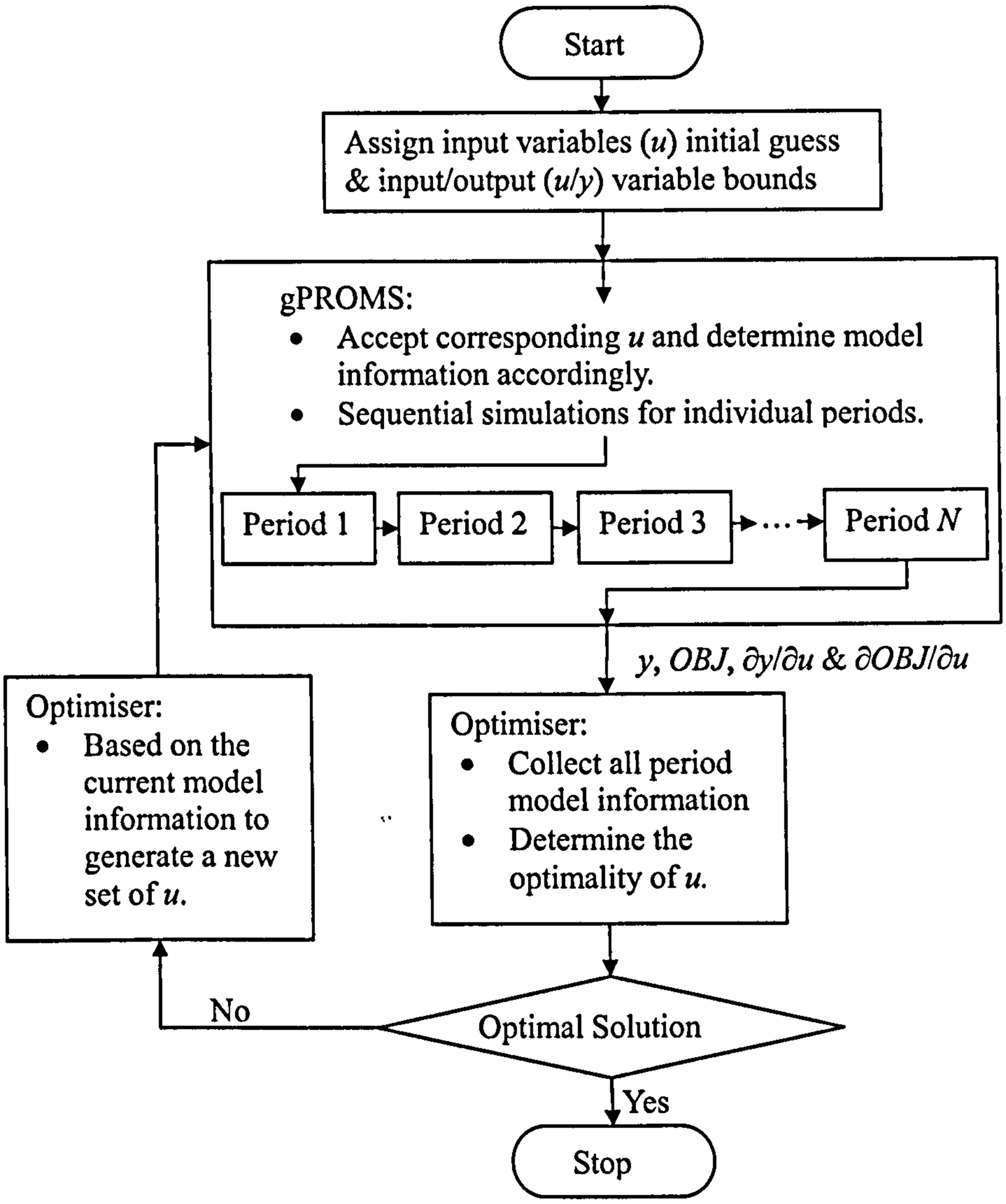

Figure 6.3: Simplified gBA-II Approach procedures flowchart.

6.3 Case Studies

Three examples are examined in this section. The first one is a single-site single-period problem based on the 5-column ethylene process described in Chapter 3. The other two are the same problems used in Chapter 5, the single-site 3-period and the single-site 4-period problems. The gBA-I program is used on all three examples to prove the feasibility of the gBA Approach idea. The gBA-II program in contrast is only tested on the 4-period problem to determine if the gBA Approach can overcome the direct optimisation difficulty. As the gBA Approach is expected to take a very long computational time, the gBA programs are executed using a Linux computer with a 2992 MHz CPU. It is about 1.7 times faster than the computer used in pervious chapters.

6.3.1 Single-site Single-period Example

A single-site single-period 5-column process model was adopted to study the gBA-I program. The process accepts ethane, propane and butane as raw materials and produces ethylene, propylene and C4 chemicals as products. It is as same as the process employed in the examples of Chapter 5, except it only contains one time period. Hence, no inventory consideration is required. In addition to the gBA-I Approach, the Simultaneous Approach was also used in the example for comparison. It however only ran on a slower machine (Linux with a 1794 MHz CPU). A base case was set up as the starting point for the approaches. The base case and other optimisation data are tabulated in Table 6.1.

Table 6.1: Single-site single-period example variables and base case values.

Input variables (u)	Base Value	Price/ Cost	Lower Bound	Upper Bound
Ethane feed flowrate (kg/s)	2.50	-0.26	2.50	15.00
Propane feed flowrate (kg/s)	2.50	-0.30	2.50	15.00
Butane feed flowrate (kg/s)	13.00	-0.43	2.50	15.00
Steam feed flowrate (kg/s)	13.00	-0.01	1.00	20.00
Reactor heat flux (kJ/m^2s)	30.00	-2E-4	30.00	45.00
Demethaniser boil-up, Bup1	2.00		0.50	3.00
Demethaniser reflux, R1	2.66		0.50	3.00
Deethaniser boil-up, Bup2	1.00		0.50	3.00
Deethaniser reflux, R2	0.78		0.50	3.00
C2 splitter boil-up, Bup3	4.76		0.50	5.00
C2 splitter reflux, R3	1.50		0.50	5.00
Depropaniser boil-up, Bup4	3.57		0.50	4.00
Depropaniser reflux, R4	1.50		0.50	4.00
C3 splitter boil-up, Bup5	5.00		0.50	5.00
C3 splitter reflux, R5	1.00		0.50	5.00
Output Variables (y)	**Base Value**	**Price/ Cost**	**Lower Bound**	**Upper Bound**
Reactor steam dilution ratio	0.6643		0.40	1.00
Reactor inlet flowrate (kg/s)	32.57		0.00	32.40
Reactor outlet pressure (kPa)	163.91		150.0	
Reactor outlet temperature (K)	1,119			1,200
Demethaniser condenser duty, Qc1 (kJ)	1.19E4	-1.05E-5		
Demethaniser reboiler duty, Qr1 (kJ)	1.12E4	-1.26E-5		
Deethaniser condenser duty, Qc2 (kJ)	1.50E3	-1.05E-5		
Deethaniser reboiler duty, Qr2 (kJ)	3.67E3	-1.26E-5		
C2 splitter condenser duty, Qc3 (kJ)	2.27E3	-1.05E-5		
C2 splitter reboiler duty, Qr3 (kJ)	1.84E3	-1.26E-5		
Depropaniser condenser duty, Qc4 (kJ)	3.60E3	-1.05E-5		
Depropaniser reboiler duty, Qr4 (kJ)	6.07E3	-1.26E-5		
C3 splitter condenser duty, Qc5 (kJ)	2.07E3	-1.05E-5		
C3 splitter reboiler duty, Qr5 (kJ)	1.53E3	-1.26E-5		
Demethaniser ratio boilup:reflux	0.7531		0.33	3.00
Deethaniser ratio boilup:reflux	1.2823		0.33	3.00
C2 splitter ratio boilup:reflux	3.1789		0.33	3.00
Depropaniser ratio boilup:reflux	2.3813		0.33	3.00
C3 splitter ratio boilup:reflux	5.0000		0.33	3.00
Ethylene product molar purity	0.9966		0.99	1.00
Ethylene production rate (kg/s)	3.12	0.587	2.00	10.00
Propylene product molar purity	0.6724		0.90	1.00
Propylene production rate (kg/s)	5.10	0.610	1.00	10.00
C4 stream propylene composition	0.0192		0.00	0.10
C4 production rate (kg/s)	4.08	0.650	0.00	
H_2/CH_4 stream flowrate	5.71		0.00	
Objective, Profit (10^6\$)	-0.2260			
Period Duration (s)	604,800			

The Simultaneous Approach took 15,474 CPU seconds (~4.30 hours) to locate an optimum. It significantly improved the profit from the base case value $\$-0.2260 \times 10^6$ to the new value $\$1.2354 \times 10^6$. The profit boost was mainly caused by changing the major feedstock from butane to ethane. The process could then produce a much more profitable product, ethylene, than in the base case.

The gBA-I Approach obtained a slightly better objective value, $\$1.2399 \times 10^6$. The pattern of the gBA-I Approach result basically is the same as in the Simultaneous Approach. They both favoured the ethane feedstock and consumed a similar amount of it. Small variations in the distillation reflux and boil-up ratios however allowed the gBA-I Approach to produce somewhat more ethylene. This consequently provided a higher profit. The gBA-I Approach was also faster than the Simultaneous Approach. It required 10,025 CPU seconds for the optimisation (~2.78 hours), which is about 1.5 times shorter. This is mainly because the gBA-I Approach used a 1.7 times faster machine. The model dimensions and selected results of the approaches are summarised in Table 6.2 and Table 6.3 respectively.

Table 6.2: Problem dimensions and optimisation tolerance in single-site single-period example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	Optimisation tolerance
Simultaneous	33,845	15	14	0.001[1]
gBA-I	30	15	14	0.001[2]

Remarks:
1. gPROMS SRQPD solver, "OptimisationTolerance". Definition can be found in (PSE, 2004a).
2. NAG E04UGA, "Major Optimality Tolerance". Definition can be found in (NAG, 2002).

Table 6.3: Single-site single-period example selected result summary.

	Base Case	Simult. Approach	gBA-I Approach	Min.	Max.
Objective, Profit (10^6\$)	-0.2260	1.2354	1.2399		
Ethane feed (kg/s)	2.50	12.67	12.66	2.50	10.00
Propane feed (kg/s)	2.50	3.46	3.48	2.50	10.00
Butane feed (kg/s)	13.00	2.50	2.50	2.50	10.00
Demethaniser boil-up, Bup1	2.00	0.86	0.89	0.50	3.00
Demethaniser reflux, R1	2.66	2.33	2.57	0.50	3.00
Deethaniser boil-up, Bup2	1.00	2.94	3.00	0.50	3.00
Deethaniser reflux, R2	0.78	0.98	1.00	0.50	3.00
C2 splitter boil-up, Bup3	4.76	4.55	4.53	0.50	5.00
C2 splitter reflux, R3	1.50	1.52	1.51	0.50	5.00
Depropaniser boil-up, Bup4	3.57	1.62	1.61	0.50	4.00
Depropaniser reflux, R4	1.50	2.10	2.10	0.50	4.00
C3 splitter boil-up, Bup5	5.00	4.36	4.44	0.50	5.00
C3 splitter reflux, R5	1.00	5.00	5.00	0.50	5.00
Reactor heat flux (kJ/m^2s)	30.00	45.00	45.00	30.00	45.00
Ethylene production (kg/s)	3.12	9.46	9.49	2.00	10.00
Ethylene product molar purity	0.9966	0.9900	0.9900	0.99	1.00

6.3.2 Single-site 3-period Example

The same single-site 3-period problem used in Chapter 5 was employed again to examine the gBA-I Approach. The problem configurations including the variable bounds and the prices/costs were unchanged. The only modification to the example was that the gBA-I Approach started the optimisation from the solution of the FOT Approach rather than from the base case. This should help reducing the gBA-I Approach solution time, as it was expected to be relatively long. The model dimensions and the optimisation tolerance used in the gBA-I Approach are reported in Table 6.4.

Table 6.4: Problem dimensions and optimisation tolerance in 3-period example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	Optimisation tolerance
gBA-I	124	63	60	0.001[1]

Remarks:
1. NAG E04UGA, "Major Optimality Tolerance". Definition can be found in (NAG, 2002).

The gBA-I Approach obtained an optimum with a profit of $\$3.5295 \times 10^6$. It is about a 3% increase from the Simultaneous Approach objective value ($\$3.4161 \times 10^6$) in Chapter 5. The gBA-I result (Figure 6.4) is very similar to the Simultaneous Approach result. They both purchased cheap ethane and produced ethylene in period 1, and kept the ethylene for selling in period 2. Also, they consumed a lot of butane to produce C4 chemicals in period 2 and raised the sales level of C4 in the same period. The only clear difference between the two results is the gBA-I Approach used more ethane in period 3 to further increase the ethylene production as well as the sales. This helped the gBA-I Approach to attain a better profit.

In terms of the computational time, the gBA-I Approach was slow even though it had a better starting point and used a faster computer. It required 67,667 CPU seconds (~18.80 hours), which is about 66% longer than the Simultaneous Approach solution time (~11.31 hours). However, the additional 3% profit from the gBA-I Approach represents an actual amount of $\$1.1340 \times 10^5$. The benefit induced by the approach definitely outweighs the extra 7 hours spent. The objective values and the computational times of the approaches investigated in Chapter 5 and those of the gBA-I Approach are summarised in Figure 6.5.

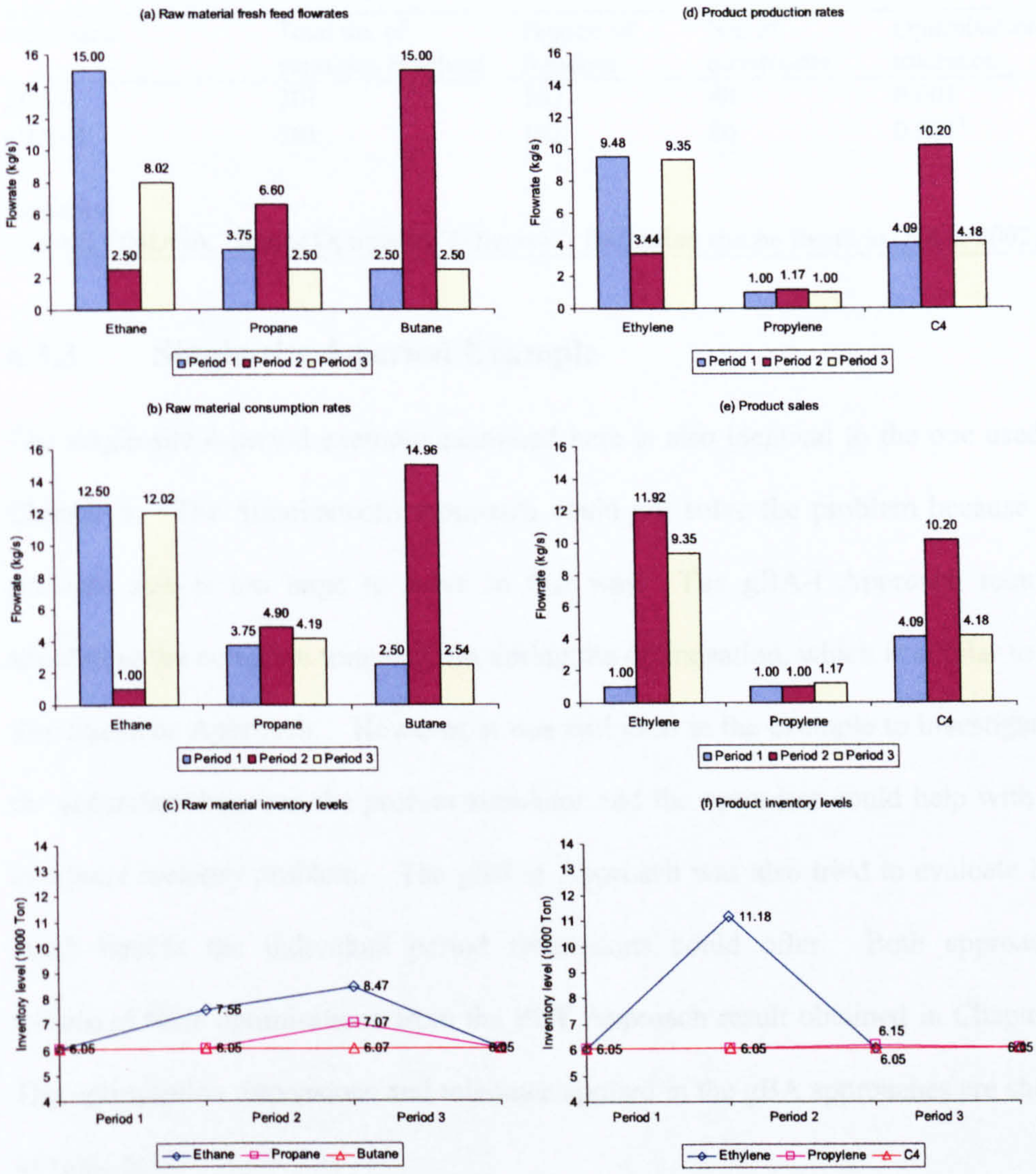

Figure 6.4: gBA-I Approach selected results of 3-period example.

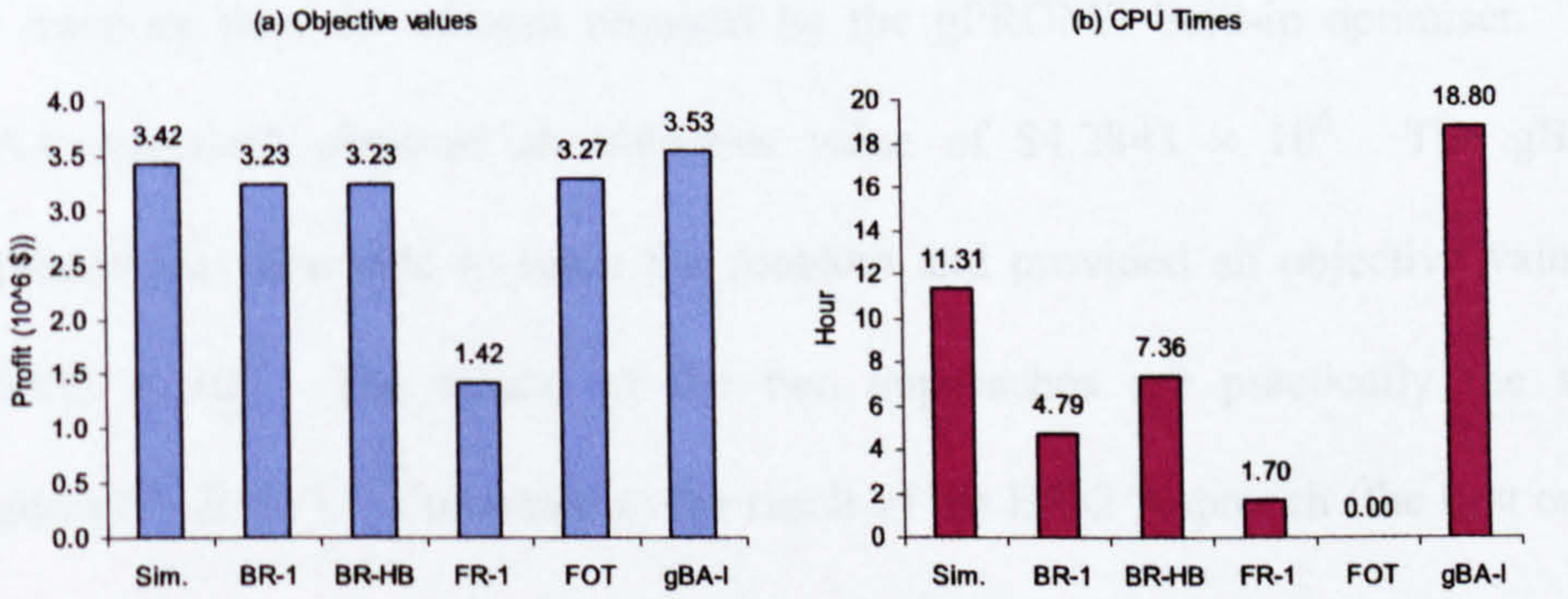

Figure 6.5: Approach objective values and CPU times of 3-period example.

Table 6.5: Problem dimensions and optimisation tolerance in 4-period example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	Optimisation tolerance
gBA-I	201	102	80	0.001[1]
gBA-II	201	102	80	0.001[1]

Remarks:
1. NAG E04UGA, "Major Optimality Tolerance". Definition can be found in (NAG, 2002).

6.3.3 Single-site 4-period Example

The single-site 4-period example examined here is also identical to the one used in Chapter 5. The Simultaneous Approach could not solve the problem because the problem size is too large to solve in that way. The gBA-I Approach requires simulating the complete time horizon during the optimisation, which is similar to the Simultaneous Approach. However, it was still used in the example to investigate if the separation between the process simulator and the optimiser could help with the computer memory problem. The gBA-II Approach was also tried to evaluate how much benefit the individual period simulations could offer. Both approaches initialised their optimisations from the FOT Approach result obtained in Chapter 5. The optimisation dimensions and tolerance applied in the gBA approaches are shown in Table 6.5.

The gBA-I Approach successfully optimised the problem without the computer memory problem. It might be because the 4-period gPROMS simulation just used less memory than the amount required by the gPROMS built-in optimiser. The gBA-I Approach obtained an objective value of \$4.2843 $\times$ 10^6. The gBA-II Approach was also able to solve the problem and provided an objective value of \$4.2836 $\times$ 10^6. The results of the two approaches are practically the same (Figures 6.6 & 6.7). Compared to the result of the BR-2 Approach (the best one in

Chapter 5), the gBA approaches provided about a 7.5% profit increase in this example. A difference is noted between the gBA results and the BR-2 result is that the gBA approaches generally kept lower inventories. They basically did not keep butane in inventory, but the BR-2 Approach had a high butane inventory level at the end of period 2. Even only with the low inventory levels, the gBA approaches still

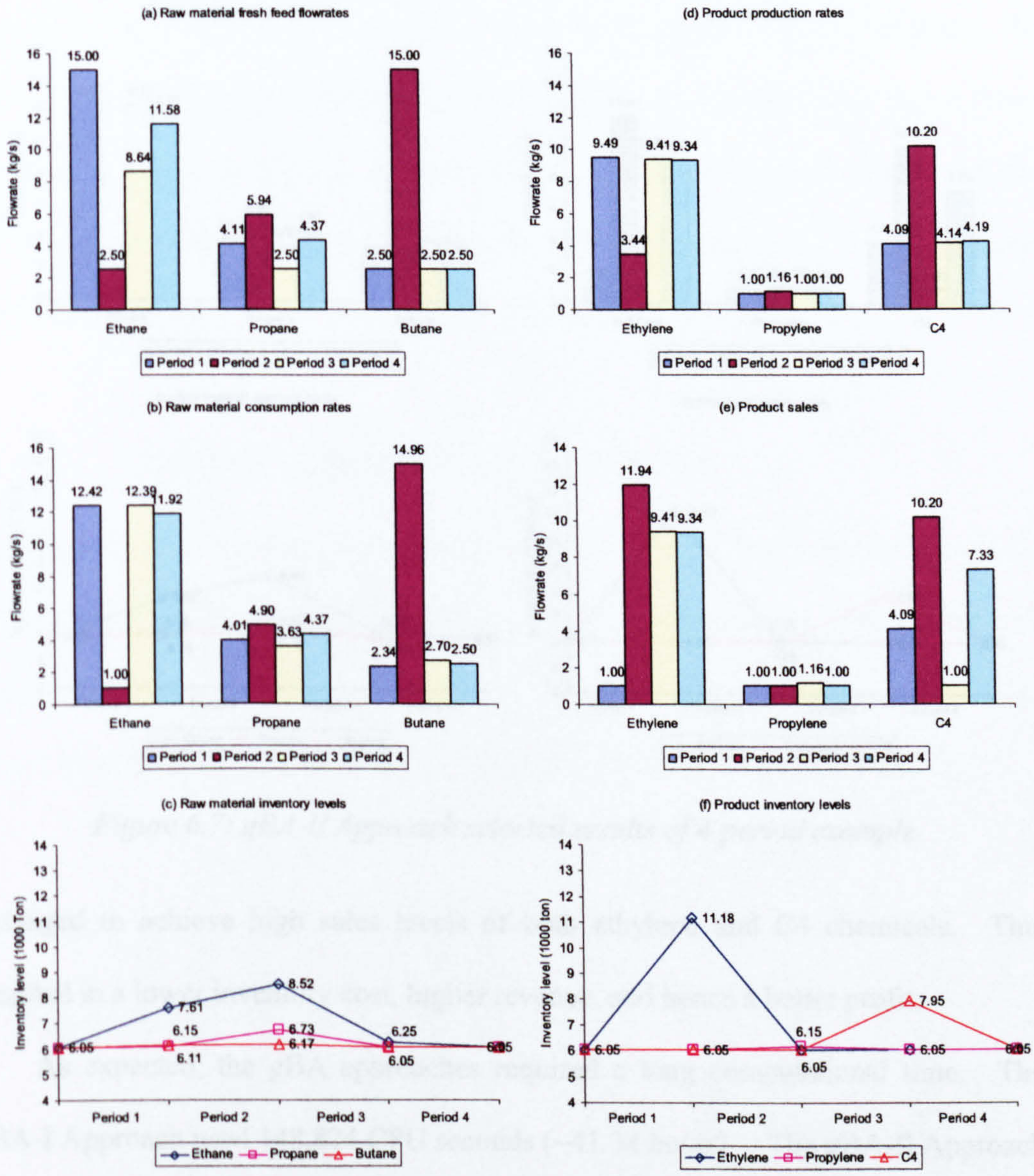

Figure 6.6: gBA-I Approach selected results of 4-period example.

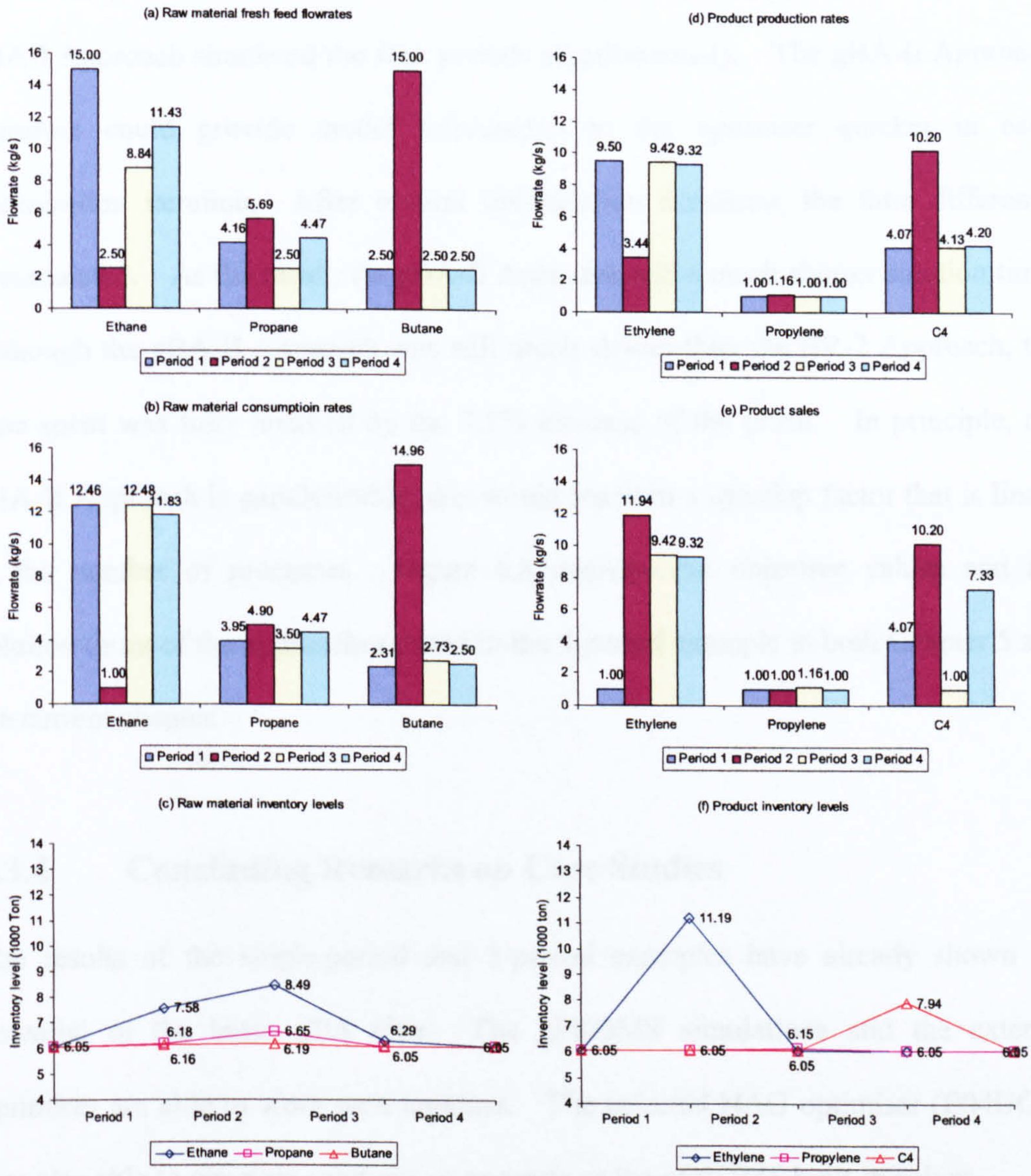

Figure 6.7: gBA-II Approach selected results of 4-period example.

managed to achieve high sales levels of both ethylene and C4 chemicals. This resulted in a lower inventory cost, higher revenue, and hence a better profit.

As expected, the gBA approaches required a long computational time. The gBA-I Approach used 148,824 CPU seconds (~41.34 hours). The gBA-II Approach was faster and required only 63,954 CPU seconds (~17.77 hours). This was because the simulation time is exponentially proportional to the problem size. The

gBA-II Approach simulated the four periods sequentially. On the other hand, the gBA-I Approach simulated the four periods simultaneously. The gBA-II Approach therefore could provide model information to the optimiser quicker in each optimisation iteration. After several optimisation iterations, the time difference accumulated. As the result, the gBA-II Approach had a much shorter solution time. Although the gBA-II Approach was still much slower than the BR-2 Approach, the time spent was fully justified by the 7.5% increase of the profit. In principle, the gBA-II Approach is parallelisable; this would result in a speedup factor that is linear in the number of processes. Figure 6.8 displays the objective values and the solution times of the approaches tested in the 4-period example in both Chapter 5 and the current chapter.

6.3.4 Concluding Remarks on Case Studies

The results of the single-period and 3-period examples have already shown the potential of the basic gBA idea. The gPROMS simulations and the external optimiser are able to work well together. The selected NAG optimiser (E04UGA) was also able to generate solutions as accurate as the gPROMS built-in solver.

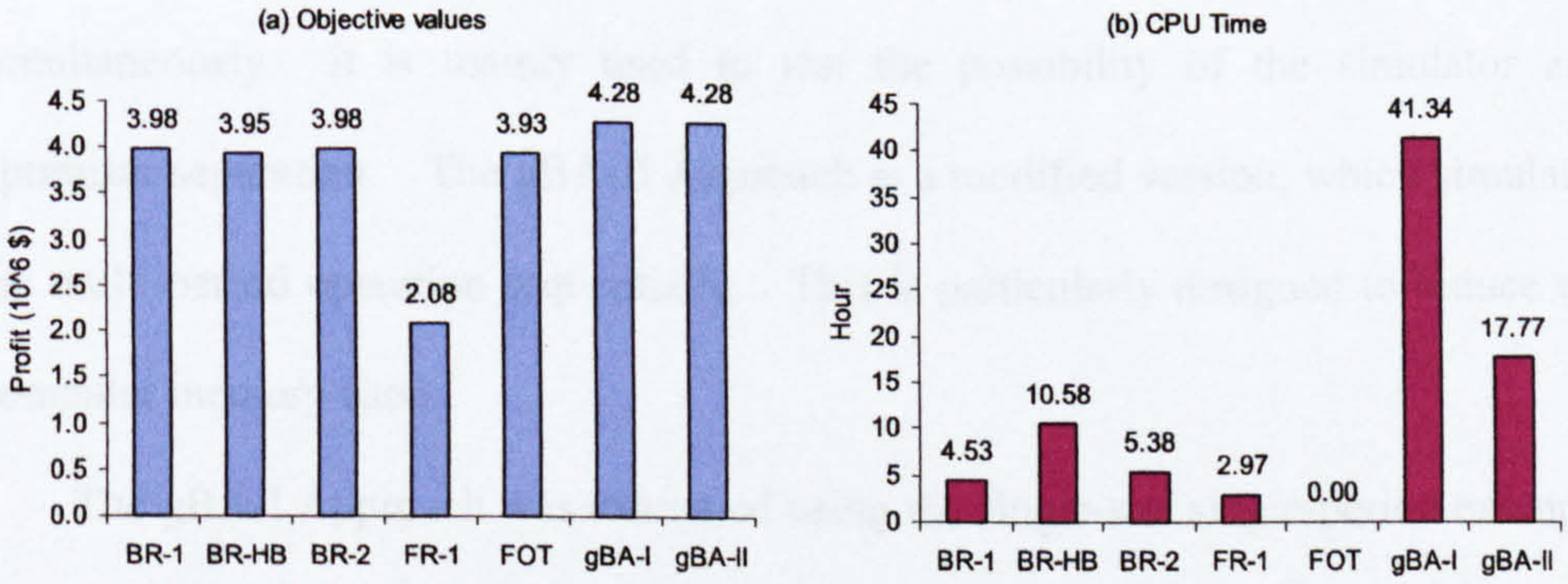

Figure 6.8: Approach objective values and CPU times of 4-period example.

The results of the 4-period example have once again proved that the direct optimisation could result in a better profit than those of the decomposition or simplification methods tested before. The example also indicated that the gBA approaches were able to overcome the memory problem in the direct optimisation. The unexpected success of the gBA-I Approach in the 4-period example suggests that the separation of the simulator and the optimiser have already improved the memory usage during the optimisation process. There is however no guarantee in more complicated problems. To enhance the reliability of the direct optimisation, the gBA-II Approach should be used. It simulated individual periods separately, so that the memory usage was minimised. That also speeded up the gBA-II computational time. With the FOT Approach to initialise the problem, the gBA-II Approach could be an effective direct optimisation approach.

6.4 Conclusions

The gBA Approach is proposed in the chapter to perform a holistic direct optimisation for the site-wide supply chain problems. The approach separates the process simulator from the optimiser in order to reduce the memory required during the optimisation. The approach has two variants, the gBA-I and gBA-II approaches. The gBA-I Approach is a basic one, which simulates the multi-period operations simultaneously. It is mainly used to test the possibility of the simulator and optimiser separation. The gBA-II Approach is a modified version, which simulates the multi-period operation sequentially. This is particularly designed to reduce the computer memory used.

The gBA-I Approach was examined using the single-site single-period example

and the single-site 3-period example. It could perform as well as the Simultaneous Approach in the first one, and slightly out-performed the Simultaneous Approach in the second one. Despite the long computational time, the idea of the gBA Approach provides a way to achieve holistic direct optimisation for site-wide problems.

The two gBA approaches were finally tested using the single-site 4-period example, which the Simultaneous Approach is not able to handle. They initialised the optimisation from the FOT Approach result, and they both successfully solved the problem. Their results are significantly better than those of other approaches in Chapter 5. This clearly justifies the long computational time spent in the gBA approaches.

The gBA-II Approach was faster than the gBA-I Approach in the 4-period example although they found practically the same result. This suggests that the gBA-II Approach is more efficient and reliable. The multi-period examples also demonstrated that the FOT Approach could be a very good initialisation tool. Therefore, the gBA-II Approach initialised by the FOT Approach has been determined as a promising technique for directly optimising site-wide supply chain problems. In the next chapter, the analysis of the optimisation technique will be extended to multi-site problems.

7 Multi-site Single-period Problem

7.1 Introduction

A chemical enterprise usually has more than one production site. Managing overall resources in the enterprise among different production sites results in another class of supply chain problem, the multi-site problem. This chapter focuses on solving the simplest form of the class, the multi-site single-period problem. The problem studied in this chapter includes several production sites and markets in different locations, but only involves a single time period. The problem does not require inventory control to be modelled. Instead, it has to optimise the operations of the production sites in order to satisfy the demands in different markets. This involves the allocation of the material flows among different production sites and markets.

This chapter uses both decomposition methods and site-wide methods to tackle the problem. The chapter proposes three decomposition methods; they are the Site/Market Decomposition Approach, Penalty Function Approach, and Rolling Site Approach. The site-wide methods employed here are the two approaches explained in previous chapters; they are the Feasible Operation Table (FOT) Approach and gPROMS-based Application (gBA) Approach. The results of the approaches are compared, and the most suitable one for the multi-site single-period problem is also determined in this chapter.

This chapter is outlined as follows. First, it describes an example of the multi-site single-period problem, which is derived from the 5-column ethylene process. The example includes four separate production sites and four discrete markets. Second, the chapter describes and explains the suggested solution approaches. After that, it uses the approaches to solve two cases studies. The case

studies are both based on the defined example, and only differ in the magnitudes of the market demands. Finally, the case study results are analysed and conclusions are drawn according to the performance of the approaches.

7.2 Problem Statement

The problem investigated in this chapter is the multi-site single-period optimisation problem. The problem includes four production sites and four markets. To generalise the problem, the four production sites are basically identical and they are all based on the 5-column ethylene process described in Chapter 3. All four production sites accept ethane, propane and butane feeds as raw materials, and they produce ethylene, propylene and C4 chemicals as products. Although the processes inside the sites are the same, the raw material costs, the utility costs and the operating conditions can be different. The products from the production sites can be sold to any one of the markets as long as the market capacity is not exceeded. The product delivery costs between a production site and different markets are varied. Each market also has its own minimum and maximum demands and its own product prices. The objective of the multi-site single-period optimisation is then to maximise the overall profit of the 4-site-4-market system, by adjusting the operating conditions in the production sites and transferring suitable amounts of products from each site to each market. Figure 7.1 shows a schematic diagram of the 4-site-4-market system used in this chapter. The mathematical representation of the multi-site single-period problem is also described below by using the notation adopted in Chapter 5, together with some additional elements.

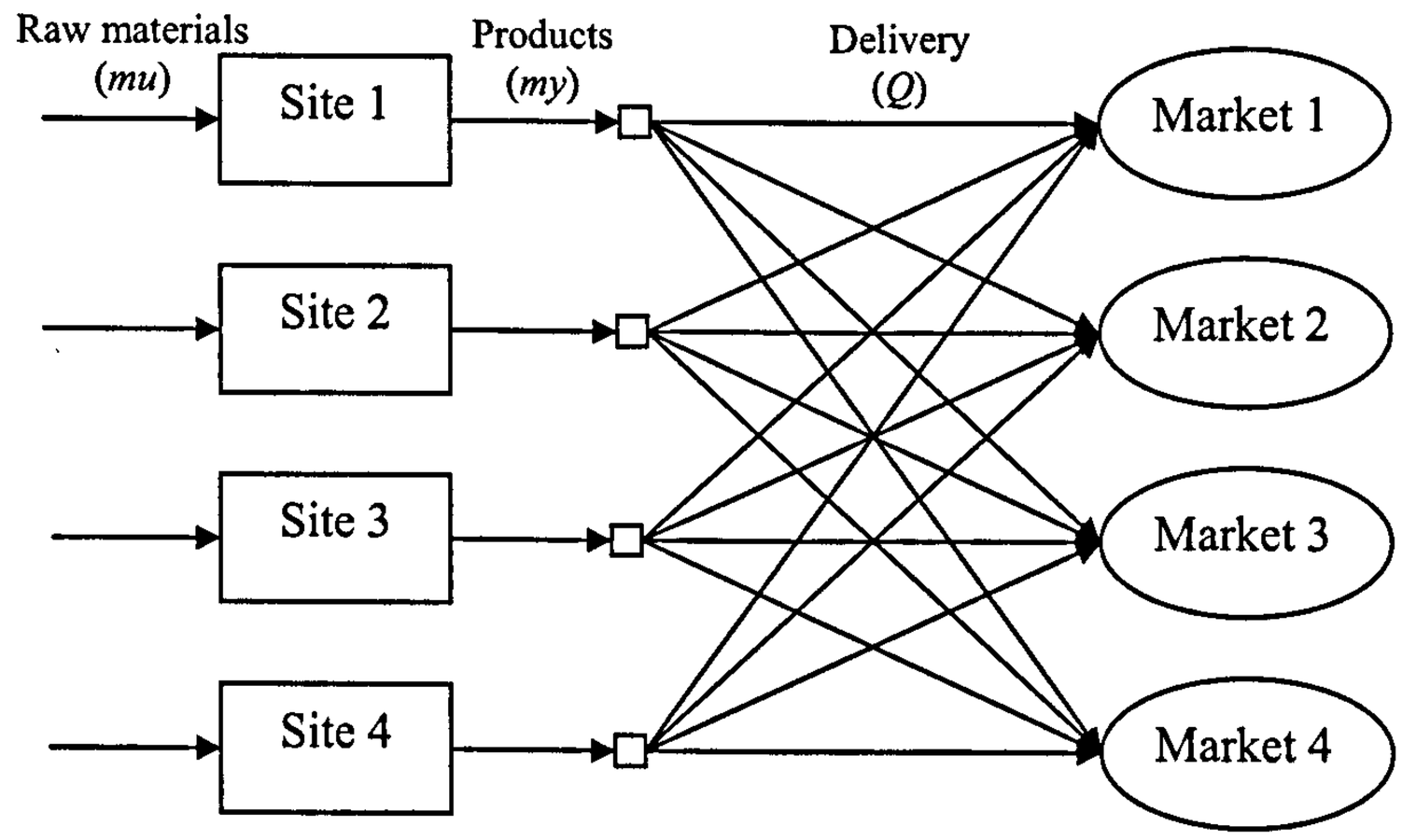

Figure 7.1: Schematic diagram of a 4-site 4-market system.

Indices:

i	Process model input variable index.
j	Process model output variable index.
k	Raw material specie index, $k \in i$.
l	Product specie index, $l \in j$.
s	Production site index.
m	Market index.

Variables:

$u_{i,s}$	Process model input variable i of site s.
$y_{j,s}$	Process model output variable j of site s.
$mu_{k,s}$	Raw material k consumption rate at site s, $mu_{k,s} \in u_{i,s}$
$my_{l,s}$	Product l production rate at site s, $my_{l,s} \in y_{j,s}$.

$D_{l,m}$	Product l sales in market m.
$Q_{l,s,m}$	Product l delivery from site s to market m.
P_s	Profit of site s.
TP	Total profit of the multi-site multi-market system.

Parameters:

$\alpha^u_{i,s}$	Price/cost associated with variable $u_{i,s}$.
$\alpha^y_{j,s}$	Price/cost associated with variable $y_{j,s}$.
$\beta^D_{l,m}$	Sale price of product l in market m.
$TC_{l,s,m}$	Transportation cost of product l from site s to market m.
$u^{\min}_{i,s}$, $u^{\max}_{i,s}$	Lower and upper bounds of input variable $u_{i,s}$ respectively.
$y^{\min}_{j,s}$, $y^{\max}_{j,s}$	Lower and upper bounds of output variable $y_{j,s}$ respectively.
$D^{\min}_{l,m}$, $D^{\max}_{l,m}$	Lower and upper bounds of product sales $D_{l,m}$ respectively.
$Q^{\min}_{l,s,m}$, $Q^{\max}_{l,s,m}$	Lower and upper bounds of product delivery $Q_{l,s,m}$ respectively.
I	The total number of the input variables $u_{i,s}$ in site s.
J	The total number of the output variables $y_{j,s}$ in site s.
PD	Duration of the single time period.

Equations:

$f_{j,s}$	Mathematical relations of y_j in terms of $\forall u_i$, both linear and nonlinear, in site s.

Process Model:

$$y_{j,s} = f_{j,s}\left(u_{1,s}, u_{2,s}, u_{3,s}, \cdots, u_{I,s}\right) \quad \text{(Eq. 7.1)}$$

$$u_{i,s}^{\min} \le u_{i,s} \le u_{i,s}^{\max} \quad \text{(Eq. 7.2)}$$

$$y_{j,s}^{\min} \le y_{j,s} \le y_{j,s}^{\max} \quad \text{(Eq. 7.3)}$$

Product Delivery from Site to Market:

$$my_{I,s} = \sum_{m} Q_{I,s,m} \quad \text{(Eq. 7.4)}$$

$$D_{I,m} = \sum_{s} Q_{I,s,m} \quad \text{(Eq. 7.5)}$$

$$D_{I,m}^{\min} \le D_{I,m} \le D_{I,m}^{\max} \quad \text{(Eq. 7.6)}$$

$$Q_{I,s,m}^{\min} \le Q_{I,s,m} \le Q_{I,s,m}^{\max} \quad \text{(Eq. 7.7)}$$

Profit of Production Site *s*:

$$P_s = \left[\sum_{i} \alpha_{I,s}^{u} \cdot u_{i,s} + \sum_{j} \alpha_{j,s}^{y} \cdot y_{j,s} + \sum_{m} \beta_{I,s}^{D} \cdot Q_{I,s,m} - \sum_{m} TC_{I,s,m} \cdot Q_{I,s,m}\right] \cdot PD \quad \text{(Eq. 7.8)}$$

Objective: Total profit

$$\max\left(TP = \sum_{s} P_s\right) \quad \text{(Eq. 7.9)}$$

7.3 Solution Approaches

This section suggests different solution approaches to attempt the multi-site single-period problem. The approaches can be classified into two categories, the

decomposition method and the site-wide method. As the problem involves several production sites together, the total problem size is large. It is likely that decomposition methods will be required to make the problem solvable. However, potential site-wide methods have been developed in previous chapters and obtained good results. This encourages the use of site-wide methods for the problem.

7.3.1 Site/Market Decomposition Approach

In the multi-site multi-market system, the production sites operate independently and they only connect to the markets by product delivery. Therefore, the system can be decomposed into separate production site models and an integrated market model via the product delivery (Figure 7.2). This type of decomposition can be classified as spatial decomposition (Kulkarni & Mohanty, 1993; Dhaenens-Flipo, 2000; van den Heever & Grossmann, 2000). The decomposition problem can be solved through some iterative procedures. Extra constraints are placed in the sub-problems to control the de-coupled variables in the master problem. The constraints are updated by other sub-problems' results through iterations. For example, the production rate in the production sub-model cannot be larger than the optimal market capacity in the market sub-model. The final solution is obtained when the de-coupled variables converge for all sub-problems' results.

For the multi-site single-period problem studied in this chapter, the production sites adopt rigorous property-based formulations, so they are nonlinear models. In contrast, the market model only deals with product sales and is linear. Based on that, the Site/Market Decomposition Approach is designed to iterate among the nonlinear production models and the linear integrated market model.

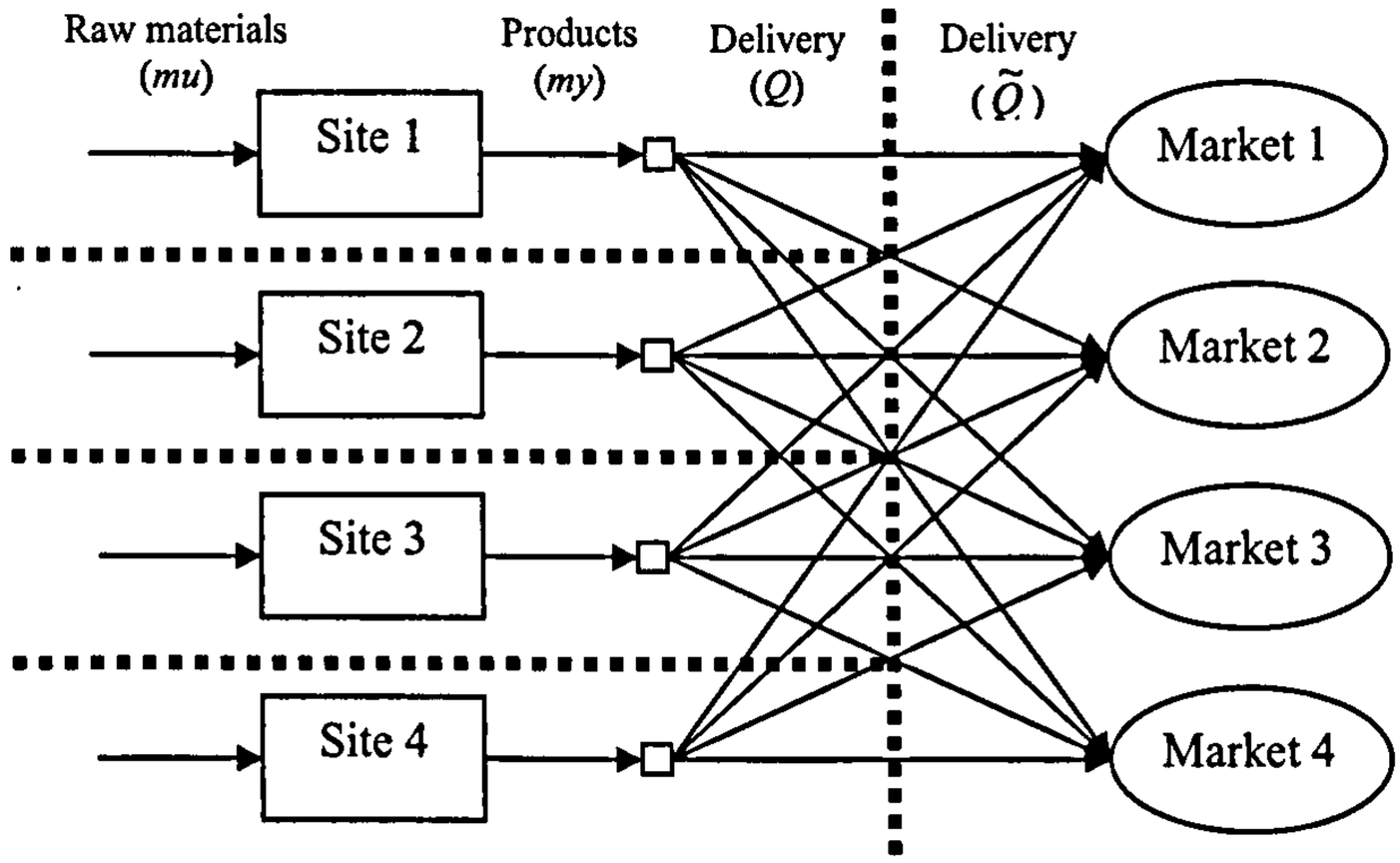

Figure 7.2: Schematic diagram of site/market decomposition.

The approach starts by optimising the production sites individually. The optimisation is to maximise the profit of the site (Eq. 7.8), which is subject to the process model (Eq. 7.1 – 7.3). From the individual production optimisations, the product delivery flowrates (Q) in the site models are determined. Based on those flowrates, the total production capacities of the products ($CAP = \sum Q$) are calculated. With the value of CAP, the integrated market model then maximises the product sales revenue (Eq. 7.10) by varying the product delivery flowrates ($\tilde{Q}$) in the market model. The total delivery flowrate in the market optimisation must be less than or equal to the production capacity determined in the site optimisations. After that, another set of production capacity values ($\tilde{C}AP = \sum \tilde{Q}$) are calculated from the market optimisation result. If the production capacities from the site optimisations (CAP) and the market optimisation ($\tilde{C}AP$) are the same, the solution approach converges. Otherwise, the production sites have to be optimised again. This time, the product delivery flowrates in the site optimisation are bounded by the

values determined in the previous market optimisation ($Q \le \tilde{Q}$). The value of CAP is then updated, and the market optimisation is executed again. The procedures are repeated until the CAP is equal to the $\tilde{C}AP$. The Site/Market Decomposition Approach is summarised in Figure 7.3.

$$\max_{\tilde{Q}_{l,s,m}} \left(\left(\sum_m \beta^D_{l,s} \cdot \tilde{Q}_{l,s,m} - \sum_m TC_{l,s,m} \cdot \tilde{Q}_{l,s,m} \right) \cdot PD \right) \qquad \text{(Eq. 7.10)}$$

1. Optimise production sites individually, maximising Eq. 7.8 as the objective.
2. Calculate $CAP_{l,s} = \sum_m Q_{l,s,m}$ from (1).
3. Optimise market model, maximising Eq. 7.10 as the objective and which is subject to $\sum_m \tilde{Q}_{l,s,m} \le CAP_{l,s}$. $CAP_{l,s}$ is fixed and obtained from (2) or (7).
4. Calculate $\tilde{C}AP_{l,s} = \sum_m \tilde{Q}_{l,s,m}$ from (3).
5. If $\tilde{C}AP_{l,s} = CAP_{l,s}$, STOP and get the final solution by substituting $\tilde{Q}_{l,m,c}$ into $Q_{l,s,m}$, else go to (6).
6. Optimise production sites again, maximising Eq. 7.8 which is subject to $Q_{l,s,m} \le \tilde{Q}_{l,s,m}$. $\tilde{Q}_{l,m,c}$ is fixed and obtained from (5).
7. Calculate $CAP_{l,s} = \sum_m Q_{l,s,m}$ from (6), and go to (3).

Figure 7.3: Site/market decomposition approach.

7.3.2 Penalty Function Approach

Similar to the Site/Market Decomposition Approach, the Penalty Function Approach also decomposes the multi-site multi-market system into separate production site models and a market model. However, its solution procedure is inspired by

Lagrangean decomposition (van den Heever *et al.*, 2001; Jackson & Grossmann, 2003). Penalty functions (Kontogiorgis & Meyer, 1998) of the de-coupled variables (i.e. product deliveries), instead of Lagrange multipliers, are placed in the objective functions of the sub-models. The penalty terms are minimised via iterations. When the penalty terms reach zero, a feasible and possibly optimal solution is obtained.

The Penalty Function Approach begins with the market model. The model is optimised to maximise Eq. 7.10 and also determine the corresponding product delivery flowrates ($\tilde{Q}$). Then optimisations of individual production sites are carried out with a modified objective function (Eq. 7.11). The new function includes a penalty term (E) to indicate the difference between the values of product delivery flowrates determined in site and market optimisations (Q and $\tilde{Q}$). The $\tilde{Q}$ values are obtained from the market optimisation and fixed in the site optimisations. The Q values instead are varied and determined from the site optimisations. If the values of E for all the production sites equal to zero, an optimal solution is found. Otherwise, the market model is optimised with the penalty term E included in the objective function (Eq. 7.13). This time, $\tilde{Q}$ is varied and Q is fixed from the previous site optimisation results. The E values are then checked for closeness to zero again. If they are zero, the approach terminates. If not, the approach will continue the loop of the site optimisations and the market optimisation until E equals to zero. The procedures of the algorithm are listed in Figure 7.4.

$$\max\left(\left(\sum_i \alpha^u_{i,s}\cdot u_{i,s}+\sum_j \alpha^y_{j,s}\cdot y_{j,s}+\sum_m \beta^D_{l,s}\cdot Q_{l,s,m}-\sum_m TC_{l,s,m}\cdot Q_{l,s,m}-\sum_{l,s,m}\pi_{l,s,m}\cdot E_{l,s,m}\right)\cdot PD\right) \quad \text{(Eq. 7.11)}$$

$$E_{l,s,m}=\left|Q_{l,s,m}-\tilde{Q}_{l,s,m}\right| \quad \text{(Eq. 7.12)}$$

$$\max_{\tilde{Q}_{l,s,m}}\left(\left(\sum_m \beta^D_{l,s}\cdot \tilde{Q}_{l,s,m}-\sum_m TC_{l,s,m}\cdot \tilde{Q}_{l,s,m}-\sum_{l,s,m}\pi_{l,s,m}\cdot E_{l,s,m}\right)\cdot PD\right) \quad \text{(Eq. 7.13)}$$

where π is the weight of the penalty term in the objective function.

1. Optimise market model, maximising Eq. 7.10 as the objective.
2. Optimise individual production sites, maximising Eq. 7.11 as the objective and which is subject to $E_{l,s,m}=\left|Q_{l,s,m}-\tilde{Q}_{l,s,m}\right|$. $\tilde{Q}_{l,m,c}$ is fixed and obtained from (1).
3. If $E_{l,s,m}=0$, STOP. Else go to (4).
4. Optimise market model again, maximising Eq. 7.13 and is subject to $E_{l,s,m}=\left|Q_{l,s,m}-\tilde{Q}_{l,s,m}\right|$. $Q_{l,s,m}$ is fixed and obtained from (2).
5. If $E_{l,s,m}=0$, STOP. Else go to (2) by setting $\pi=2\pi$ in Eq. 7.11 and Eq. 7.13.

Figure 7.4: Penalty function approach.

7.3.3 Rolling Site Approach

The "Rolling Site" Approach is a counterpart of the Rolling Horizon Approach, where the former is for multi-site problems and the latter is for multi-period problems. The Rolling Site Approach also has a similar advantage of the Rolling Horizon Approach; its solution time is only linear in the number of sites. This should be helpful to speed up the solution process from the previous two iterative approaches.

The first step of the Rolling Site Approach is to rank the sites involved in the problem. There are different criteria to do this, but basically the sites are ranked by their economical potential. The most economical one should be placed first. Then the sites are optimised sequentially from the first rank to the last rank. After each site optimisation, the remaining demand capacities of the markets ($\tilde{D}_{l,m}^{\max} = D_{l,m}^{\max} - Q_{l,s,m}$) are calculated. The values are passed on to the next site optimisation, and the product delivery amounts ($Q_{l,s,m}$) are constrained by them ($Q_{l,s,m} \le \tilde{D}_{l,m}^{\max}$). When all the production sites are optimised and products are allocated to different markets, violations on some markets' minimum sales ($D_{l,m}^{\min}$) might occur. This is because the production site optimisations only consider selling the products at the highest price market. If the highest price market still has capacity, the products will be sent to it. This however does not take account of the minimum sales in other lower price markets. To eliminate the violations, the integrated market model with a modified penalty objective function (Eq. 7.14) is used, and the penalty term (E') calculation is also modified to Eq. 7.15. By fixing $Q_{l,s,m}$ obtained from the site optimisations, the market optimisation is executed to re-allocate the product deliveries in order to match the sites' production amounts as well as to satisfy the demand capacity constraints in the markets. The algorithm of the Rolling Site Approach is shown in Figure 7.5.

$$\max_{\tilde{Q}_{l,s,m}} \left(\left(\sum_{m} \beta_{l,s}^{D} \cdot \tilde{Q}_{l,s,m} - \sum_{m} TC_{l,s,m} \cdot \tilde{Q}_{l,s,m} - \sum_{l,s} \pi_{l,s} \cdot E'_{l,s} \right) \cdot PD \right) \qquad \text{(Eq. 7.14)}$$

$$E'_{l,s} = \left| \sum_{m} Q_{l,s,m} - \sum_{m} \tilde{Q}_{l,s,m} \right| \qquad \text{(Eq. 7.15)}$$

1. Rank the sites (R: ranking).
2. Start from the Rank 1 site. Set $\tilde{D}_{l,m}^{\max} = D_{l,m}^{\max}$.
3. Optimise current site, using Eq. 7.8 as the objective function and which is subject to $Q_{l,s,m} \le \tilde{D}_{l,m}^{\max}$.
4. If R ≠ the last rank, update $\tilde{D}_{l,m}^{\max} = D_{l,m}^{\max} - Q_{l,s,m}$ from (3) and go to (5). Else go to (6).
5. Set R as the next rank and go to (3).
6. Optimise market model by using Eq. 7.14 as the objective function and being subject to $E'_{l,s} = \left| \sum_m Q_{l,s,m} - \sum_m \tilde{Q}_{l,s,m} \right|$. $Q_{l,s,m}$ is fixed and obtained from (3).
7. Obtain the final solution by substituting $\tilde{Q}_{l,m,c}$ into $Q_{l,s,m}$.

Figure 7.5: Rolling site approach.

7.3.4 Feasible Operation Table Approach

The Feasible Operation Table (FOT) Approach is a site-wide method, which applies model simplification. The rigorous process models are simplified into a table of operation modes. The process optimisation hence becomes a selection of the most suitable operation mode. The single-site multi-period version of the approach has already been explained in Chapter 5. Based on that version, a few modifications on the MILP model are carried out to optimise the approach for the multi-site single-period problem.

Indices:

md Operation mode index.

Binary variables:

$z_{md,s}$ Status of the operation mode *md* in site *s*. 1 is on and 0 is off.

Parameters:

$UO_{i,md}$ Value of input variable u_i in operation mode *md*.

$YO_{j,md}$ Value of output variable y_j in operation mode *md*.

$MUO_{k,md}$ Value of raw material consumption rate mu_k in operation mode *md*.

$MYO_{l,md}$ Value of product production rate my_l in operation mode *md*.

Equations for process operations:

$$u_{i,s} = \sum_{md} \left(UO_{i,md} \times z_{md,s} \right) \quad \text{(Eq. 7.16)}$$

$$y_{j,s} = \sum_{md} \left(YO_{j,md} \times z_{md,s} \right) \quad \text{(Eq. 7.17)}$$

$$mu_{k,s} = \sum_{md} \left(MUO_{k,md} \times z_{md,s} \right) \quad \text{(Eq. 7.18)}$$

$$my_{l,s} = \sum_{md} \left(MYO_{l,md} \times z_{md,s} \right) \quad \text{(Eq. 7.19)}$$

$$\sum_{md} z_{md,s} = 1, \; z_{md,s} = 0 \text{ or } 1. \quad \text{(Eq. 7.20)}$$

Equations (Eq. 7.16 – Eq. 7.20) formulate the operation mode selections for the production sites. They replace the rigorous process models (Eq. 7.1 – Eq. 7.3) and form a complete MILP model for the multi-site single-period problem with other

original equations (Eq. 7.4 – Eq. 7.8) and the objective function (Eq, 7.9). As the FOT Approach presented here is principally identical to the one in Chapter 5, they should share the same advantages. The MILP model is relatively small, so the approach can handle many sites and markets simultaneously without decomposition. Also, the MILP model is easy to solve. It should be able to offer a very quick solution time to the approach.

7.3.5 gBA Approach

The gBA Approach is a technique, developed in Chapter 6, to directly execute large-scale supply chain optimisations. It combines the strengths of the gPROMS process simulator and the NAG optimiser to tackle the task. The details of the approach have been described in Chapter 6. Although Chapter 6 only concentrated on solving multi-period problems, the principle of the approach can also be applied to solving the multi-site problem. This is because both multi-period and multi-site systems are fundamentally collections of individual processes. The approach can easily handle the production sites of the multi-site problem in the same manner as handling the periods of the multi-period problem. The gBA approach has two varieties, the gBA-I and gBA-II Approaches. Figures 7.6 and 7.7 illustrate the procedures of the two gBA approaches used in this chapter.

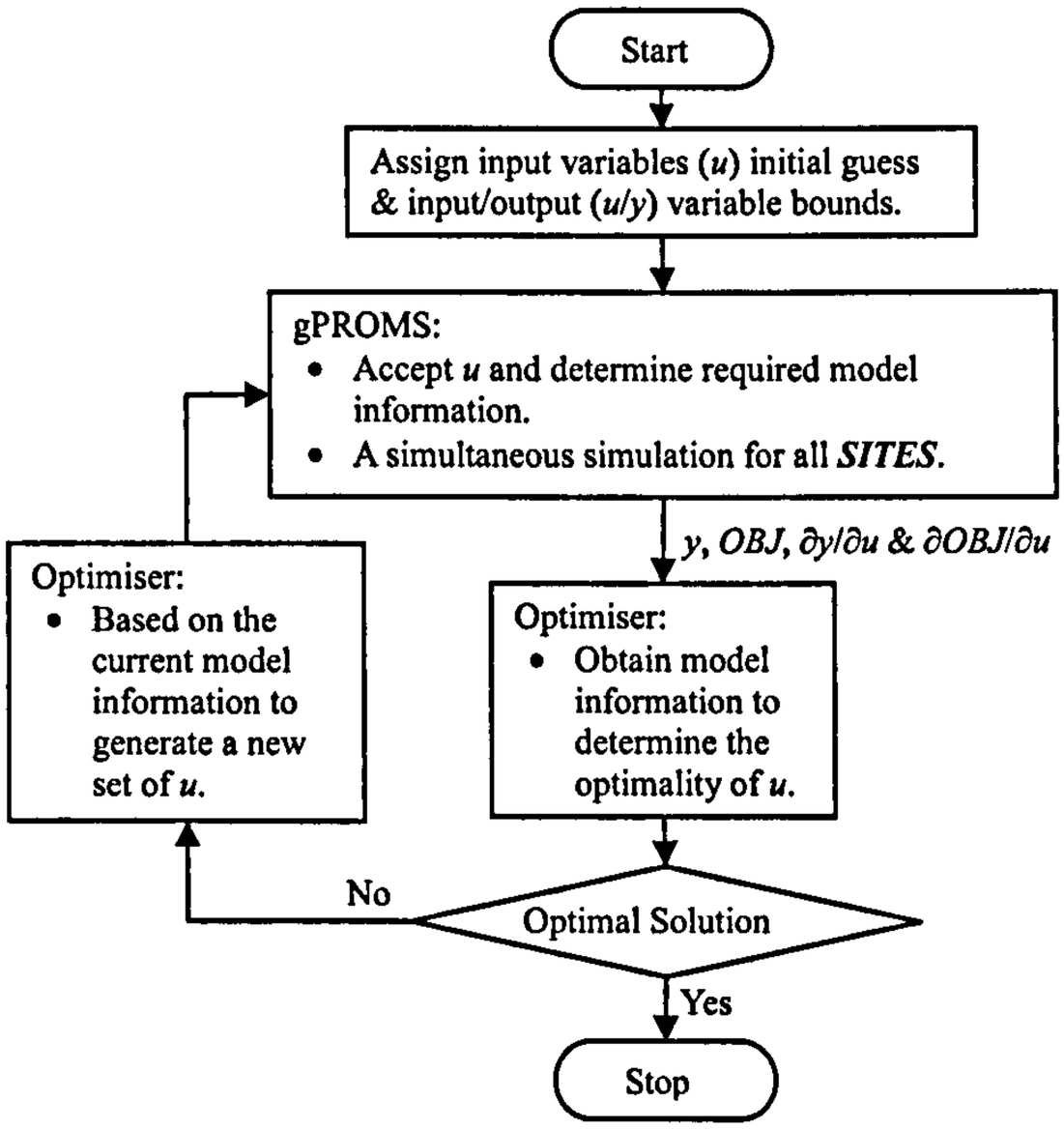

Figure 7.6: gBA-I Approach procedures for multi-site single-period problem.

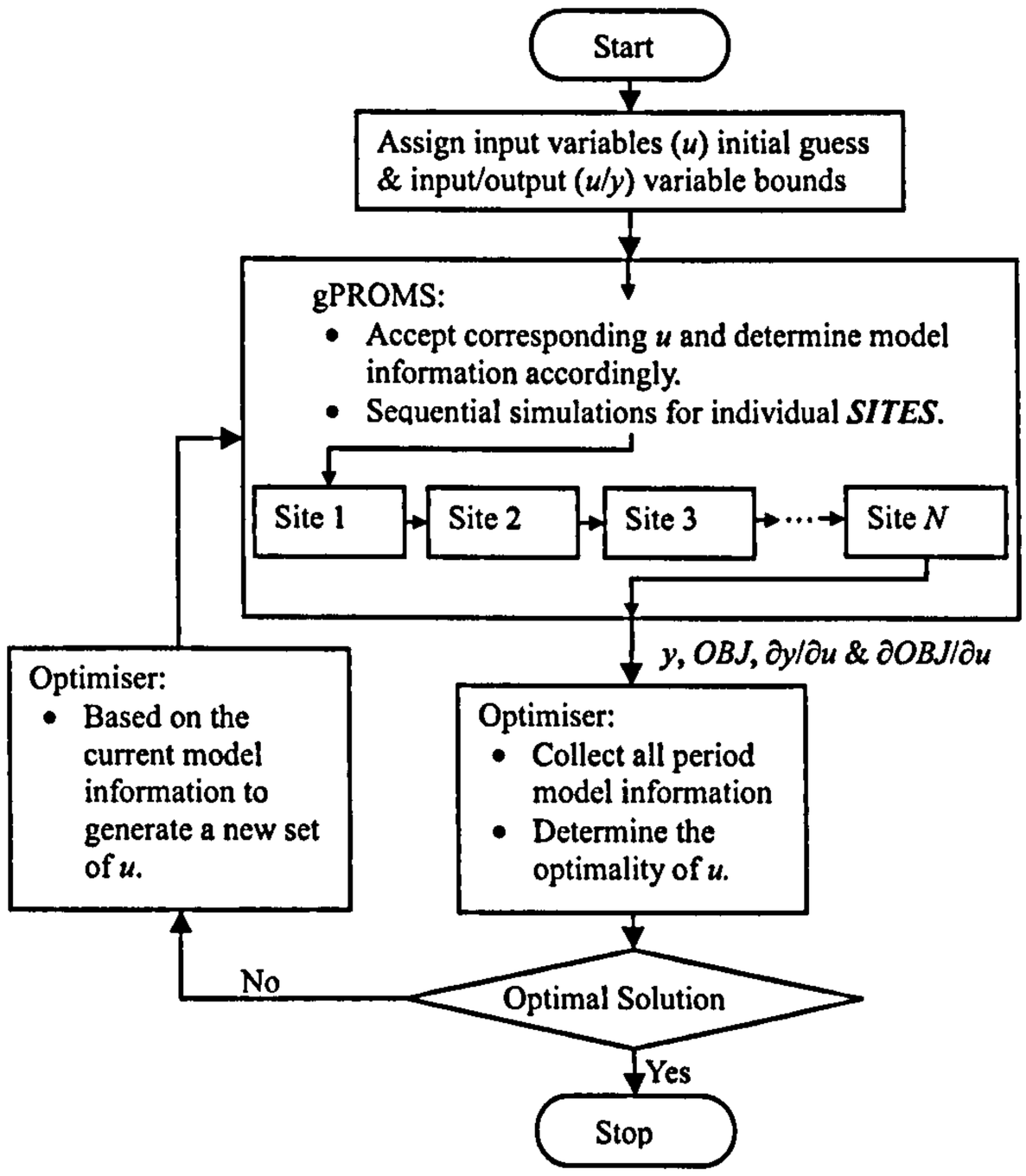

Figure 7.7: gBA-II Approach procedures for multi-site single-period problem.

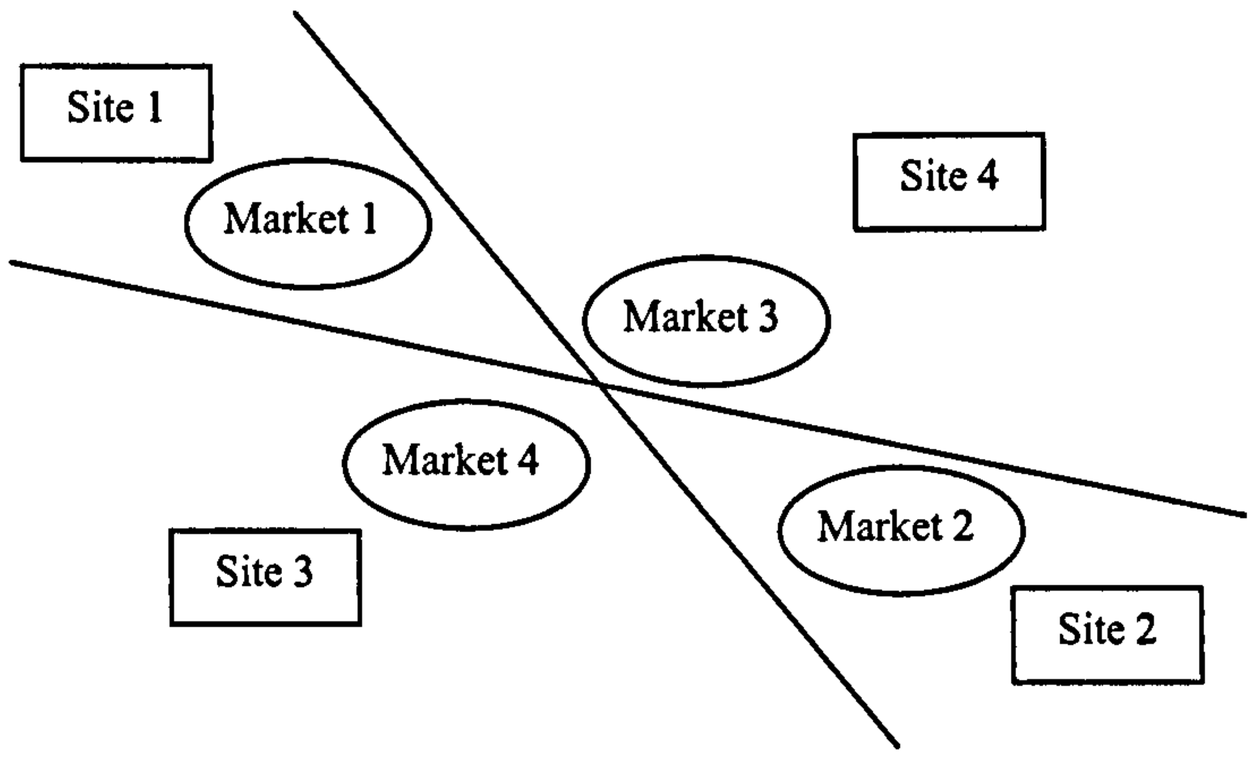

Figure 7.8: Approximated distance representation of the site/market system.

7.4 Case Studies

This section examines two examples; they are four-site four-market problems and use the same site-market system (Figure 7.8). The first example has a higher product demand in the markets. All the approaches suggested in the previous section are tested using it. The second example reduces the product demand, and only those approaches that have potential on the first example are employed to solve the problem. As the gBA Approach is expected to require more computational effort, a faster Linux computer with CPU speed 2992 MHz is assigned to the approach. Other approaches use a slower machine with CPU speed 1794 MHz instead.

7.4.1 High Demand Example

The example contains four production sites and four markets. The 5-column ethylene process is employed for all the production sites involved in the example. It allows the production sites to accept ethane, propane and butane as the raw materials,

and produces ethylene, propylene and C4 chemicals as products. The production sites can supply any product to any market, although different markets have their own product demands (Table 7.1). The sites are supposed to operate in a single period, and the period lasts for 604,800 seconds (7 days). The objective of the example is to maximise the overall profit of the four-site four-market system in the single period.

In the example, the processes in the production sites are basically the same as the one used in the single-site single-period example of Section 6.3.1. They adopt the same set of lower and upper bounds to constrain their input and output variables. The data is in Table 6.1 of Chapter 6. The price/cost values however are different from those of the example in Section 6.3.1. The price/cost values in fact vary across the production sites and the markets. The product delivery costs are also proportional to the distances between sites and markets. The distances are roughly illustrated in Figure 7.8. The price/cost data are shown in Tables 7.2 to 7.4.

Table 7.1: Market product demand capacities of high demand example.

Ethylene demand (kg/s)	Market 1	Market 2	Market 3	Market 4
Max.	5.0	5.0	10.0	10.0
Min.	2.0	2.0	1.0	1.0
Propylene demand (kg/s)	Market 1	Market 2	Market 3	Market 4
Max.	5.0	5.0	5.0	5.0
Min.	1.0	1.0	1.0	1.0
C4 chemicals demand (kg/s)	Market 1	Market 2	Market 3	Market 4
Max.	7.0	7.0	7.0	7.0
Min.	1.0	1.0	1.0	1.0

N.B. Delivery flowrates ($Q_{l,s,m}$) are bounded by $0.0 \leq Q_{l,s,m} \leq 10.0$.

Table 7.2: Raw material and product prices.

Raw material price	Site 1	Site 2	Site 3	Site 4
Ethane ($/kg)	0.260	0.280	0.230	0.300
Propane ($/kg)	0.300	0.310	0.270	0.350
Butane ($/kg)	0.430	0.440	0.380	0.500
Product price	Market 1	Market 2	Market 3	Market 4
Ethylene (kg/s)	0.587	0.650	0.600	0.550
Propylene ($/kg)	0.610	0.610	0.671	0.549
C4 chemicals ($/kg)	0.650	0.650	0.585	0.715

Table 7.3: Site utility prices.

	Site 1	Site 2	Site 3	Site 4
Process steam ($/kg)	0.01	0.02	0.01	0.02
Furnace fuel (in terms of heat flux) ($/kJ-m2)	2.00E-4	2.10E-4	3.00E-4	2.00E-7
Column heating ($/kJ)	1.26E-5	1.30E-5	1.26E-5	2.00E-5
Column cooling ($/kJ)	1.05E-5	1.20E-8	1.05E-5	1.80E-5

Table 7.4: Product delivery costs from production sites to markets.

Ethylene	Unit	Market 1	Market 2	Market 3	Market 4
Site 1	$/kg	0.001	0.050	0.015	0.020
Site 2	$/kg	0.050	0.001	0.020	0.030
Site 3	$/kg	0.040	0.020	0.030	0.022
Site 4	$/kg	0.020	0.030	0.010	0.035
Propylene	Unit	Market 1	Market 2	Market 3	Market 4
Site 1	$/kg	0.001	0.048	0.014	0.019
Site 2	$/kg	0.048	0.001	0.019	0.029
Site 3	$/kg	0.038	0.019	0.029	0.021
Site 4	$/kg	0.020	0.029	0.010	0.033
C4 chemicals	Unit	Market 1	Market 2	Market 3	Market 4
Site 1	$/kg	0.001	0.045	0.014	0.018
Site 2	$/kg	0.045	0.001	0.018	0.027
Site 3	$/kg	0.036	0.018	0.027	0.019
Site 4	$/kg	0.018	0.027	0.009	0.032

7.4.1.1 Site/Market Decomposition Approach Result

The Site/Market Decomposition Approach used the gPROMS SQP solver to handle the nonlinear production site optimisations, and applies GAMS/Cplex to solve the linear market model. It required only one iteration to solve the problem. The total computational time of the approach is 47,709 CPU seconds (~ 13 hours), and the objective value obtained is $\$2.8701 \times 10^6$.

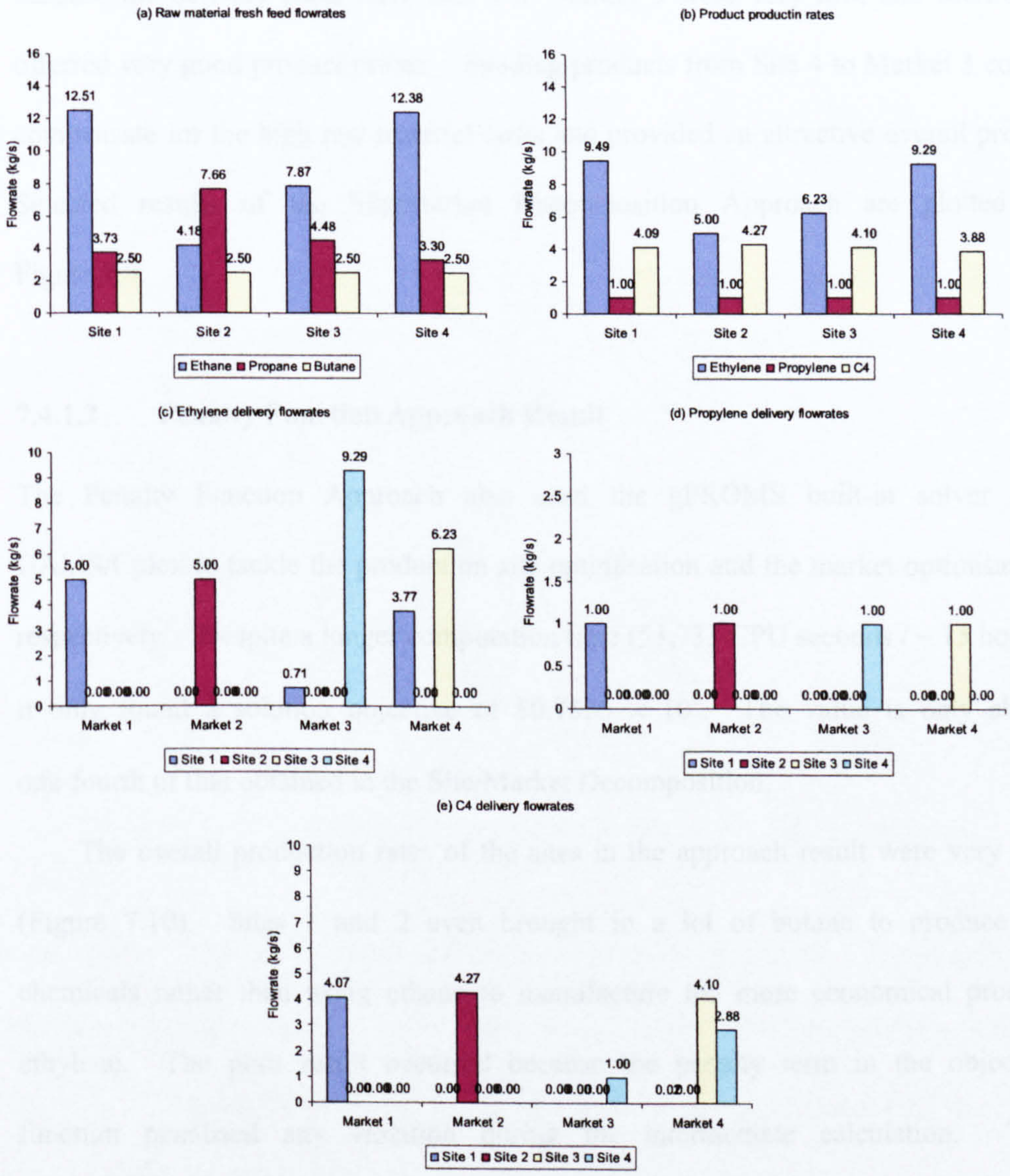

Figure 7.9: Site/market decomposition approach selected results for high demand example.

From the result, it is observed that the product delivery costs greatly influence the delivery pattern. Production sites 1 and 2 are the nearest sites of Markets 1 and 2 respectively. Their delivery costs are lower than the others. This resulted in Markets 1 and 2 basically only receiving products from Sites 1 and 2 respectively. The delivery costs also affect the production rates in the sites. Sites 2 and 4 had higher raw material costs. The high cost usually leads to a low production rate, as in Site 2. However, the production rates of Site 4 were relatively high. This is because the delivery costs from Site 4 to Market 3 were very low, and Market 3 offerred very good product prices. Sending products from Site 4 to Market 3 could compensate for the high raw material costs and provided an attractive overall profit. Selected results of the Site/Market Decomposition Approach are plotted in Figure 7.9.

7.4.1.2 Penalty Function Approach Result

The Penalty Function Approach also used the gPROMS built-in solver and GAMS/Cplex to tackle the production site optimisation and the market optimisation respectively. Despite a longer computation time (53,733 CPU seconds / ~ 15 hours), it only found a solution objective of $\$0.7535 \times 10^6$. The value is only about one-fourth of that obtained in the Site/Market Decomposition.

The overall production rates of the sites in the approach result were very low (Figure 7.10). Sites 1 and 2 even brought in a lot of butane to produce C4 chemicals rather than using ethane to manufacture the more economical product ethylene. The poor result occurred because the penalty term in the objective function penalised any violation during the intermediate calculation. This

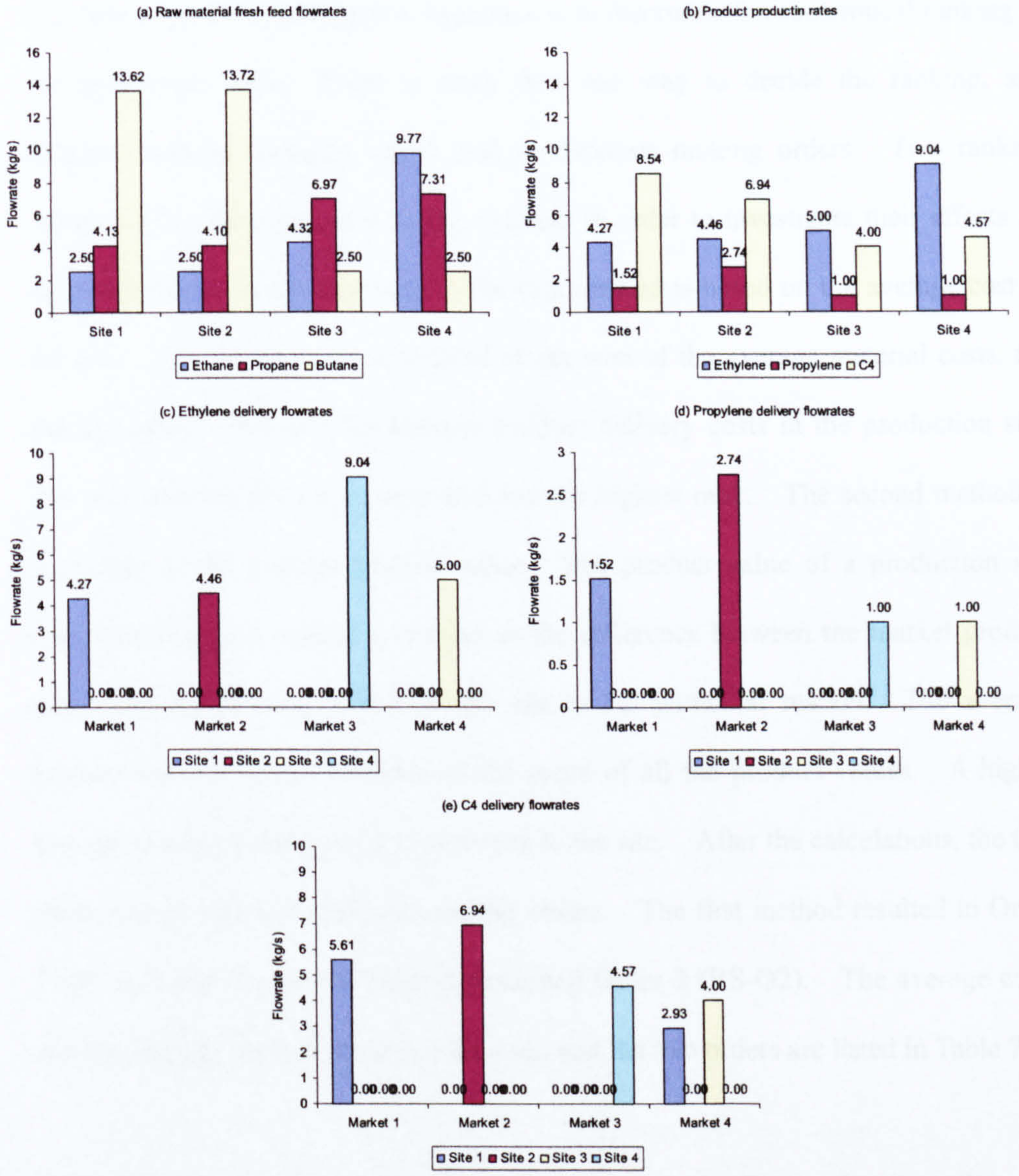

Figure 7.10: Penalty function approach selected results for high demand example.

unintentionally confined the approach to a small solution region. Eventually, the approach could only locate a feasible local solution instead of the global optimum. To improve the situation, the weight of the penalty term (π) should be carefully specified. Unfortunately, it is not straightforward to achieve that.

7.4.1.3 Rolling Site Approach

The first step of the Rolling Site Approach is to determine the economical ranking of the production sites. There is more than one way to decide the ranking, and different ranking methods might lead to different ranking orders. Two ranking methods were therefore used in the example in order to investigate their effects on the performance of the approach. The first method is based on the average cost of the site. The average cost is defined as the sum of the average material costs, the average utility costs and the average product delivery costs in the production site. The site with the lowest average cost has the highest rank. The second method is according to the average product value. The product value of a production site corresponding to a market is defined as the difference between the market product price and the delivery cost from the site to the particular market. The average product value of a site is therefore the mean of all the product values. A higher average product value gives a higher rank to the site. After the calculations, the two methods provided two different ranking orders. The first method resulted in Order 1 (RS-O1) and the second method generated Order 2 (RS-O2). The average costs and the average product values of the sites, and the two orders are listed in Table 7.5.

Table 7.5: Average costs, average product values and rolling orders in rolling site approach.

	Site 1	Site 2	Site 3	Site 4
Average cost	0.3529	0.3723	0.3224	0.4110
Average product values	0.5985	0.5949	0.5924	0.5963
Order 1 (based on average cost)	Site 3 >	Site 1 >	Site 2 >	Site 4
Order 2 (based on average product value)	Site 1 >	Site 4 >	Site 2 >	Site 3

The results of Order 1 and Order 2 are shown in Figures 7.11 and 7.12 respectively. It is noted that in the Order 1 result, the total ethylene production rate of the four sites (30.30 kg/s) is actually larger than the total ethylene market demand (30.00 kg/s). A similar situation also occurred in the result of Order 2. The total ethylene production rate is 31.83 kg/s and the total market demand is 30.00 kg/s. The excess ethylene produced actually had no destination to go to, as the problem did not consider any inventory. This means the results are effectively infeasible.

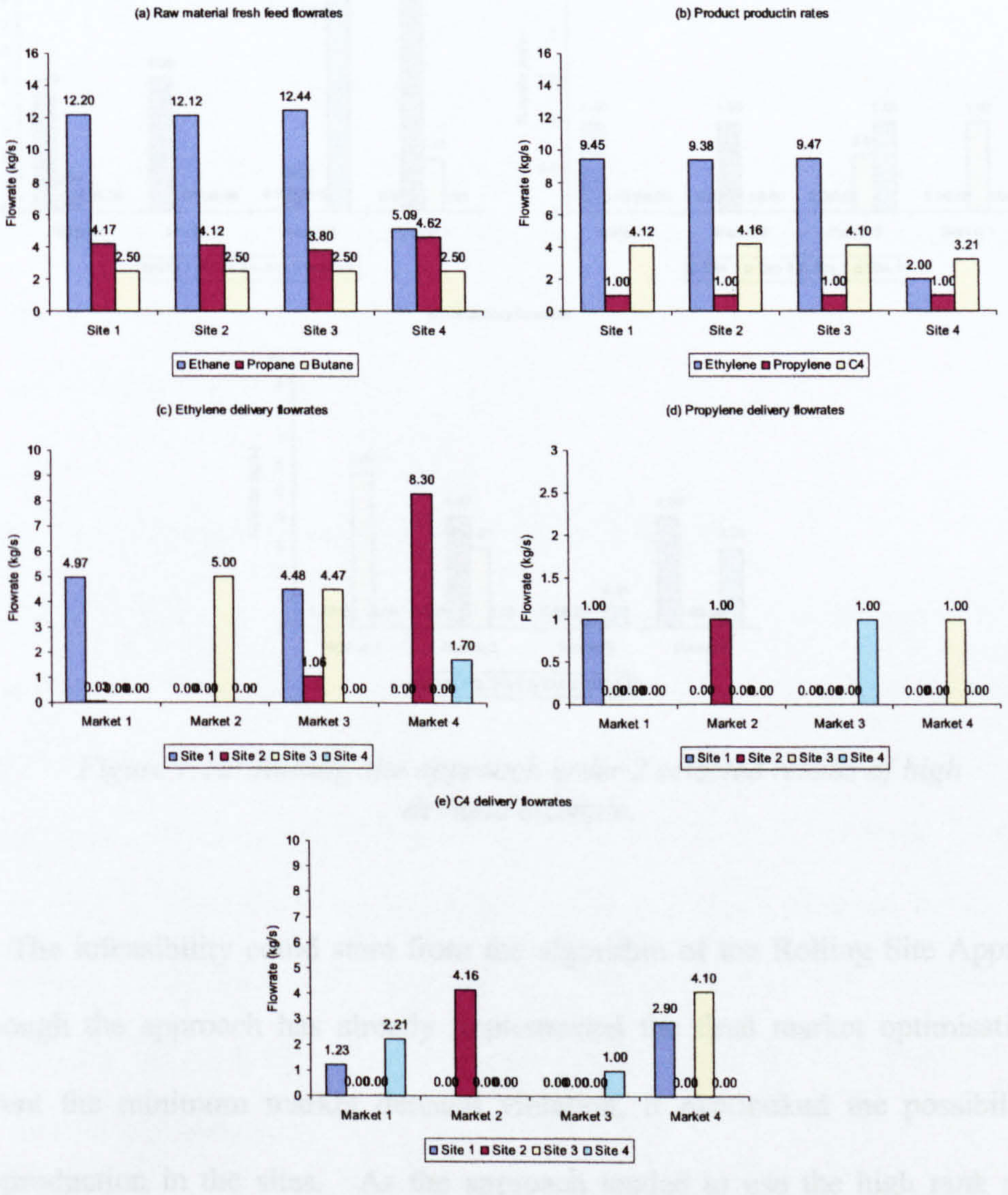

Figure 7.11: Rolling site approach order 1 selected results of high demand example.

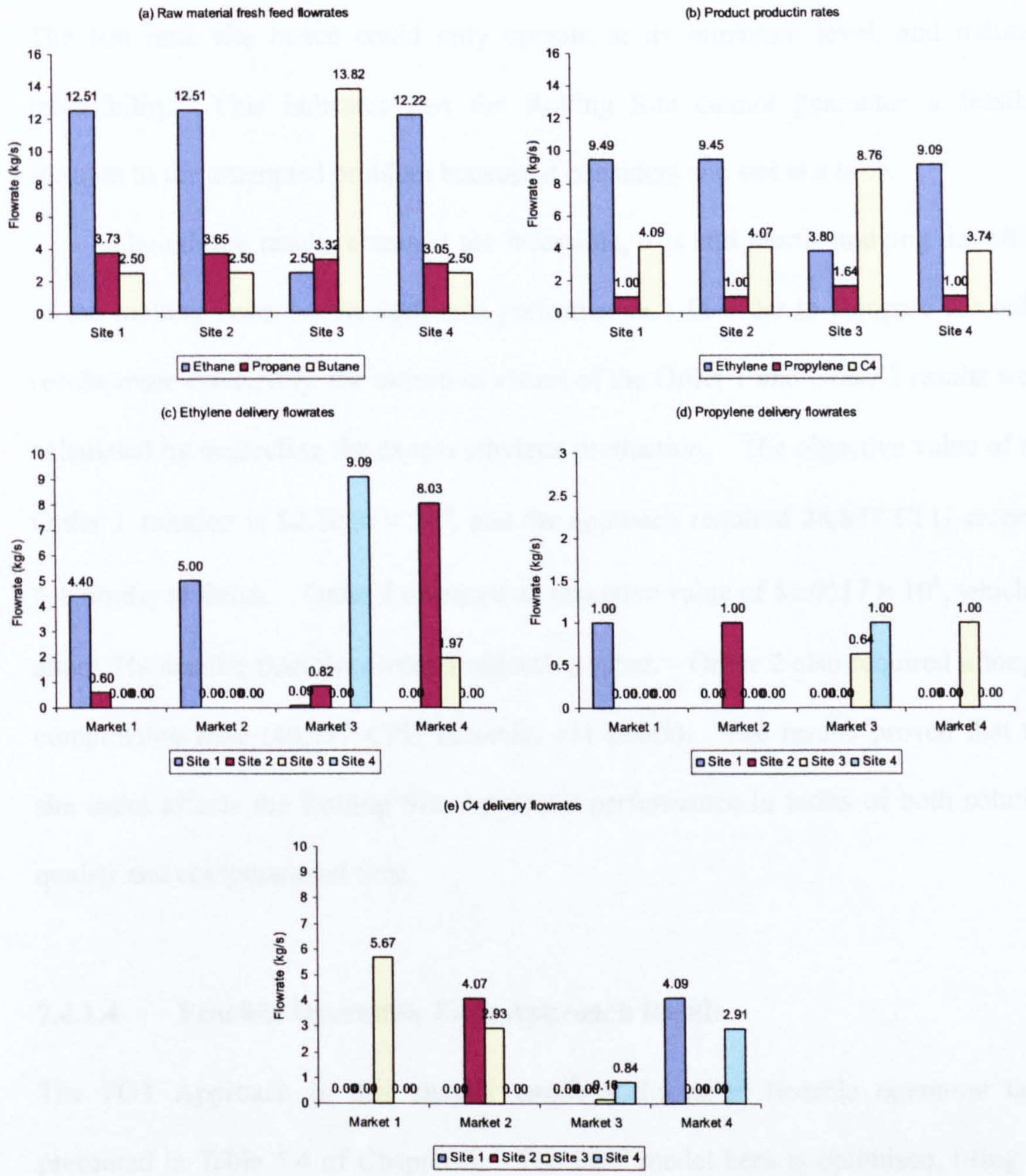

Figure 7.12: Rolling site approach order 2 selected results of high demand example.

The infeasibility could stem from the algorithm of the Rolling Site Approach. Although the approach has already implemented the final market optimisation to prevent the minimum market demand violation, it overlooked the possibility of overproduction in the sites. As the approach tended to use the high rank site to fulfil the market demands as far as possible, the remaining demand for the last rank

site was too small. That was even smaller than the site's minimum production rate. The last rank site hence could only operate at its minimum level, and induced infeasibility. This indicates that the Rolling Site cannot guarantee a feasible solution to the attempted problem because it considers one site at a time.

Although the results obtained are infeasible, it is still worth studying the effect of the ranking order on the approach performance. In order to compare the order results more effectively, the objective values of the Order 1 and Order 2 results were calculated by neglecting the excess ethylene production. The objective value of the Order 1 solution is $\$2.2010 \times 10^6$, and the approach required 28,877 CPU seconds (~8 hours) to finish. Order 2 obtained an objective value of $\$2.0517 \times 10^6$, which is about 7% smaller than the Order 1 objective value. Order 2 also required a longer computation time (40,197 CPU seconds, ~11 hours). The results proved that the site order affects the Rolling Site Approach performance in terms of both solution quality and computational time.

7.4.1.4 Feasible Operation Table Approach Result

The FOT Approach in this chapter employs the same feasible operation table presented in Table 5.4 of Chapter 5. The FOT model here is optimised, using the solver GAMS/Cplex, to select suitable operation modes for different sites. The resulted mode allocation is Site 1:Mode 1; Site 2:Mode 7; Site 3:Mode 1 and Site 4:Mode 7. Based on that allocation, the overall profit obtained by the FOT Approach is $\$2.7411 \times 10^6$. Although the FOT objective value is about 4.5% less than that of the Site/Market Decomposition Approach, the FOT Approach only required 3 CPU seconds.

One of the main differences between the results of the FOT and Site/Market Decomposition approaches is in the ethylene production rates of the Sites 3 and 4. Site 3 had a higher production rate than Site 4 in the FOT results; in the Site/Market Decomposition approaches it is the opposite. The arrangement of the FOT Approach resulted in the ethylene demand not being completely fulfilled and induced

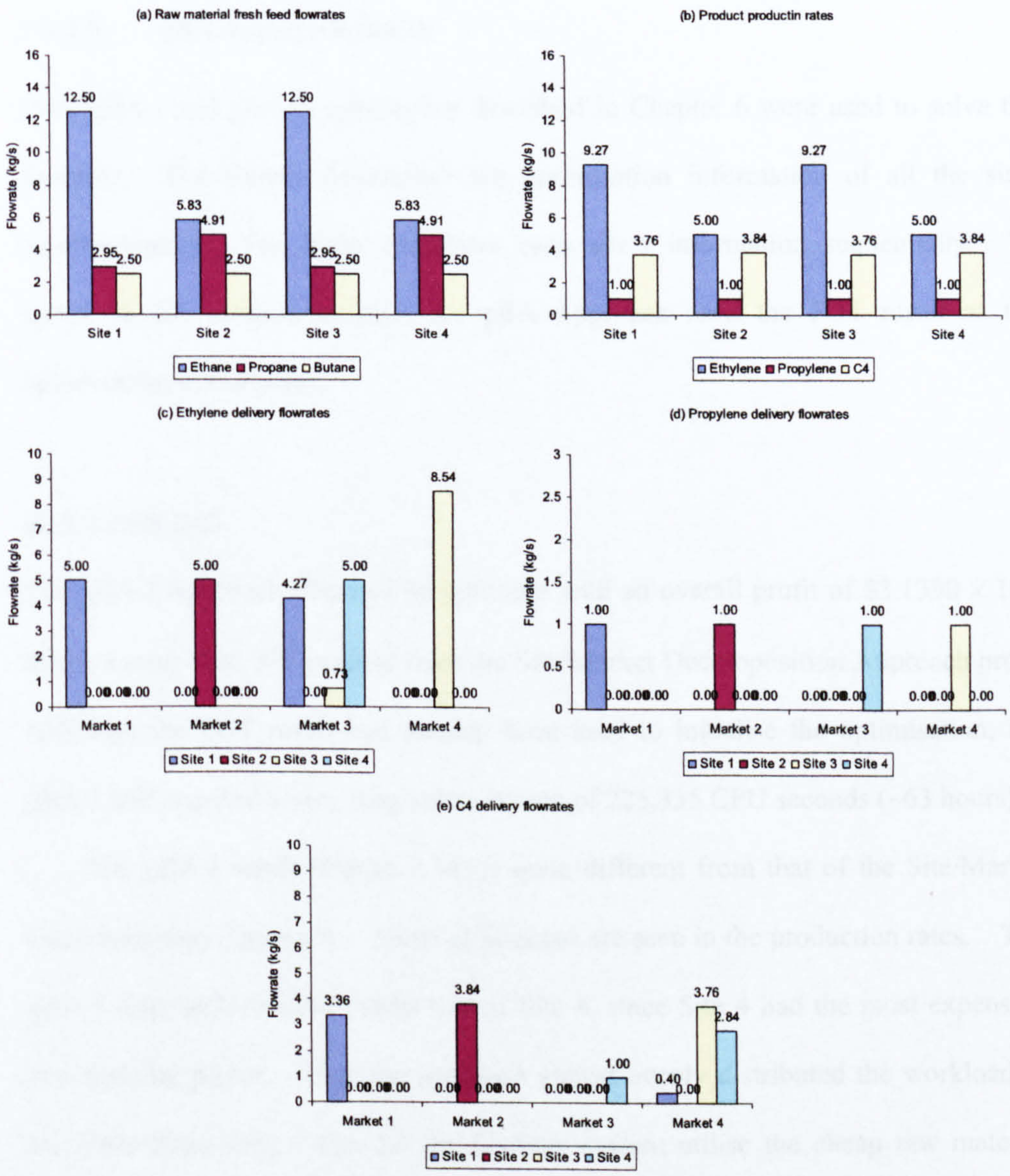

Figure 7.13: FOT approach selected results of high demand example.

some profit loss. This should be because the production rates of the process were limited by the operation modes in the FOT Approach. If a site changes its operation mode to one with higher production, the maximum demand capacity might be violated. Therefore, the FOT Approach had to sacrifice some productivity in order to attain the best possible feasible solution with the available operation modes. Figure 7.13 plots selected results of the FOT Approach.

7.4.1.5 gBA Approach Result

Both gBA-I and gBA-II approaches described in Chapter 6 were used to solve the example. The former determines the optimisation information of all the sites simultaneously. The latter calculates each site's information sequentially. To speed up the solution process, the gBA Approach used the FOT result as the optimisation initial point.

gBA-I Approach

The gBA-I Approach obtained an optimum with an overall profit of $\$3.1390 \times 10^6$; this is a more than 9% increase from the Site/Market Decomposition Approach profit. Although the FOT result had already been used to initialise the optimisation, the gBA-I still required a very long solution time of 225,335 CPU seconds (~63 hours).

The gBA-I result (Figure 7.14) is quite different from that of the Site/Market Decomposition Approach. Some differences are seen in the production rates. The gBA-I Approach reduced production at Site 4, since Site 4 had the most expensive raw material prices. Then the approach almost evenly distributed the workload to the other three sites. This let the four-site system utilise the cheap raw material

more effectively. At the same time, the system could also satisfy completely the overall demand of ethylene, the most economical product. This opportunity had just been missed by the other decomposition methods.

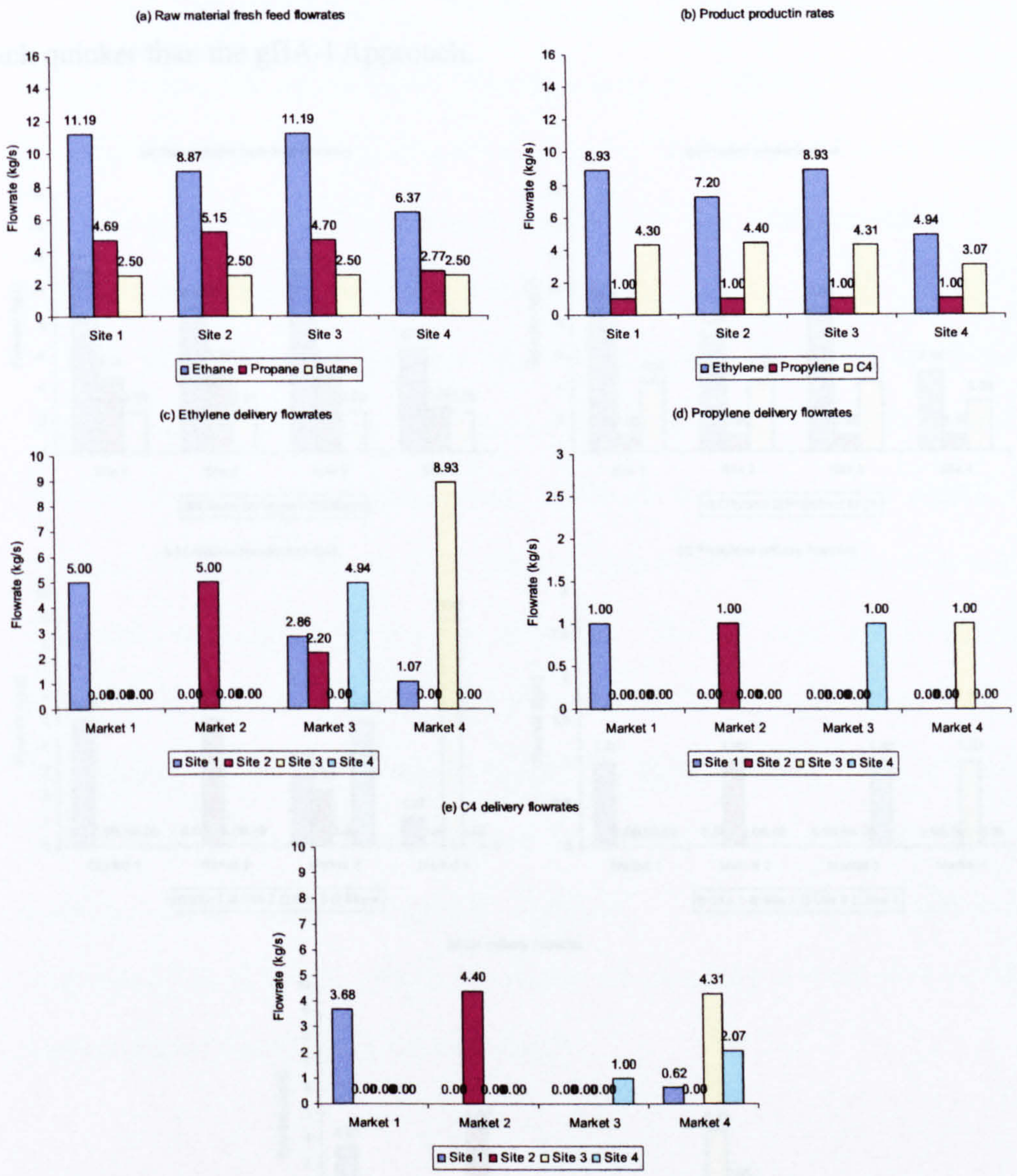

Figure 7.14: gBA-I approach selected results of high demand example.

gBA-II Approach

The gBA-II Approach practically located the same solution of the gBA-I Approach (Figure 7.15). The objective value found is $\$3.1389 \times 10^6$, but the required solution time was greatly reduced to 55,784 CPU seconds (~15.5 hours). This follows the result of the 4-period example in Chapter 6 of indicating that the gBA-II Approach is much quicker than the gBA-I Approach.

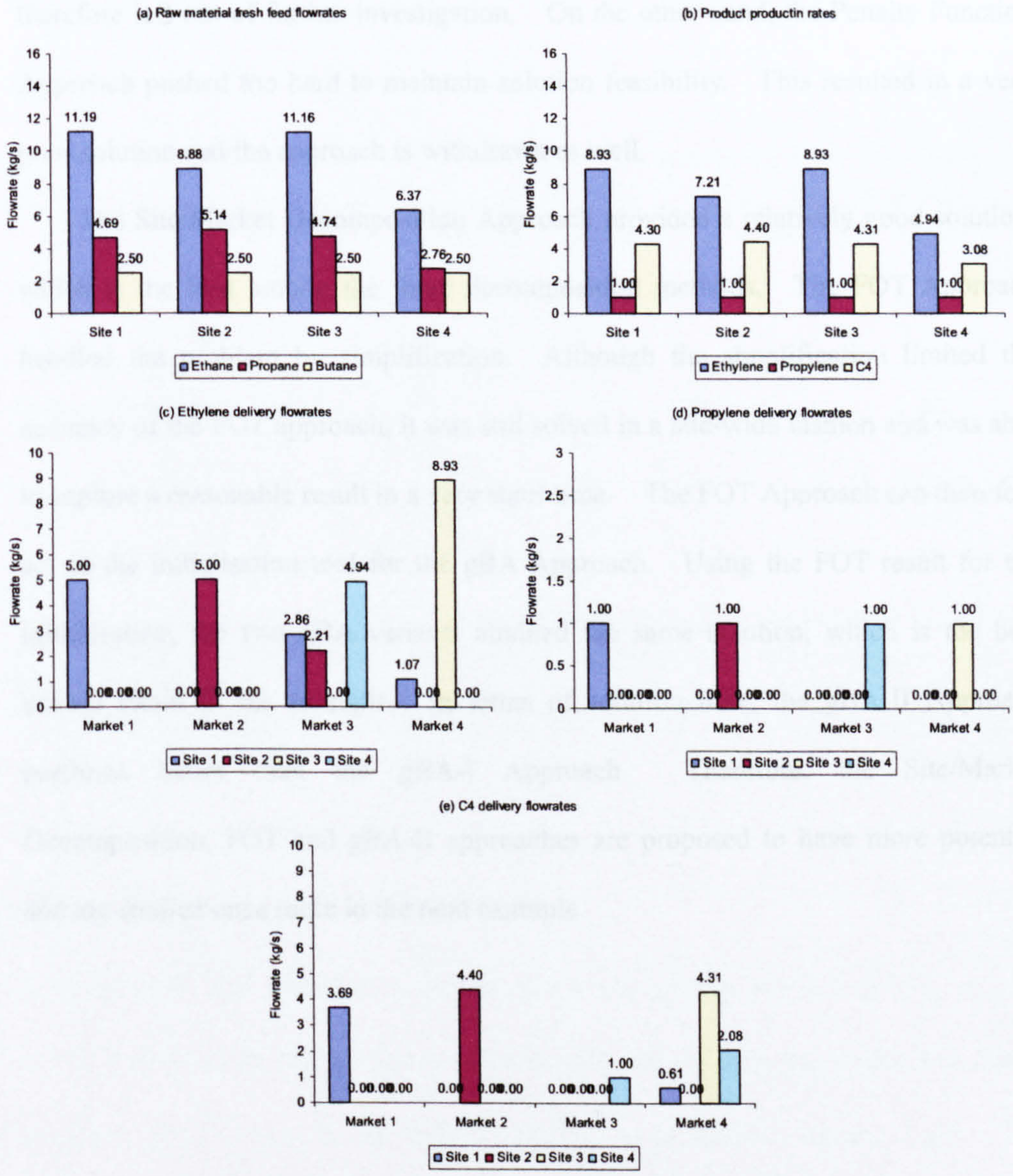

Figure 7.15: gBA-II approach selected results of high demand example.

7.4.1.6 Results Analysis

The Site/Market Decomposition, Penalty Function, Rolling Site, FOT and gBA approaches were investigated in this high demand multi-site single-period example. The objective values and the solution times of the approaches are shown in Figure 7.16. The optimisation dimensions and tolerance settings of the approaches are also summarised in Table 7.6. The Rolling Site approach tried two different site ranking orders, but neither could provide a feasible solution. The approach is therefore left out of further investigation. On the other hand, the Penalty Function Approach pushed too hard to maintain solution feasibility. This resulted in a very poor solution and the approach is withdrawn as well.

The Site/Market Decomposition Approach provided a relatively good solution, which is the best among the three decomposition methods. The FOT Approach handled the problem by simplification. Although the simplification limited the accuracy of the FOT approach, it was still solved in a site-wide fashion and was able to capture a reasonable result in a very short time. The FOT Approach can therefore act as the initialisation tool for the gBA Approach. Using the FOT result for the initialisation, the two gBA variants attained the same solution, which is the best overall result in the example. In terms of solution time, the gBA-II Approach performs better than the gBA-I Approach. Therefore, the Site/Market Decomposition, FOT and gBA-II approaches are proposed to have more potential and are studied once more in the next example.

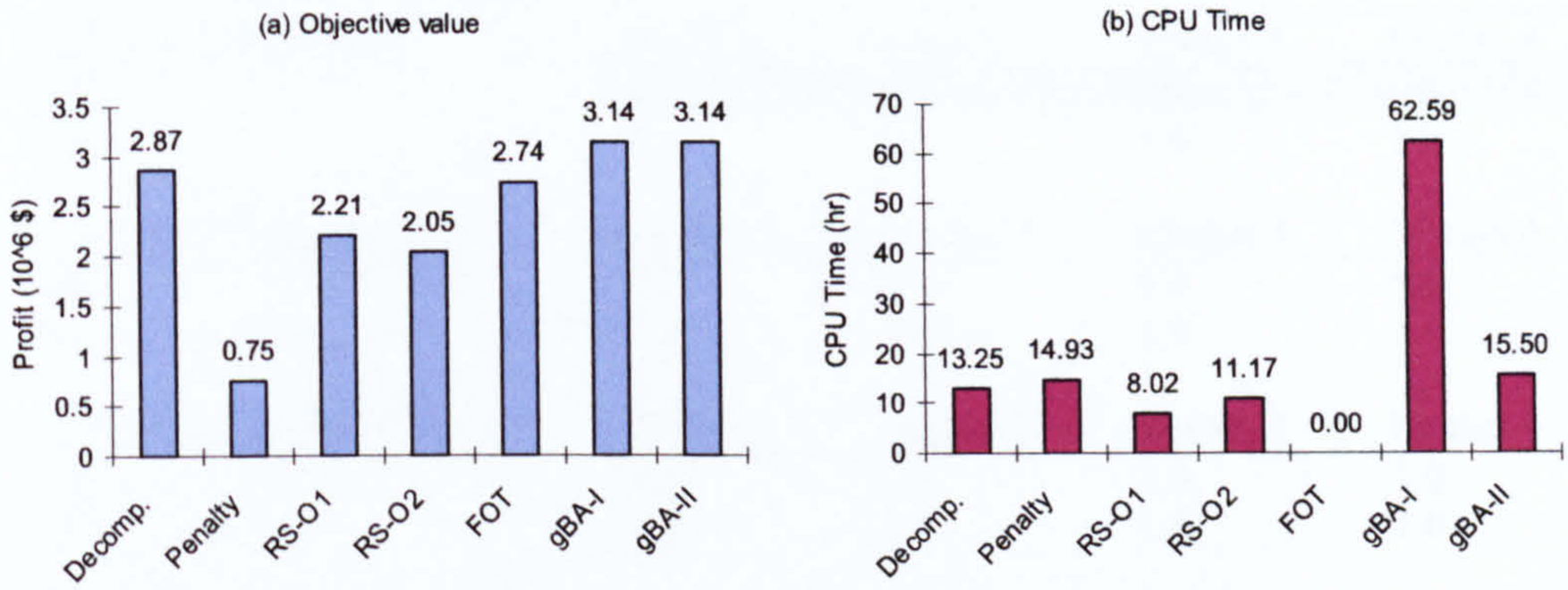

Figure 7.16: Approach objective values and CPU times of high demand example.

Table 7.6: Problem dimensions and optimisation tolerance in high demand example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	No. of binary variables	Optimisation tolerance
Decomp. (each iteration)	33,888	24	17		0.001[1]
Penalty (each iteration)	33,903	24	17		0.001[1]
RS-O1 (each iteration)	33,888	24	17		0.001[1]
RS-O2 (each iteration)	33,888	24	17		0.001[1]
FOT	702	96	68	28	0.0[2]
gBA-I	189	108	68		0.001[3]
gBA-II	189	108	68		0.001[3]

Remarks:
1. gPROMS SRQPD solver, "OptimisationTolerance". Definition can be found in (PSE, 2004a).
2. GAMS Cplex solver, option "optcr": relative termination tolerance for MILP. Definition can be found in (GAMS, 2007).
3. NAG E04UGA, "Major Optimality Tolerance". Definition can be found in (NAG, 2002).

7.4.2 Reduced Demand Example

Product demands and prices of petrochemicals are usually stable but they are still subject to variation as the market condition changes. Once the product demands and/or prices are changed, it unavoidably affects the production supply chain. This example is set up to test the stability of the optimisation approaches with different demand levels.

Table 7.7: Market product demand capacities of reduced demand example.

Ethylene demand (kg/s)	Market 1	Market 2	Market 3	Market 4
Max.	6.0	6.0	6.0	6.0
Min.	2.0	2.0	1.0	1.0
Propylene demand (kg/s)	Market 1	Market 2	Market 3	Market 4
Max.	5.0	5.0	5.0	5.0
Min.	1.0	1.0	1.0	1.0
C4 chemicals demand (kg/s)	Market 1	Market 2	Market 3	Market 4
Max.	7.0	7.0	7.0	7.0
Min.	1.0	1.0	1.0	1.0

N.B. Shaded cells represent modifications from the high demand example.

The example uses the same problem configurations of the previous example, including the site-market structure, the production constraints and the cost/price data. The only difference between two examples is the ethylene product demand. This example reduced the total ethylene demand of the markets, but there are slight increases of the ethylene demands in Markets 1 and 2. The modified demand data is shown in Table 7.7.

7.4.2.1 Site/Market Decomposition Approach Result

The approach took 37,124 CPU seconds (~10 hours) to solve the problem and found an objective of $\$2.0048 \times 10^6$. From the result, the total ethylene production decreased from the previous example, especially at Sites 3 and 4. The product delivery pattern however still followed the magnitudes of the delivery cost. In general, Sites 1 and 2 produced products for Markets 1 and 2 respectively. Also, Sites 3 and 4 sent products to Markets 4 and 3. Selected results of the approach are summarised in Figure 7.17.

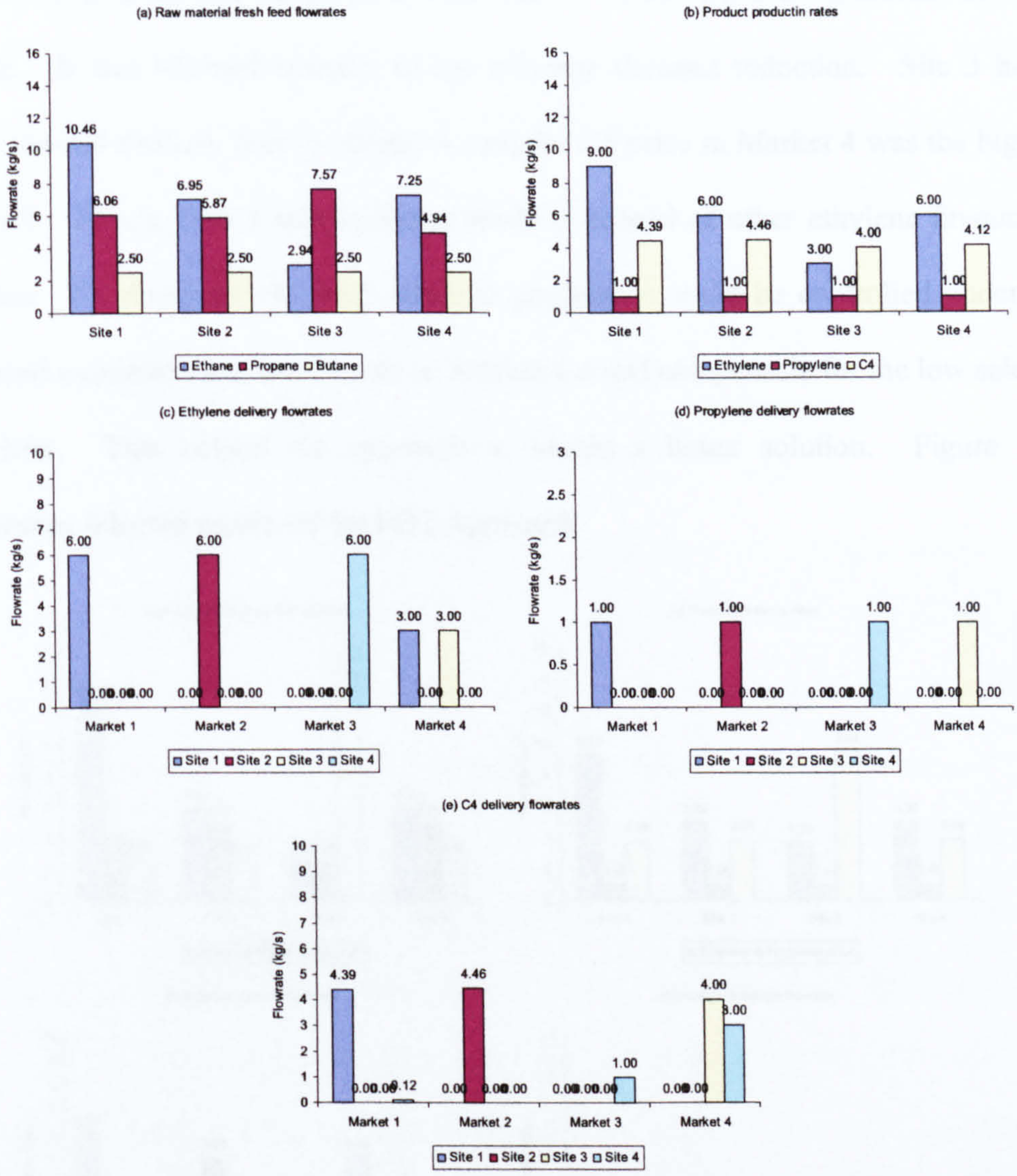

Figure 7.17: Site/market decomposition approach selected results of reduced demand example.

7.4.2.2 Feasible Operation Table Approach

Using the same operation table (Table 5.4 in Chapter 5), the FOT Approach optimised the example in only 3 CPU seconds. The overall profit calculated is $\$2.1112 \times 10^6$. It is about 5% higher than that of the Site/Market Decomposition Approach. In the solution, the FOT Approach chose Mode 1 for Site 1, Mode 7 for

Site 2, Mode 6 for Site 3 and Mode 7 for Site 4. Mode 6 is a C4 chemicals oriented mode. It was selected because of the ethylene demand reduction. Site 3 had a very low C4 delivery cost to Market 4, and the C4 price in Market 4 was the highest overall. Hence, Site 3 was assigned Mode 6 instead of other ethylene favourable modes. By doing so, the total ethylene production could be controlled under the demand maximum and the C4 sold in Market 4 could compensate for the low sales of ethylene. This helped the approach to obtain a better solution. Figure 7.18 illustrates selected results of the FOT Approach.

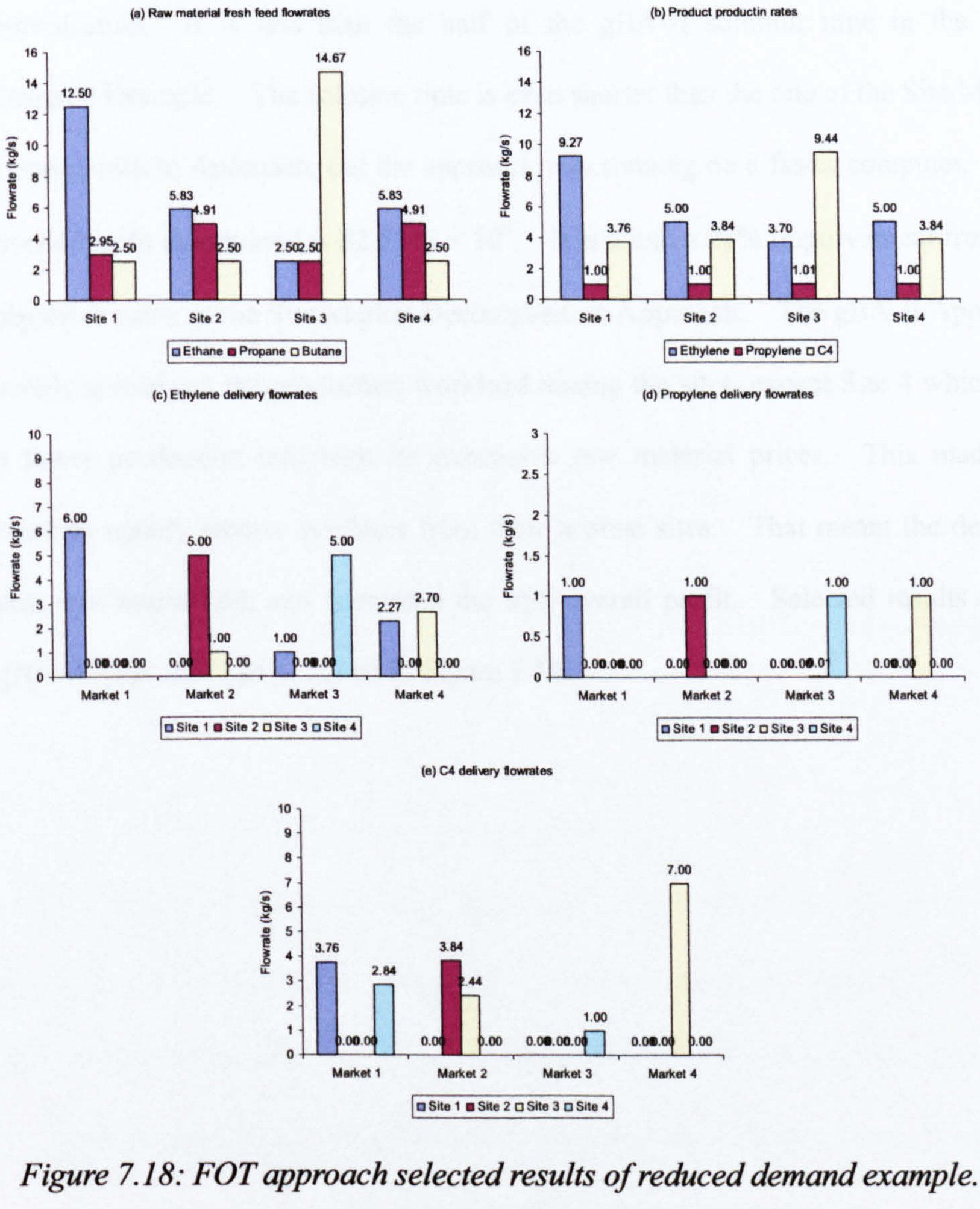

Figure 7.18: FOT approach selected results of reduced demand example.

7.4.2.3 gBA-II Approach Result

The configurations of the current example are the same as the previous example. They only differ in the values of the ethylene demand maximum. In this situation, the NAG optimiser employed by the gBA Approach can capture useful information from the previous example's optimal solution to "warm start" the optimisation for the current example. The "warm start" should greatly speed up the solution process.

The gBA-II Approach was the only gBA variant to be tested in this example, since it has exhibited a quicker solution time before. With the warm start, the gBA-II Approach just required 24,352 CPU seconds (~6.7 hours) to compete the optimisation. It is less than the half of the gBA-II solution time in the High Demand Example. The solution time is even shorter than the one of the Site/Market Decomposition Approach, but the approach was running on a faster computer. The overall profit determined is $\$2.5313 \times 10^6$. It is about a 26% improvement from the objective value of the Site/Market Decomposition Approach. The gBA-II Approach evenly spread out the production workload among the sites, except Site 4 which had a lower production rate with its expensive raw material prices. This made the markets mainly receive products from their nearest sites. That meant the delivery cost was minimised, and generated the best overall profit. Selected results of the gBA-II Approach can be found in Figure 7.19.

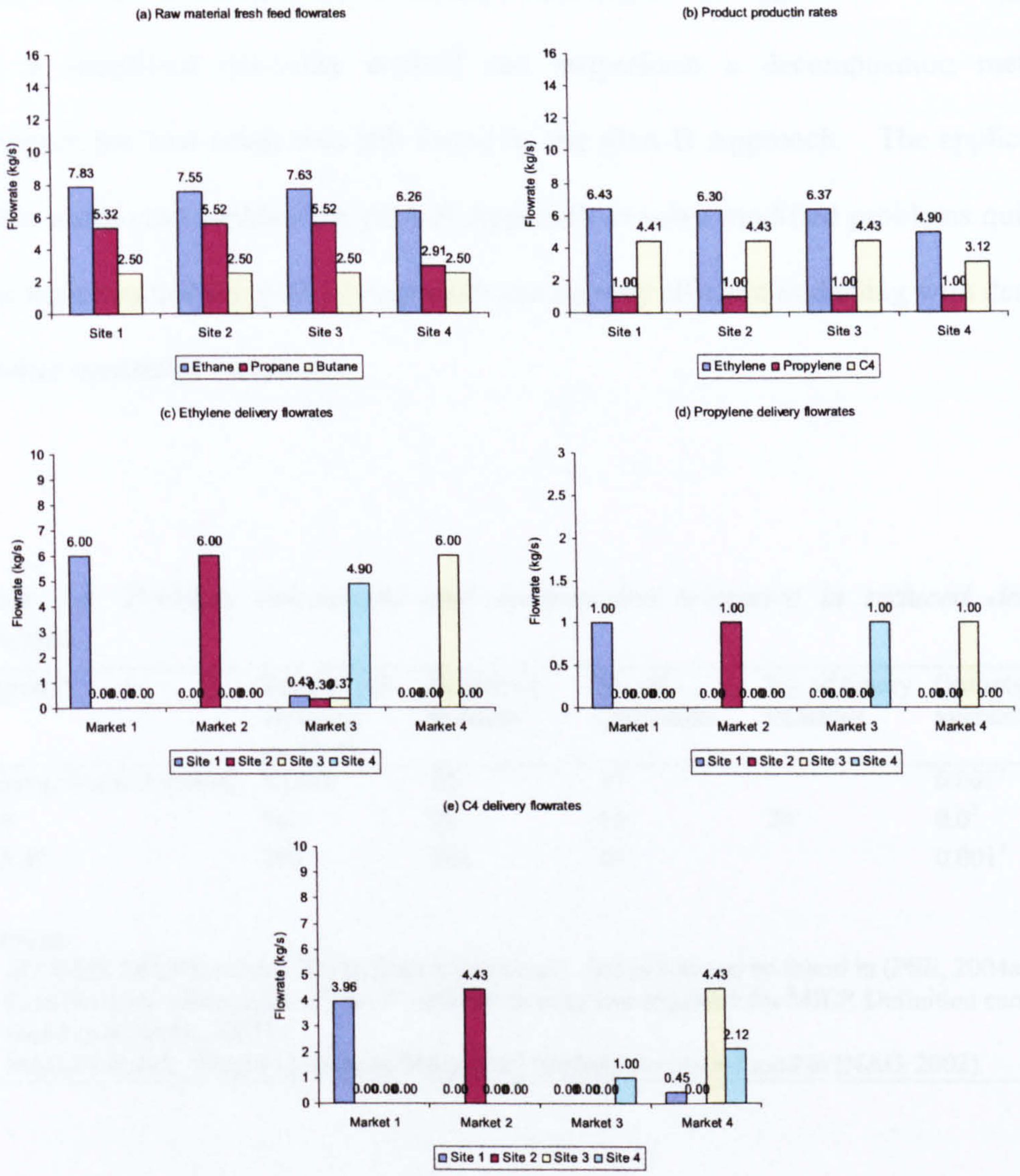

Figure 7.19: gBA-II approach selected results of reduced demand example.

7.4.2.4 Results Analysis

Only the Site/Market Decomposition, FOT and gBA-II approaches were examined using the Reduced Demand Example. The optimisation dimensions of the approaches are shown in Table 7.8. The objective values and computational times are summarised in Figure 7.20. In this example, the FOT Approach provided a

better solution than that of the Site/Market Decomposition Approach. This suggests that a simplified site-wide method can outperform a decomposition method. However, the best result was still found by the gBA-II Approach. The application of the warm start enabled the gBA-II Approach to solve modified problems quickly. This indicates that the gBA-II Approach can be very efficient in dealing with demand or other constraint variations.

Table 7.8: Problem dimensions and optimisation tolerance in reduced demand example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	No. of binary variables	Optimisation tolerance
Decomp. (each iteration)	33,888	24	17		0.001[1]
FOT	702	96	68	28	0.0[2]
gBA-II	189	108	68		0.001[3]

Remarks:
1. gPROMS SRQPD solver, "OptimisationTolerance". Definition can be found in (PSE, 2004a).
2. GAMS Cplex solver, option "optcr": relative termination tolerance for MILP. Definition can be found in (GAMS, 2007).
3. NAG E04UGA, "Major Optimality Tolerance". Definition can be found in (NAG, 2002).

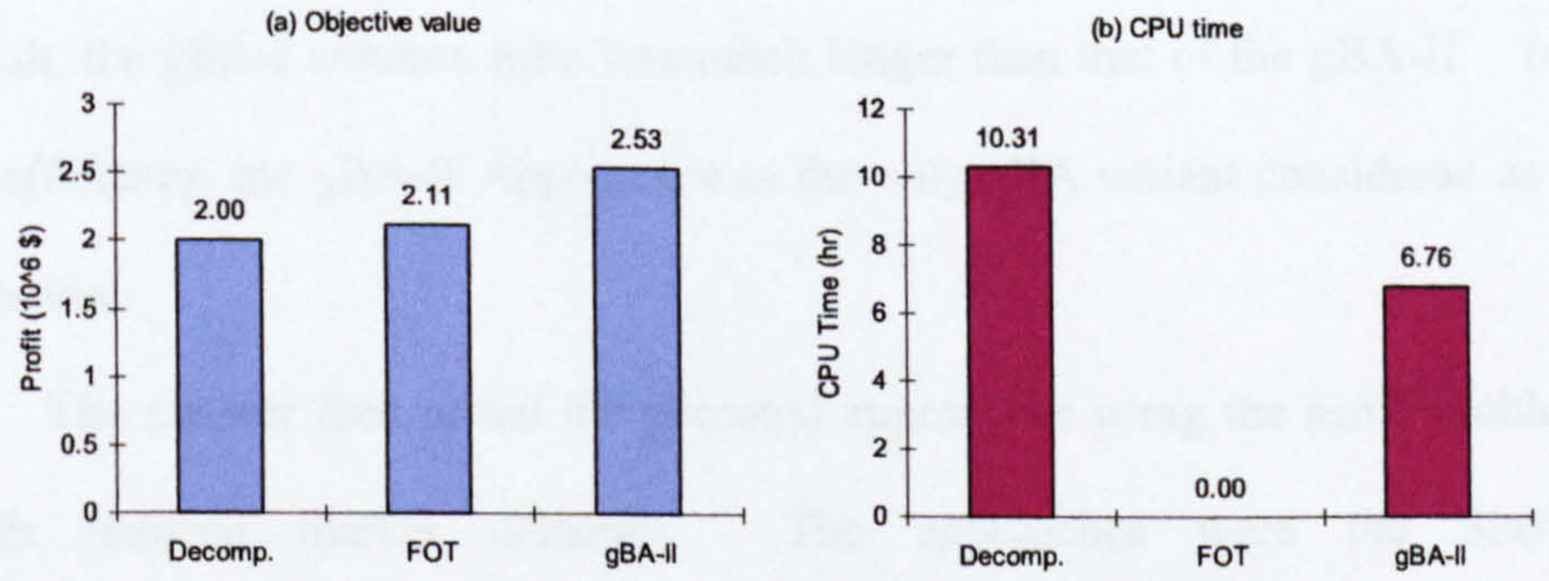

Figure 7.20: Approach objective values and CPU times of reduced demand example.

In the two examples, only the gBA variants could locate the best solutions. The gBA Approach improved the objective value of the Site/Market Decomposition Approach by 9% in the High Demand Example, and by 26% higher in the Reduced Demand Example. This matched the results (better solutions from the gBA Approach) obtained in Chapter 6, and once again verified the benefit of using direct optimisation to tackle site-wide supply chain problems. As the gBA-II Approach required less computational effort than the gBA-I Approach, it was considered as the most suitable approach for the multi-site single-period problems.

7.5 Conclusions

This chapter performed an investigation into solution approaches for multi-site single-period problems. Several approaches were tested, including the Site/Market Decomposition, Penalty Function, Rolling Site, FOT and gBA approaches. The chapter first used a four-site four-market problem to determine the most promising approaches. Based on the example result, the Penalty Function and Rolling Site approaches were screened out. This was because they provided very poor or infeasible solutions. The gBA-I Approach, one of the gBA variants, was also dropped. Although both the gBA-I and gBA-II approaches could determine the best result, the gBA-I solution time was much longer than that of the gBA-II. In terms of efficiency, the gBA-II Approach was the only gBA variant considered as having potential.

The chapter then tested the potential approaches using the same problem, but with reduced market demands. The approaches were the Site/Market Decomposition, FOT and gBA-II approaches. In the modified problem, the FOT

Approach performance had improved and it outperformed the Site/Market Decomposition Approach. The gBA-II Approach however still obtained the best result for the example. It also could reach the optimum in a relatively short time with the help from the warm start and the faster computer. Due to its high accuracy and its better efficiency among the gBA variants, the gBA-II Approach was observed as the most promising solution approach in the chapter. In the next chapter, the extension of gBA-II application to the multi-site multi-period case is examined.

8 Multi-site Multi-period Problem

8.1 Introduction

A realistic operation of a chemical enterprise supply chain usually involves both material transport and inventory storage. To optimise this sort of system, the multi-site single-period model of Chapter 7 has to be extended into a multi-site multi-period model. That makes the model the most complicated one in this thesis. The model includes a multi-site multi-market system as well as a series of time periods. The model hence can manage material transfer among different production sites and markets. In addition, it can consider material inventory across the planning horizon. With those settings, the enterprise can utilise the model to maximise its own profit by optimising supply chain operation.

Direct optimisation is the most reliable and accurate method to solve the supply chain problems studied here. Although its solution time is very long, the experience from previous chapters has shown that benefits offered by the direct optimisation approach exceed the drawbacks. Throughout the studies presented before, the gBA-II Approach with the FOT initialisation has emerged as the most efficient direct optimisation method. Therefore, this chapter only plans to demonstrate the application of the method to the multi-site multi-period problem, rather than comparing different solution approaches. The chapter aims to verify the reliability of the gBA-II Approach together with the FOT initialisation, by applying it to this class of problem.

Following this section, the chapter defines a multi-site multi-period problem and presents the problem's mathematical representation. After that, the FOT and gBA-II approaches are reviewed. Then the chapter sets up a case study and applies

the FOT and gBA-II approaches to solve the multi-site multi-period problem. Finally, a conclusion is drawn based on the case study result.

8.2 Problem Statement

The multi-site multi-period problem is the most complex problem examined in this thesis. It involves a multi-site multi-market system for production and sales. In the system, a production site can sell its products to any one of the markets. A site can also keep raw material and product inventories across the time horizon for its own use. A multi-period framework is hence required in the problem (Figure 8.1).

In this chapter, the site-market system contains four production sites and four markets. The sites in the system are all developed from the 5-column ethylene process explained in Chapter 3. The system also has a two-period planning horizon. The periods are only connected by inventories. Although the processes in different sites and different periods are basically the same, their operating conditions and price/cost data can vary. Differences also occur in the markets. The product delivery costs, product prices and product demands can have different values in different markets and periods. The objective of the problem is then to maximise the overall profit of the site-market system in the two periods. This is achieved by altering the operating conditions of the sites, the product delivery to the markets and the inventory stored across the periods. Modified from the models of Chapter 5 and Chapter 7, the mathematical representation of the multi-site multi-period problem is presented below.

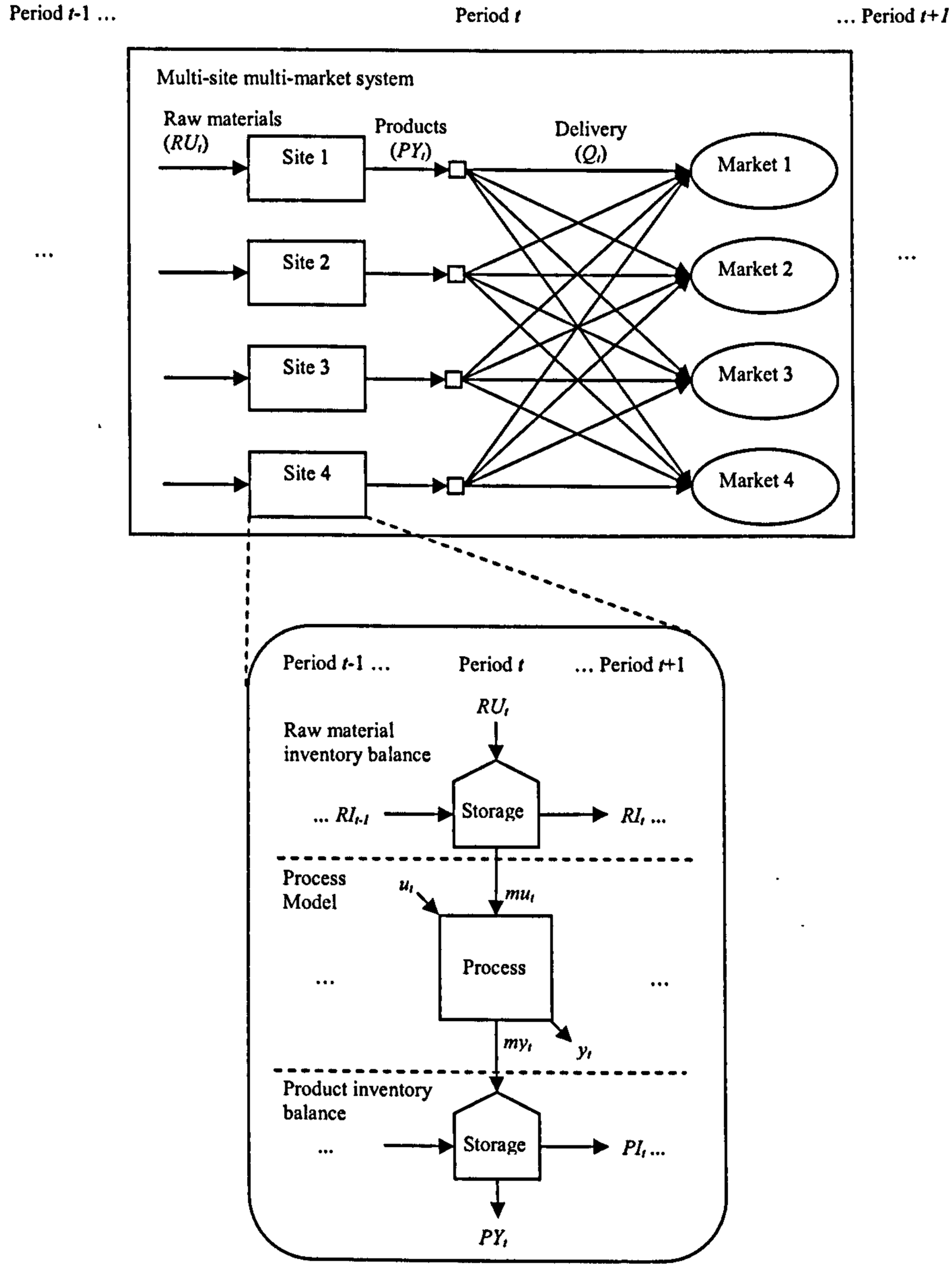

Figure 8.1: Schematic diagram of a multi-site multi-period model.

Indices:

i	Process model input variable index.
j	Process model output variable index.
k	Raw material specie index, $k \in i$.
l	Product specie index, $l \in j$.
s	Product site index.
m	Market index.
t	Time period index.

Variables:

$u_{i,s,t}$	Process model input variable i of site s at time period t.
$mu_{k,s,t}$	Raw material k consumption rate of site s at time period t, $mu_{k,t} \in u_{i,t}$
$y_{j,s,t}$	Process model output variable j of site s at time period t.
$my_{l,s,t}$	Product l production rate of site s at time period t, $my_{l,t} \in y_{j,t}$.
$RU_{k,s,t}$	Fresh feed flowrate of raw material k of site s at time period t.
$RI_{k,s,t}$	Inventory of raw material k of site s at the end of time period t.
$PY_{l,s,t}$	Sale of product l of site s at time period t.
$PI_{l,s,t}$	Inventory of product l of site s at the end of time period t.
$D_{l,m,t}$	Product l sales in market m at time period t.
$Q_{l,s,m,t}$	Product l delivery from site s to market m at time period t.
$P_{s,t}$	Profit of site s at time period t.
PP_t	Profit of all sites at time period t.
TP	Total profit of the time horizon.

Parameters:

$\alpha^{u}_{i,s,t}$	Price/cost associated with variable $u_{i,s,t}$.
$\alpha^{y}_{j,s,t}$	Price/cost associated with variable $y_{j,s,t}$.
$\beta^{RU}_{k,s,t}$	Purchasing cost of raw material k of site s at time period t.
$\beta^{D}_{l,m,t}$	Sale price of product l in market m at time period t.
$TC_{l,s,m,t}$	Delivery cost of product l from site s to market m at period t.
$\gamma^{RI}_{k,s,t}$	Inventory cost of raw material k of site s at time period t.
$\gamma^{PI}_{l,s,t}$	Inventory cost of product l of site s at time period t.
$u^{\min}_{i,s,t}$, $u^{\max}_{i,s,t}$	Lower and upper bounds of input variable $u_{i,s,t}$ respectively.
$y^{\min}_{j,s,t}$, $y^{\max}_{j,s,t}$	Lower and upper bounds of output variable $y_{j,s,t}$ respectively.
$D^{\min}_{l,m,t}$, $D^{\max}_{l,m,t}$	Lower and upper bounds of product sales $D_{l,m,t}$ respectively.
$Q^{\min}_{l,s,m,t}$, $Q^{\max}_{l,s,m,t}$	Lower and upper bounds of product delivery $Q_{l,s,m,t}$ respectively.
$RU^{\min}_{k,s,t}, RU^{\max}_{k,s,t}$	Lower and upper bounds of raw material feedstock $RU_{k,s,t}$ respectively.
$RI^{\min}_{k,s,t}, RI^{\max}_{k,s,t}$	Lower and upper bounds of raw material inventory $RI_{k,s,t}$ respectively.
$PY^{\min}_{l,s,t}, PY^{\max}_{l,s,t}$	Lower and upper bounds of product sale $PY_{l,s,t}$ respectively.
$PI^{\min}_{l,s,t}, PI^{\max}_{l,s,t}$	Lower and upper bounds of product inventory $PI_{l,s,t}$ respectively.
I	The total number of the input variables $u_{i,s,t}$ in site s.
J	The total number of the output variables $y_{j,s,t}$ in site s.
PD_t	Duration of the time period t.

Equations:

$f_{j,s,t}$ Mathematical relations of y_j in terms of $\forall u_i$, both linear and nonlinear, in site s at time period t.

Process model:

$$y_{j,s,t} = f_{j,s,t}\left(u_{1,s,t}, u_{2,s,t}, u_{3,s,t}, \cdots, u_{I,s,t}\right) \quad \text{(Eq. 8.1)}$$

$$u_{i,s,t}^{\min} \le u_{i,s,t} \le u_{i,s,t}^{\max} \quad \text{(Eq. 8.2)}$$

$$y_{j,s,t}^{\min} \le y_{j,s,t} \le y_{j,s,t}^{\max} \quad \text{(Eq. 8.3)}$$

Product delivery from site to markets:

$$PY_{l,s,t} = \sum_{m} Q_{l,s,m,t} \quad \text{(Eq. 8.4)}$$

$$D_{l,m,t} = \sum_{s} Q_{l,s,m,t} \quad \text{(Eq. 8.5)}$$

$$D_{l,m,t}^{\min} \le D_{l,m,t} \le D_{l,m,t}^{\max} \quad \text{(Eq. 8.6)}$$

$$Q_{l,s,m,t}^{\min} \le Q_{l,s,m,t} \le Q_{l,s,m,t}^{\max} \quad \text{(Eq. 8.7)}$$

Raw material inventory balance:

$$RI_{k,s,t} = RI_{k,s,t-1} + RU_{k,s,t} - mu_{k,s,t} \cdot PD_t \quad \text{(Eq. 8.8)}$$

$$RI_{k,s,t}^{\min} \le RI_{k,s,t} \le RI_{k,s,t}^{\max} \quad \text{(Eq. 8.9)}$$

$$RU_{k,s,t}^{\min} \le RU_{k,s,t} \le RU_{k,s,t}^{\max} \quad \text{(Eq. 8.10)}$$

Product inventory balance:

$$PI_{l,s,t} = PI_{l,s,t-1} + my_{l,s,t} \cdot PD_t - PY_{l,s,t} \quad \text{(Eq. 8.11)}$$

$$PI_{l,s,t}^{\min} \le PI_{l,s,t} \le PI_{l,s,t}^{\max} \quad \text{(Eq. 8.12)}$$

$$PY_{l,s,t}^{\min} \le PY_{l,s,t} \le PY_{l,s,t}^{\max} \quad \text{(Eq. 8.13)}$$

Profit of production site *s*:

$$\begin{aligned} P_{s,t} = \Bigg[& \sum_i \alpha_{i,s,t}^{u} \cdot u_{i,s,t} + \sum_j \alpha_{j,s,t}^{y} \cdot y_{j,s,t} - \sum_k \beta_{k,s,t}^{RU} \cdot RU_{k,s,t} \\ & + \sum_{l,m} \beta_{l,m,t}^{D} \cdot Q_{l,s,m,t} - \sum_{l,m} TC_{l,s,m,t} \cdot Q_{l,s,m,t} \\ & - \sum_k \gamma_{k,s,t}^{RI} \cdot \tfrac{1}{2}\left(RI_{k,s,t} + RI_{k,s,t-1}\right) - \sum_l \gamma_{l,s,t}^{PI} \cdot \tfrac{1}{2}\left(PI_{l,s,t} + PI_{l,s,t-1}\right) \Bigg] \cdot PD_t \end{aligned} \quad \text{(Eq. 8.14)}$$

At $t = 1$, $RI_{k,s,t-1}$ and $PI_{k,s,t-1}$ are the initial inventory levels and their values are given as constants in the optimisation.

Profit of all sites at time period *t*:

$$PP_t = \sum_s P_{s,t} \quad \text{(Eq. 8.15)}$$

Objective: Total profit

$$\max\left(TP = \sum_t PP_t\right) \quad \text{(Eq. 8.16)}$$

8.3 Solution Approaches

The chapter only employs the Feasible Operation Table (FOT) and gPROMS-based Application – Variant II (gBA-II) approaches to solve the multi-site multi-period

problem. This is because the chapter aims to examine the reliability of direct optimisation for this problem. It does not require the comparison of different solution techniques. In addition, the gBA-II approach with FOT initialisation has been determined to be the most efficient direct optimisation approach in previous chapters.

8.3.1 Feasible Operation Table (FOT) Approach

The FOT approach was first suggested in Chapter 5, and it is a site-wide simplification method. The approach applies a tailor-made operation table to simplify the rigorous process model. This transforms the complicated nonlinear (NLP) supply chain model into a simple mixed-integer linear (MILP) model. The problem information is reduced in the MILP model, and this results in a relatively small model size. This makes the approach suitable to tackle multiple production sites, markets and time periods without decomposition. The linearity and small size also ensure a fast solution time. Due to the advantages, the approach is selected as the initialisation tool for direct optimisation.

The FOT MILP model used in this chapter keeps most of the linear parts of the supply chain model. They are the equations of the product delivery (Eq. 8.4 – 8.7), the material inventory (Eq. 8.8 – 8.13), the profit calculation (Eq. 8.14 – 8.16), and the objective function (Eq. 8.16). The model however discards the nonlinear process model, and substitutes it with the linear operation mode selection equations (Eq. 8.17 – 8.21). Those equations express the key idea of the MILP model used to solve the multi-site multi-period problem. The following shows the elements

involved in the operation mode selection, and they are derived from the FOT MILP model in Chapter 5.

Indices:

md Operation mode index.

Binary variables:

$z_{md,s,t}$ Status of the operation mode *md* at site *s* at period *t*. 1 is on and 0 is off.

Parameters:

$UO_{i,s,md}$ Value of input variable $u_{i,s}$ in operation mode *md*.

$YO_{j,s,md}$ Value of output variable $y_{j,s}$ in operation mode *md*.

$MUO_{k,s,md}$ Value of raw material consumption rate $mu_{k,s}$ in operation mode *md*.

$MYO_{l,s,md}$ Value of product production rate $my_{l,s}$ in operation mode *md*.

Equations for process operations (Operation mode selection):

$$u_{i,s,t} = \sum_{md} \left(UO_{i,s,md} \times z_{md,s,t} \right) \quad \text{(Eq. 8.17)}$$

$$y_{j,s,t} = \sum_{md} \left(YO_{j,s,md} \times z_{md,s,t} \right) \quad \text{(Eq. 8.18)}$$

$$mu_{k,s,t} = \sum_{md} \left(MUO_{k,s,md} \times z_{md,s,t} \right) \quad \text{(Eq. 8.19)}$$

$$my_{l,s,t} = \sum_{md} \left(MYO_{l,s,md} \times z_{md,s,t} \right) \quad \text{(Eq. 8.20)}$$

$$\sum_{md} z_{md,s,t} = 1 \,,\; z_{md,s,t} = 0 \text{ or } 1. \quad \text{(Eq. 8.21)}$$

8.3.2 gPROMS-Based Application Approach – Variant II (gBA-II)

The gBA-II Approach is developed to combine the gPROMS simulator and the NAG optimiser, in order to optimise the large-scale supply chain problem directly. It is recommended instead of another gBA variant (gBA-I) because it requires less computational effort. The approach has been successfully applied in different multi-period and multi-site examples. Together with the initialisation tool, FOT Approach, it is believed that the gBA-II approach can also perform efficiently on the multi-site multi-period problem.

The gBA-II approach is specially designed to handle problems with multiple processes, whether multi-period or multi-site. Therefore, the approach is able to solve the multi-site multi-period problem without major modifications. It only needs to make sure that the gPROMS simulator retrieves information from every process in the multiple sites within every period. The gBA-II procedures used to solve multi-site multi-period problems are illustrated in Figure 8.2.

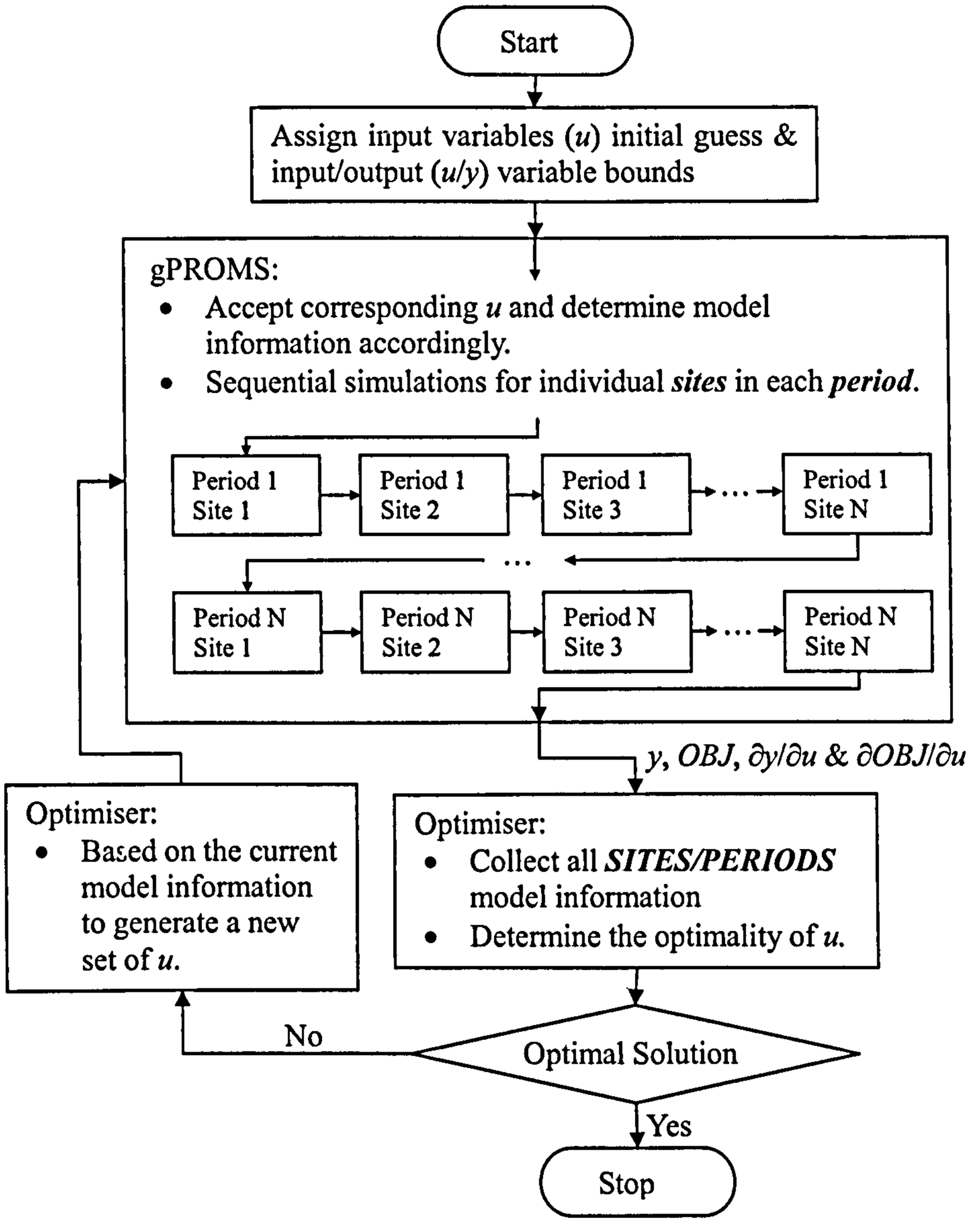

Figure 8.2: gBA-II Approach procedures for multi-site multi-period problem.

8.4 Case Study

8.4.1 Example Definition

Based on the problem statement, a multi-site multi-period example is developed to investigate the performance of the FOT and gBA-II approaches. The example involves a four-site four-market system. The operation of the system is considered under a two-period (604,800 seconds or 7 days per period) framework. In the site-market system, the four sites are all based on the 5-column ethylene process. That means they accept ethane, propane and butane as raw materials, and also produce ethylene, propylene and C4 chemicals as products. Although the process operating conditions can be different from site to site and from time to time, the operations are constrained by the same set of upper and lower bounds. The bound values are basically duplicated from the example of Section 6.3.1, but a summary is listed in Table 8.1. The production sites can also store inventory for their own use. The inventory levels are limited by the values tabulated in Table 8.2, and the bounds are unchanged across sites and periods. However, there are also data variations in the example. Market demands, product delivery costs and utility costs change in different sites and/or markets (Tables 8.3 – 8.5). The raw material and product prices even vary with each site/market and each time period (Tables 8.6 & 8.7). With the variable constraints and price/cost data ready, the example is optimised to maximise the overall profit within the planning horizon. The example is solved by the suggested approach on a Linux computer with CPU clock speed 2992 MHz.

Table 8.1: Bounds of ethylene process operation.

	Min.	Max.
Ethane feed (kg/s)	2.5	15.0
Propane feed (kg/s)	2.5	15.0
Butane feed (kg/s)	2.5	15.0
Steam feed (kg/s)	1.0	20.0
Reactor inlet flowrate (kg/s)	0.0	32.4
Reactor steam dilution ratio	0.4	1.0
Furnace heat flux (kJ/m^2-s)	30.0	45.0
Furnace outlet temperature (K)	0.0	1,200
Furnace outlet pressure (kPa)	150.0	N/A
Column Boilup:Reflux	0.33	3.00
Ethylene production rate (kg/s)	2.0	10.0
Ethylene product molar purity	0.99	1.00
Propylene production rate (kg/s)	1.0	10.0
Propylene product molar purity	0.90	1.00
C4 production rate (kg/s)	0.0	10.0
Propylene composition in C4 stream	0.00	0.10

Table 8.2: Initial, minimum and maximum levels of inventories.

Inventory level	Ethane	Propane	Butane	Ethylene	Propylene	C4
Initial (kTon)	6.048	6.048	6.048	6.048	6.048	6.048
Max. (kTon)	12.096	12.096	12.096	12.096	12.096	12.096
Min. (kTon)	6.048	6.048	6.048	6.048	6.048	6.048

Table 8.3: Market demand capacities.

Ethylene demand	Market 1	Market 2	Market 3	Market 4
Max. (kg/s)	10.0	10.0	10.0	10.0
Min. (kg/s)	1.0	1.0	1.0	1.0

Propylene demand	Market 1	Market 2	Market 3	Market 4
Max. (kg/s)	7.0	7.0	7.0	7.0
Min. (kg/s)	1.0	1.0	1.0	1.0

C4 chemicals demand	Market 1	Market 2	Market 3	Market 4
Max. (kg/s)	7.0	7.0	7.0	7.0
Min. (kg/s)	1.0	1.0	1.0	1.0

Table 8.4: Product delivery costs from production sites to markets.

Ethylene	Unit	Market 1	Market 2	Market 3	Market 4
Site 1	$/kg	0.001	0.050	0.015	0.020
Site 2	$/kg	0.050	0.001	0.020	0.030
Site 3	$/kg	0.040	0.020	0.030	0.022
Site 4	$/kg	0.020	0.030	0.010	0.035

Propylene	Unit	Market 1	Market 2	Market 3	Market 4
Site 1	$/kg	0.001	0.048	0.014	0.019
Site 2	$/kg	0.048	0.001	0.019	0.029
Site 3	$/kg	0.038	0.019	0.029	0.021
Site 4	$/kg	0.020	0.029	0.010	0.033

C4 chemicals	Unit	Market 1	Market 2	Market 3	Market 4
Site 1	$/kg	0.001	0.045	0.014	0.018
Site 2	$/kg	0.045	0.001	0.018	0.027
Site 3	$/kg	0.036	0.018	0.027	0.019
Site 4	$/kg	0.018	0.027	0.009	0.032

Table 8.5: Utility costs of different production sites.

	Site 1	Site 2	Site 3	Site 4
Process steam ($/kg)	0.01	0.02	0.01	0.02
Furnace fuel (in terms of heat flux) ($/kJ/m^2)	2.00E-4	2.10E-4	3.00E-4	2.00E-4
Column heating ($/kJ)	1.26E-5	1.30E-5	1.26E-5	2.00E-5
Column cooling ($/kJ)	1.05E-5	1.20E-5	1.05E-5	1.80E-8

Table 8.6: Raw material prices of production sites in different periods.

Period 1	Site 1	Site 2	Site 3	Site 4
Ethane ($/kg)	0.260	0.280	0.230	0.300
Propane ($/kg)	0.300	0.310	0.270	0.350
Butane ($/kg)	0.430	0.440	0.380	0.500

Period 2	Site 1	Site 2	Site 3	Site 4
Ethane ($/kg)	0.281	0.271	0.246	0.304
Propane ($/kg)	0.358	0.298	0.294	0.419
Butane ($/kg)	0.347	0.419	0.403	0.449

Table 8.7: Product prices of markets in different periods.

Period 1	Market 1	Market 2	Market 3	Market 4
Ethylene ($/kg)	0.587	0.650	0.600	0.550
Propylene ($/kg)	0.610	0.610	0.671	0.549
C4 chemicals ($/kg)	0.650	0.650	0.585	0.715
Period 2	**Market 1**	**Market 2**	**Market 3**	**Market 4**
Ethylene ($/kg)	0.607	0.524	0.564	0.543
Propylene ($/kg)	0.566	0.709	0.781	0.551
C4 chemicals ($/kg)	0.697	0.622	0.627	0.786

8.4.2 FOT Approach Result

The production sites involved in the problem are all based on the 5-column process, so they all can be represented by the same feasible operation table (Table 5.4) employed in Chapter 5. Using the operation table and the MILP model presented before, the FOT Approach solved the problem in just 4 CPU seconds and obtained an overall profit of $\$7.2181 \times 10^6$. The approach assigned Mode 1 to all sites in both periods. This can be observed from the identical production pattern in the sites over the planning horizon (Figure 8.3 (b)). Mode 1 favours a high production of ethylene. The mode assignment in the FOT approach suggests that ethylene is the most profitable product and the market capacity is also large enough to accept a high ethylene production from all sites. This also reflects on the product deliveries (Figure 8.3 (c, d & e)). The four markets all received quite a high level of ethylene, but propylene and C4 chemicals were sold in smaller quantities as by-products.

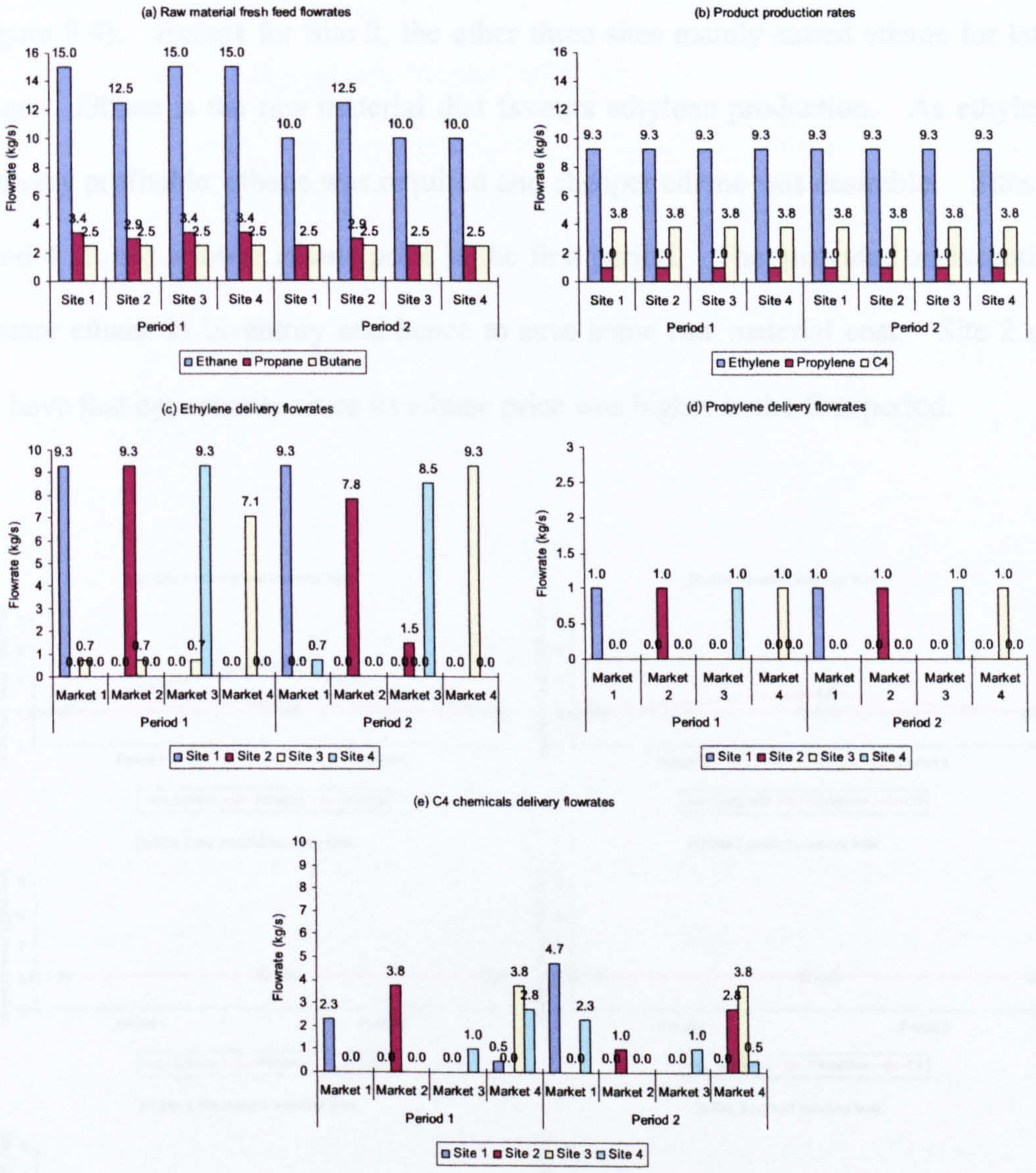

Figure 8.3: Raw material, production and delivery flowrates of FOT result.

In the product delivery plan, the sites tried to transport products to markets with the lowest delivery cost. This makes Site 1 and Site 2 prefer Market 1 and Market 2 respectively. Site 3 and Site 4, on the other hand, tend to sell products in Market 4 and Market 3 respectively. The pattern helps the production system to minimise the delivery cost in order to exploit the product prices offered by the markets.

It is also noted that raw material inventories were kept in the FOT results (Figure 8.4). Except for Site 2, the other three sites mainly stored ethane for later usage. Ethane is the raw material that favours ethylene production. As ethylene was very profitable, ethane was required and cheaper ethane was desirable. Sites 1, 3 and 4 all had a lower ethane price in the first period. That provided an incentive to store ethane in inventory and hence to save some raw material cost. Site 2 did not have that opportunity since its ethane price was higher in the first period.

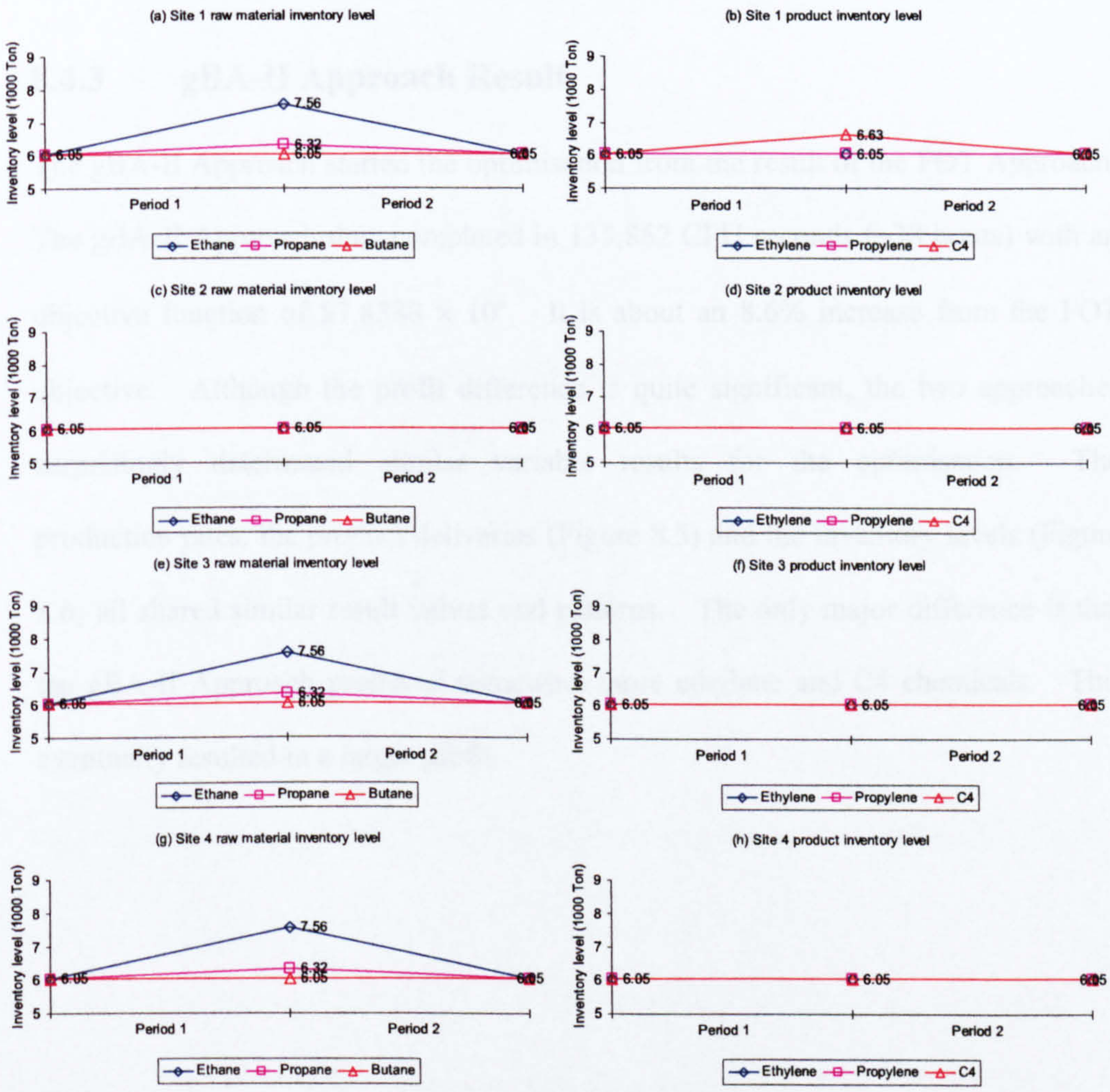

Figure 8.4: Inventory levels of FOT result.

A different picture however is observed for the product inventory. There was almost no product inventory kept for all sites during the planning periods. In a multi-site multi-market system, the sites could send products to the best price market immediately after the production. It reduced the significance of keeping product inventory to wait for future better prices. Furthermore, storage would incur inventory costs. If the future product prices are less attractive than the current best market price in all considerations, product inventory should not be kept. This situation occurred in the example, and only a small amount of C4 chemicals was stored in Site 1 at the end of Period 1.

8.4.3 gBA-II Approach Result

The gBA-II Approach started the optimisation from the result of the FOT Approach. The gBA-II Approach then completed in 135,862 CPU seconds (~38 hours) with an objective function of $\$7.8388 \times 10^6$. It is about an 8.6% increase from the FOT objective. Although the profit difference is quite significant, the two approaches surprisingly determined similar variable results for the optimisation. The production rates, the product deliveries (Figure 8.5) and the inventory levels (Figure 8.6) all shared similar result values and patterns. The only major difference is that the gBA-II Approach produced somewhat more ethylene and C4 chemicals. This eventually resulted in a larger profit.

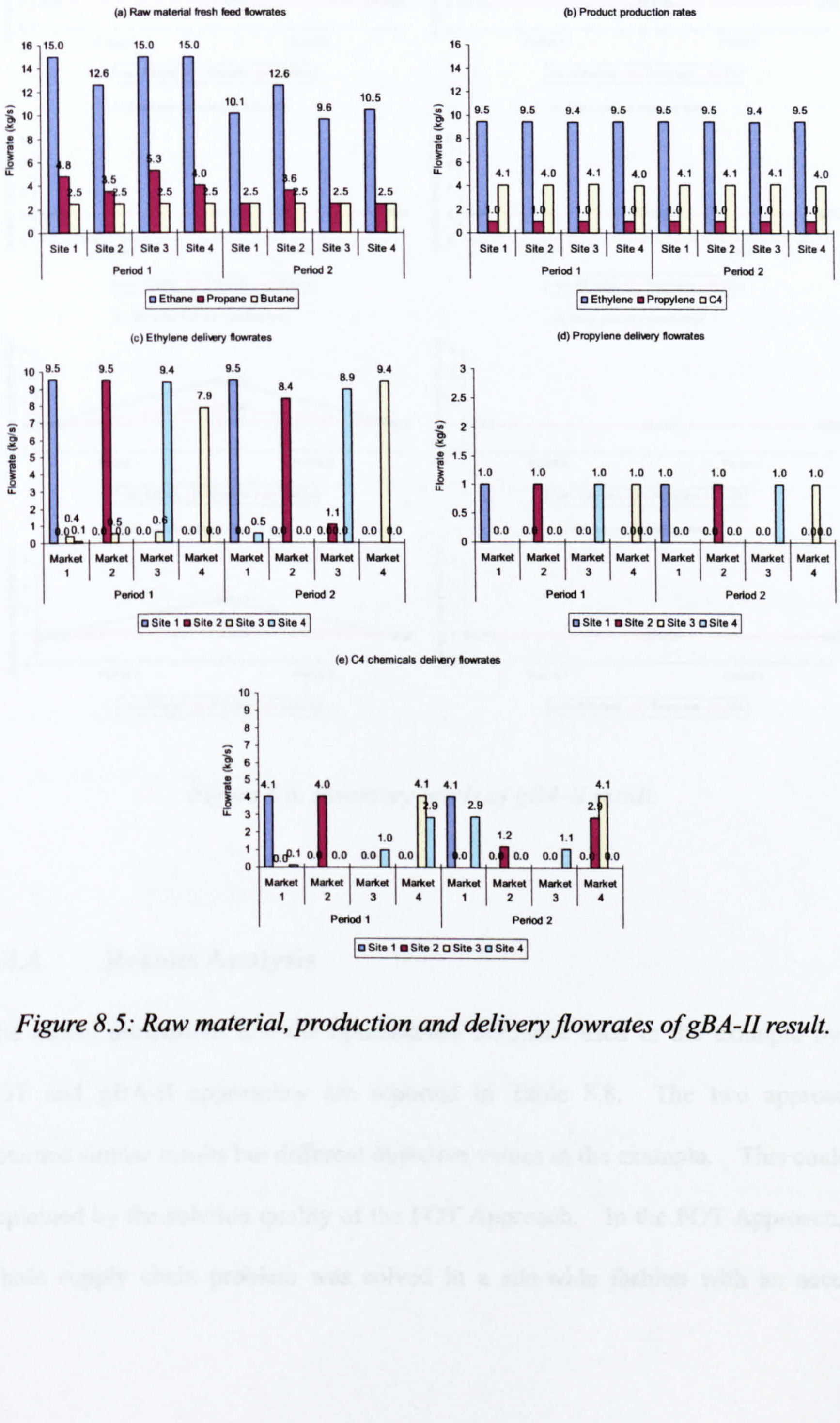

Figure 8.5: Raw material, production and delivery flowrates of gBA-II result.

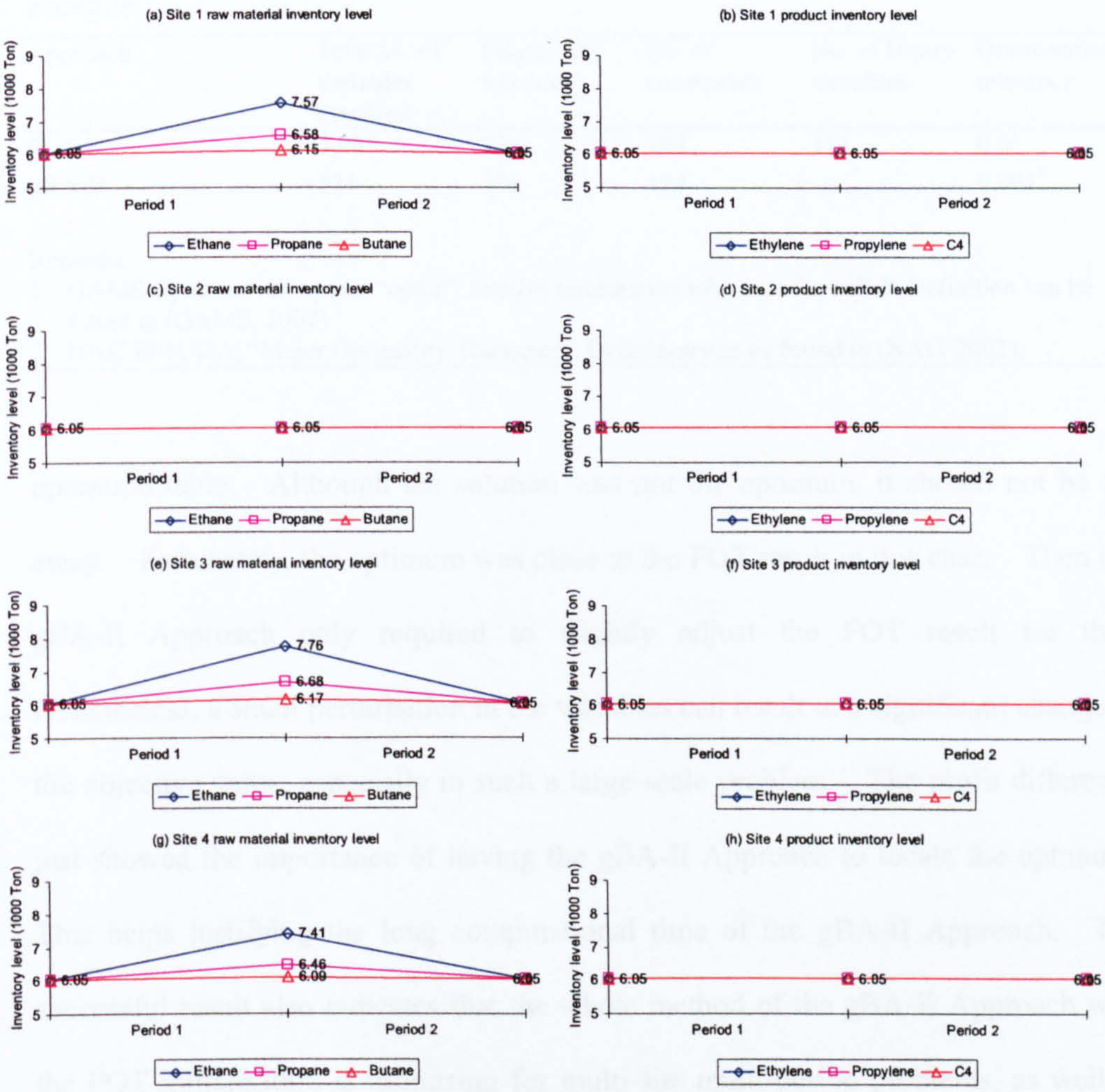

Figure 8.6: Inventory levels of gBA-II result.

8.4.4 Results Analysis

The model dimensions and the optimisation tolerance used in the example by the FOT and gBA-II approaches are reported in Table 8.8. The two approaches obtained similar results but different objective values in the example. This could be explained by the solution quality of the FOT Approach. In the FOT Approach, the whole supply chain problem was solved in a site-wide fashion with an accurate

Table 8.8: Problem dimensions and optimisation tolerance in multi-site multi-period example.

Approach	Total no. of variables involved	Degree of freedom	No. of constraints	No. of binary variables	Optimisation tolerance
FOT	3,097	228	184	112	0.0[1]
gBA-II	521	288	184		0.001[2]

Remarks:
1. GAMS Cplex solver, option "optcr": relative termination tolerance for MILP. Definition can be found in (GAMS, 2007).
2. NAG E04UGA, "Major Optimality Tolerance". Definition can be found in (NAG, 2002).

operation table. Although the solution was not the optimum, it should not be far away. Fortunately, the optimum was close to the FOT result in this case. Then the gBA-II Approach only required to slightly adjust the FOT result for that. Nonetheless, a small perturbation in the variables can result in a significant change in the objective value, especially in such a large-scale problem. The profit difference just showed the importance of having the gBA-II Approach to locate the optimum. This helps justifying the long computational time of the gBA-II Approach. The successful result also indicates that the whole method of the gBA-II Approach with the FOT initialisation is promising for multi-site multi-period problems, as well as the problems studied in previous chapters.

8.5 Conclusions

An application of the gBA-II Approach with the FOT initialisation on a multi-site multi-period problem has been demonstrated in this chapter. The FOT Approach was first used to locate a near-optimal solution for the problem in a short time. Then the gBA-II Approach was applied to determine the exact optimum based on the FOT result. The method was executed on the four-site four-market two-period

example. The gBA-II Approach successfully increased (by 8.6%) the objective value from the FOT result by only making small changes to the optimisation variables. The objective increment clearly revealed the potential benefits from the gBA-II Approach. This not only justified the gBA-II's long computational time, it also confirmed the reliability of the whole gBA-II and FOT method for the multi-site multi-period problem.

9 Conclusions and Future Work

9.1 Conclusions

Supply chain management is an essential exercise for every business to survive in today's ever-changing economy. Optimisation is a viable technique that has always found applications in this area. To obtain the best supply chain result, the optimisation process should include all relevant information in a "site-wide" fashion. The petrochemical industry has already employed optimisation techniques to deal with supply chain problems for decades. The continuous chemical process is a typical process type in the petrochemical industry. Complexity and a vast number of process units in a continuous chemical process, however, trigger a lot of difficulties for site-wide supply chain optimisation. The industry has found it difficult to achieve the utmost benefit from supply chain management. This has introduced an opportunity to develop a practical site-wide supply chain optimisation tool for the continuous chemical process.

In order to exploit the opportunity, objectives were defined for the thesis. The first objective was to establish a holistic model to accurately formulate process and supply chain operations. In Chapter 3, ethylene production was chosen as the example process. Based on the literature, detailed reaction kinetics and rigorous distillation calculations were implemented in the "property-based" formulations. They offered precise representations for the two major components of the process, the steam cracking reactor and the distillation column. This greatly enhanced the accuracy of the process unit operation models. The unit models were then built and connected together to form a site-wide process model by using the modelling package, gPROMS. The hierarchical modelling structure of gPROMS also has the

capability to extend the standalone site-wide model into a multi-site or multi-period model, which was found to be very useful to formulate supply chain problems. With the help of the "property-based" unit representations and the software gPROMS, an accurate holistic model was successfully constructed to capture both unit operations and supply chain at the same time.

The second objective was to develop a practical approach to solve the site-wide supply chain model. The thesis started with a single-site single-period problem in Chapter 4. The chapter showed that site-wide methods had the greatest potential to tackle the supply chain problem. The idea was further verified in Chapter 5 using the single-site multi-period problem. To utilise the idea, a site-wide method, the gPROMS-based Application (gBA) Approach, was developed in Chapter 6. The gBA Approach joined forces between the powerful simulator of gPROMS and a robust optimiser from the Fortran NAG Library to achieve the objective. The gPROMS simulator retrieved information from each site and each period individually. This helped the approach to overcome the computer memory shortage caused by the process complexity and the large problem size. The information from each site and period was then collected together and sent to the NAG optimiser for optimisation. Therefore, the gBA Approach was able to execute the supply chain optimisation in a truly site-wide fashion and to obtain a better result.

The final objective was to compare the holistic approach with other solution approaches, in order to investigate the most promising method. The other approaches were mainly in the category of decomposition method, such as the Rolling Horizon Approach in Chapter 5 and Site/Market Decomposition Approach in Chapter 7. There was also a site-wide simplification method proposed, the Feasible

Operation Table (FOT) Approach. Together with the gBA Approach, different approaches were examined using different types of supply chain problems from Chapter 4 to Chapter 7. The problem types included the single-site single-period, single-site multi-period and multi-site single-period. In the problems attempted, the gBA Approach was always able to locate the best solutions. However, it also required the longest computational time. To speed up the solution process, a more efficient variant of the gBA Approach (gBA-II) together with a swift initialisation using the FOT Approach were used to solve the problems. Although the gBA-II and FOT arrangement still required quite a long time, it improved the process profit from the decomposition methods by at least 3%. The few percentages increment of the profit actually represents a huge amount of money. This suggested the long solution time was worth investing in. In addition, Chapter 8 further confirmed the reliability of the gBA-II and FOT arrangement using the most complicated multi-site multi-period problem. Based on those results, it is clear that the holistic approach outperformed other decomposition methods on solving the site-wide supply chain problems. Therefore, the gBA-II Approach with the FOT initialisation was determined as the most promising approach.

9.2 Future Work

Although a potential solution method has been developed for the continuous process supply chain optimisation, there are still a lot of opportunities to improve the supply chain results. The following topics are suggested for future investigation.

9.2.1 More Detailed Process Representation

The ethylene process used in the thesis supply chain models was simplified from a realistic process, though it was reasonably accurate. This was because the complexity of the real process was too severe for the solution method development. As a potential method has already been established, a more detailed process representation should be applied. For example, the process should include rigorous models of drying units and acid gas removal units. They are represented by a black box or ignored in the current process model. It is believed that a more detailed model should provide a more accurate result, and hence more benefits from the potential solution method.

9.2.2 Advanced Optimiser in gBA Approach

The optimisation capability of the gBA Approach greatly depends on the optimiser implemented. The approach currently uses the optimiser E04UGA from the Fortran NAG Library. The optimiser basically adapts a Sequential Quadratic Programming (SQP) technique to tackle the optimisation. It is robust and able to provide accurate results, however, its solution time should be able to be shortened. An optimiser with a more sophisticated algorithm might be helpful. The optimiser IPOPT developed by Wächter and Biegler (2006) is one of the potential candidates; it employs an advanced primal-dual interior-point algorithm. The optimiser was designed for large-scale nonlinear programming problems and was reported to have a robust and efficient performance. The IPOPT and other potential optimisers should therefore be investigated in the gBA Approach. Their performance should be compared with the NAG solver in order to determine the most promising one.

9.2.3 Multi-computer gBA Method

Another major time determining factor of the gBA Approach is the model information retrieval performed by the gPROMS simulator. Supply chain models always involve a lot of production sites and time periods. To overcome the computer memory shortage problem, the gPROMS simulator has to obtain the information from each site and each period one by one. Currently, the gBA Approach only executes a problem using a single computer, and receives the information for each site and each period sequentially. However, multi-computer processing would be promising since techniques of computer networking have been continuously developed. Via the computer network, the gBA Approach should be able to assign a site or a period to each computer inside the network. Then the computers could calculate the required information simultaneously. This should make the information of the whole supply chain model available more quickly. As the information retrieval is a repeated procedure in the optimisation, the time saved by it would be accumulated and eventually greatly reduces the total solution time of the gBA Approach. Therefore, a further investigation of a multi-computer gBA method is strongly recommended.

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