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**Planning the Petrochemical Industry in
Kuwait Using Economic and Safety
Objectives**

By

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Abstract

Kuwait, one of the major oil producing countries in the Middle East, is in the process of globalizing its operation in petroleum and petrochemical production. Kuwaiti officials have expressed interest in accelerating development of the country's relatively small petrochemical industry. The development is to produce new valuable chemicals from the available basic feedstock chemicals.

Two of the important planning objectives for a petrochemical industry are the economic gain and the industrial safety involved in the development.

For the economic evaluation of the industry, and for the proposed final product chemicals in the development, a long-range plan is needed to identify trends in chemical prices. The chemical prices are related to the oil price, which is considered an important motivator for the whole petrochemical industry. Price trend modelling is performed to be able to forecast these prices for the planning horizon.

Safety, as the second objective, is considered in this study as the risk of chemical plant accidents. Risk, when used as an objective function, has to have a simple quantitative form to be easily evaluated for a large number of possible plants in the petrochemical network. The simple quantitative form adopted is a risk index that enables the number of people affected by accidents resulting in chemical releases to be estimated.

The two objectives, when combined with constraints describing the desired or the possible structure of the industry, will form an optimization model. For this study, the petrochemical planning model consists of a Mixed Integer Linear Programming (MILP) model to select the best routes from the basic feedstocks available in Kuwait to the desired final products with multiple objective functions.

The economic and risk objectives usually have conflicting needs. The presence of several conflicting objectives is typical when planning. In many cases,

where optimization techniques are utilized, the multiple objectives are simply aggregated into one single objective function. Optimization is then conducted to get one optimal result. However, many results are obtained for different aggregations of the objectives and eventually a set of solutions is obtained. Other tools, such as strategic tools, are used to select the best solution from the set.

This study, which is concerned with economic and risk objectives, leads to the identification of important factors that affect the petrochemical industry. Moreover, the procedure, of modelling and model solution, can be used to simplify the decision-making for complex or large systems such as the petrochemical industry. It presents the use of simple multiple objective optimization tools within a petrochemical planning tool formulated as a mixed integer linear programming model. Such a tool is particularly useful when the decision-making task must be discussed and approved by officials who often have little experience with optimization theories.

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Abbreviations

ABS	Acrylonitrile Butadiene Styrene
ARIP	Accidental Release Information Program
ARX	Auto-Regression with exogenous variable
BCG	Boston Consulting Group
CEI	Chemical Exposure Index
EPa	Environmental Public authority (Kuwait)
EPA	Environmental Protection Agency.
F&EI	Fire and Explosion Hazard Index
GCC	Gulf Cooperation Council
GDP	Gross Domestic Product
GE	General Electric
HAZOP	Hazard and Operability Study
HSE	Health, Safety and Environmental
KNPC	Kuwait National Petroleum Company
KPC	Kuwait Petroleum Corporation
K-wave	Kondratieff wave
LC ₅₀	Median Lethal Concentration 50
LD ₅₀	Median Lethal Dose 50
LP	Linear Programming
MILP	Mixed Integer Linear Programming
MO	Multiple Objectives
NFPA	National Fire Protection Association
OPEC	Organization of the Petroleum Exporting Countries
PIC	Petrochemical Industries Company (Kuwait)
PS	Polystyrene
PVC	Polyvinyl Chloride
RMP*info	Risk Management Plans database
SO	Single Objective
SOPDT	Second Order Plus Dead Time
SRI	Stanford Research Institute

TLV	Threshold Limit Value
VAM	Vinyl Acetate Monomer

Nomenclature

a_{na}	Coefficient for the previous na output variable in ARX forecast
Bg	Budget available for the development, \$
B_j	Minimum economic production rate of plant j , kg/yr
b_{nb}	Coefficient for the previous nb input variable in ARX forecast
cap_j	Capital investment cost for plant j , \$
C_i	Price (or cost) of chemical i , \$/kg
D_i	World demand of chemical i , kg/yr
e	Noise in data for ARX forecast
F_i	Annual amount of chemical i used as a feedstock, kg/yr
f_m	Objective function number m
$Freq$	Frequency of accidents, number of accidents per process per year
H	Valid upper bound on production rates, kg/yr
Haz	Hazardous effect of a chemical, number of people affected per tonne of chemical released
Inv	Inventory of chemical released, tonne per accident
k	Gain of transfer function, (\$/kg)/(\$/bbbl)
K	Risk index, people affected per year
M	Total number of plants
N	Total number of chemicals
na	Number of previous output variables used in ARX forecast
nb	Number of previous input variables used in ARX forecast
nk	Number of delay in input variables used in ARX forecast
o_{ij}	Output coefficient of chemical i from plant j
p	Exponent for the distance-based method
P	Number of the desired final product
Q_i	Annual amount produced of chemical i , kg/yr
S_i	Supply availability of feedstock chemical i , kg/yr
s	Laplace transform variable
$Size$	Size of plant, number of major processes in plant
t	Time, yr

U	Upper limit of the country's share in petrochemical market, %
u	Input variable (independent variable)
V	Total number of objective functions
w_m	Weighting coefficient for the objective function number m
X_j	Annual level of production for plant j , kg/yr
y	Output variable (dependent variable)
Y_j	Binary variable for selecting plant j
ζ	Damping factor for transfer function
θ	Dead time for transfer function, yr
τ	Time constant for transfer function, yr

Chapter 1

Introduction

Petroleum is the most valuable feedstock for both fuels and chemicals. It is clear that the value of products from a barrel of oil is far higher than the selling price of that barrel of oil, even when considering the cost of manufacturing. Very wide ranges of chemicals are manufactured from oil and gas. They consist of synthesis resins and plastics, textile fibres, rubber, industrial chemicals, agricultural chemicals, solvents, pesticides, and detergents. Chemicals can be standard chemicals, such as ammonia, acetone, glycerol, etc., or speciality chemicals such as plastics, detergents, sulfates, pesticides, etc.

The structure of the petrochemical industry is cross-linked and can be visualized as a network of chemical processes connecting basic feedstock chemicals to the desired final products. Rudd (1975) did the first formulation of a petrochemical model and it was a Linear Programming model that was used to model the petrochemical industry of the United States. Since that time, many researchers have expanded and improved the model. A major change to the model was done by Jimenez et al. (1982) which was the transfer to a Mixed Integer Programming model. These models have been used extensively to model, plan and improve the performance of petrochemical plants; they translate the petrochemical network into mathematical relations and utilize the available resources in an optimal way.

Petrochemical Modelling started in the early seventies, but its application to the petrochemical industry within the major oil countries in the Middle East started later. Since the early nineties, oil producing countries in the Middle East have started to look closely at the prospect of a more added-value petrochemical industry. Kuwait, as an example of these countries, is now opening up all its resources and aims all its strategies to a larger and more globalized petrochemical industry. The petrochemical industry is considered to be the most suitable sector for development in Kuwait with the economic justification of: (1) the availability of cheap natural gas, which is the

feed stock for basic petrochemicals; (2) the availability of labour which Kuwait has in excess to encourage labour-intensive petrochemical industries; and (3) the formation of an integrated industry consisting of basic feedstocks, intermediates, and final products. Historically, Kuwait's Petrochemical Industries Company (PIC) has manufactured mainly low-value bulk products such as urea, ammonia, and fertilizer for export. Now, many advanced technologies and new added-value products have entered the petrochemical industry and their production has provided an enormous improvement in the infrastructure of the country. These new developments in the industry are still insufficient according to Kuwait's resources and needs and therefore further developments are required.

One of the widely recognized goals for development is Sustainability. Therefore, it has been selected in this study as the objective function for the optimal petrochemical development in Kuwait. Sustainability is defined as "economic development that meets the needs of the present generation without compromising the ability of future generations to meet their own needs" (Engel and Engel 1990). Sustainability, as an objective, has many indicators, the most important of which are the economical gain and Health, Safety and Environmental (HSE) protection.

The petrochemical industry is large and is affected by different types of economic forces. The economic environment in which a chemical plant operates is a dynamic rather than a static one, and it undergoes continuous change. During the life of the plant, the demand and prices for its product will change, as will all the factors that determine its profitability, e.g., labour, raw material, and utilities costs. Many of these factors must be included in a complete economic evaluation of the industry.

The petrochemical industry is now affected by other forces i.e. the HSE legislations. Over the last 20 years, there has been a very rapid growth in HSE legislation affecting all industries. Regulations now cover products, air and water quality, waste disposal, safety precautions in the work environment, and related matters. Looking ahead a further 20 years, it seems likely that the global petrochemical industry will face a major challenge in responding to the political and

social imperatives of continuous improvement in HSE performance whilst, at the same time, ensuring its economic and financial viability. However, the huge task of identifying and then trying to quantify the HSE issues makes most modelling efforts concentrate on certain indicators at the expense of the others, depending on their importance to the industry.

In the wake of the September 11 attacks, and from the history of chemical accidents, the risk from deliberate acts or large accidents are now considered both real and credible. Risks associated with these accidents must be estimated so that adequate countermeasures are provided. Only recently, the petrochemical industry equated risk to the scale of a disaster in terms of financial, structural, environmental and human losses. Therefore, good risk quantification, especially due to accidents, and continual improvement in safety planning has become a very important objective for the petrochemical industry.

The focus of this work is to perform early planning and decision-making for a petrochemical plants network, producing desired final product chemicals. The aim is to structure this network for maximum economical gain, with long-range economical insight, and for minimum risk to people from possible chemical accidents. This thesis consists of seven chapters and three appendices. Chapter 2 describes the petrochemical industry in Kuwait which is to be modelled and planned. Chapter 3 reviews the work that has been done by researchers on modelling the petrochemical industry. Chapter 4 identifies and forecasts, with different mathematical tools, the price trends for the desired chemicals and relates them to the oil price; hence, this chapter is an economical evaluation for planning. Chapter 5 deals with the safety part of planning and includes the formulation of a new risk index. Chapter 6 demonstrates the application of a Mixed Integer Linear Programming model with multiple objectives as a decision support system for planning Kuwait's petrochemical industry; this model uses the concepts presented in the previous chapters. Conclusions, from this work, and recommendations for future work are presented in the last chapter. In the appendices, a list of the plants used in the petrochemical models, a sample output of the optimization program and papers published from this work are listed.

Chapter 2

The Petrochemical Industry in Kuwait: Current Status and Future Outlook

This chapter gives an overview of Kuwait and its petrochemical industry; an economic, environmental and safety overview is presented. The current status of the industry owned by the Petrochemical Industries Company (PIC) is presented together with the proposed final products. The products relative importance to the global petrochemical industry and their relevance for the development of the petrochemical industry in Kuwait is also described. At this point, the need for the development of the petrochemical industry in Kuwait will be demonstrated and the direction in which it should concentrate will be identified.

2.1 Overview

Kuwait is situated on the northern shore of the Arabian (Persian) Gulf. Its population is estimated to be 2,335,648 in the year 2005. The country's 17,818 square kilometres of mostly desert land is bounded on the north and west by Iraq, on the east by the Gulf, and on the south and southeast by Saudi Arabia. The state includes some islands, of which one, "Failakah" is inhabited. There are no springs or streams on the surface; thus, the scarcity of water is one of the major physical problems. The weather represents another physical constraint. The temperature normally ranges from a minimum of 5°C in winter, with high relative humidity and occasional rain, to a maximum of about 50°C in the summer with frequent sandstorms.

2.1.1 Economic Overview

Because of the physical constraints of land and weather, Kuwait's agriculture is very limited. Only 8.6 percent of the total land area is cultivatable and only 0.3 percent is presently being cultivated with crops and vegetables. Therefore, the contribution of the agricultural sector to the Kuwaiti economy is minimal; it only

contributes upto 0.5 percent of the Gross Domestic Product (GDP) (Country Report 2004).

The prospects for economic development in Kuwait took on an entirely new dimensions since oil was first discovered in 1938. Before the oil era, the lack of economic opportunities, especially land resources, combined with Kuwait's geographical location, stimulated the Kuwaitis to attain proficiency in marine industries, particularly pearling, fishing, boat building and sea-going trade. However, people were drawn away from these traditional activities by the expansion of job opportunities generated through the oil sector and the growth of the cultured pearls industry, led by Japan. The Kuwaitis moved from pearling and shipbuilding to more stable and lucrative jobs. Trade has continued to flourish, and Kuwaitis, with their long background of international exposure, came to be known as "internationally minded, thriving on free trade" and their oil based affluence has moved them into a much higher league of activities.

During the 1970s and 1980s, Kuwait moved heavily into activities downstream of oil and gas production including local refining, transport, overseas refining, and distribution of products through the acquisition of foreign assets. Refining and the overseas distribution of products, besides generating higher profits, provided market protection during gluts in crude oil. Kuwait also entered the field of overseas exploration and production.

After a period of reorganization in the late 1970s and the acquisition of foreign corporations in the 1980s, Kuwait's oil industry, supervised by the Ministry of Oil, is controlled today by:

- Kuwait Petroleum Corporation (KPC) as the overall coordinating body.
- Kuwait Oil Company (KOC) carries out exploration and crude production.
- Kuwait National Petroleum Company (KNPC) manages refineries and domestic marketing.
- Kuwait Oil Tanker Company (KOTC) undertakes transportation.

- Petrochemicals Industries Company (PIC) produces petrochemicals.
- Kuwait Foreign Petroleum Exploration Company (KUFPEC) handles exploration of oil overseas.
- Kuwait Petroleum International (KPI) manages downstream operations in Europe.
- Kuwait Aviation Fuelling Company supplies fuel to aircraft that use Kuwait International Airport.
- Sante Fe International Corporation provides expertise in exploration, drilling, pipelines, etc. Sante Fe's wholly owned subsidiary, C.F. Braun & Company, provides refinery engineering services.

As a member of the Organization of the Petroleum Exporting Countries (OPEC), Kuwait owns about 10 per cent of the world's proven oil reserves. Its reserves of 96.5 billion barrels are expected to last more than 100 years. The country's gas reserves, in 1999, were at 52.4 trillion cubic feet, or 1.1 per cent of the world's proven reserves. These figures, however, include half of the oil and gas obtained from operations in the Neutral Zone border area, which is shared with Saudi Arabia (Annual Statistical Abstract 2002).

The destruction of Kuwait's oil industry during the Iraqi occupation was extensive, but damage to exploitable reserves was estimated to be only about 2 per cent. Several hundred oil wells and all of the gathering stations required replacement. All the three domestic refineries were beyond operation. By mid-1994, however, nominal production capacity of crude from Kuwait and its share of the Neutral Zone was around 2.4 million barrels per day, and the refineries capacity was back to pre-invasion levels.

Today, the industry has recovered fully from the Iraqi invasion. The State-owned KPC is estimated to be the seventh largest oil company in the world. It has extensive overseas operations including refineries and large downstream distribution networks in Western Europe. Non-Arab states are Kuwait's main customers and some

73 per cent of its petrochemical products are exported to them (Annual Statistical Abstract 2002).

2.1.2 Environment and Safety Overview

Minimizing the risks arising from industrial and economic development and the resultant degradation of the environment has been a matter of great concern to Kuwait for a number of years. Various institutions have come together for the preservation of the environment. These integrated efforts resulted in the passing of a decree in 1980, which enforced basic rules for the protection of the environment in Kuwait.

The Environmental Public authority (EPa) was established in 1995; in 1996 a High Council of the EPa was created to define the EPa's aims, objectives and policy. The High Council is headed by the First Deputy Prime Minister and the Foreign Minister and has the following members:

- The Minister for Health.
- The Minister for Planning.
- The Minister for Oil.
- The Minister for Commerce and Industry.
- The Minister for Communications.
- The Municipality Chief.
- The Chairman - the Director General of the Public Authority for the Agriculture Affairs and Fish Resources.
- The Director General of Kuwait Institute for Scientific Research.

The High Council of the EPa also includes, for four renewable years, three qualified and experienced individuals in the field of environment protection. The EPa has recently promulgated a 10-year strategy aimed at protecting Kuwait's environment, and addressing specific concerns about the atmosphere, water resources, environment preservation, education and awareness as well as industry and power. It

also provides an environmental framework to protect and preserve components of the infrastructure and the urban environment.

In spite of the unfavourable global business environment and the unusual events witnessed in the Arabian Gulf during the past few years, KPC proceeded with efforts to constantly promote the level of occupational safety at its various facilities to ensure optimal safety of both employees and the installations and to protect the environment outside, as well as within, its production areas. The achievements of KPC in the field of occupational safety and industrial security are outlined below (KPC annual report 2002/2003):

- Opening a dedicated training centre for industrial safety and occupational environmental health at Mina Al-Ahmadi Refinery.
- Executing over 23% of the “Health Safety and Environmental Management System” scheme at KNPC’s Refinery
- Achieving four million accident-free work hours in the new Southern Pier Project and Mina Al-Ahmadi Refinery Rehabilitation Project.
- Conducting several evacuation and emergency drills at manufacturing facilities and headquarters of KPC and its subsidiaries.
- Conducting a sweeping inspection of buried pipes at all production facilities.
- Organizing several awareness campaigns and contests on safety issues, which included dissemination of bulletins, media flyers and posters.

2.2 Kuwait’s Current and Future Petrochemical Outlooks

The reconstruction of Kuwait following the Iraqi invasion provided unique opportunities for foreign investors and contractors as the country rapidly rebuilt its infrastructure and its oil industry. The economy is dominated to an unusual extent by the oil sector, which provides well over 84% of national revenues (Country Report 2004). Kuwait’s oilfields are a crucial feature as are its oil port and shipping facilities.

It also has large oil refineries and processing facilities and has invested in a range of light industries, including glass, textiles, paper, furniture, mineral and construction materials.

Petrochemical Industries Company (PIC), a subsidiary of KPC, was established by an Amiri Decree issued on July 23, 1963, to develop the ammonia and nitrogen fertilizers industry in Kuwait. Petrochemical derivatives constitute one of the main building blocks of the modern industrial economy. The market's exponential growth in recent years has led PIC to embark upon several ambitious projects for petrochemical production in Kuwait. Over the years, PIC's plants have undergone expansion and new plants have been installed for the production of liquid ammonia with a total capacity of 858,000 tonnes/year and three urea plants with a total capacity of 792,000 tonnes/year. In 1997, the company started a polypropylene plant with an annual capacity of 100,000 tonnes.

PIC has also approved building two new petrochemical complexes, one for the production of aromatics and methanol and one for the production of olefins that could enter production in 2008. The first stage of the \$1.4 billion aromatic complex has been granted by the Kuwait Petroleum Company (KPC). The complex, which was first suggested in 1995, will be established and run by PIC. The complex will produce 1,000,000 tonnes/year of aromatic compounds such as para-xylene, benzene and toluene for the manufacture of synthetic fibres, using naphtha from the country's refineries. The olefin complex is planned to have a production of 850,000 tonne/year ethylene and 600,000 tonnes/year ethylene oxide/ethylene glycol.

2.3 The Proposed Final Products for Developing the Petrochemical Industry

Kuwaiti officials have expressed interest in accelerating development of the country's relatively small petrochemical industry. This would accomplish several goals: boosting the value of Kuwait's crude oil reserves, helping to protect Kuwait's revenues during periods of low crude prices, and boosting Kuwait's revenues while adhering to OPEC crude oil quota limitations. The proposed final products for the development of the petrochemical industry are:

- Vinyl acetate monomer
- Polystyrene
- Polyvinyl chloride
- Acrylonitrile Butadiene Styrene
- Cumene

The desired final products were defined by the criteria of their importance to the global petrochemical industry and the relevance of each final product to Kuwait. The economic importance for the proposed chemicals is discussed below.

Vinyl Acetate Monomer (VAM):

Vinyl Acetate Monomer is a chemical building block in the manufacturing of a wide variety of industrial consumer products. Including Polyvinyl acetate (PVA), emulsion polymers used in paints, adhesives, textile sizing and finishes, non-woven textile binders, paper coating and special coating for flexible substrates. Nearly half of the VAM produced in the US is used in PVA production, Polyvinyl alcohol, ethylene-vinyl acetate copolymers, and ethylene-vinyl alcohol. Vinyl Acetate Monomer can be produced by the reaction of ethylene, acetylene or ethane with acetic acid.

Polystyrene (PS):

Polystyrene was first produced in 1831 but has only become commercially significant over the last 50 years. Present consumption is measured in millions of tonnes per year. Polystyrene is made industrially in large quantities because the equipment is expensive and the process requires several days between intake and discharge. Benzene under pressure is added to ethylene in the presence of aluminium trichloride to produce ethyl benzene. The product is reduced to styrene monomer by passing it over an oxide catalyst at high temperatures. Free styrene is then mixed with peroxide and the resulting polymer is passed through a cylindrical tower where the reaction is controlled by heaters. It is extruded and granulated.

The characteristics of styrene-based polymers include:

- Wide range of properties
- Low cost of basic material.
- Low cost of processing because of relatively low processing temperature.
- Low mould shrinkage.
- Low water absorption.
- Clear and transparent.
- Easily produced as foam.
- Excellent dielectric properties.

Polyvinyl Chloride (PVC):

Polyvinyl chloride is manufactured from the polymerization of vinyl chloride monomer, which in turn is produced from ethylene, either directly, or with an ethylene dichloride intermediate. By itself, PVC is brittle and susceptible to heat decomposition. The use of a plasticizer, however, produces PVC having much more desirable properties, and indeed a wide range of properties depending on the amount and type of plasticizer used.

PVC can be manufactured to be either rigid or flexible. Some uses for rigid PVC include pipe and tubing, ductwork and credit cards. Other uses are film and sheet, electrical insulation, floor coverings, hoses, footwear (soles and heels), packaging, coating, adhesives, toys, and household goods.

Acrylonitrile Butadiene Styrene (ABS):

ABS plastics are a family of thermoplastics offering a balance of properties, the most outstanding being impact resistance, tensile strength and scratch resistance. Three methods of manufacturing are employed for ABS plastics: emulsion, suspension and bulk polymerization. In emulsion and suspension polymerization, the monomer and the many chemicals used to control the reaction are finely dispersed or dissolved in water. In bulk polymerization, the monomer itself serves as a solvent for the polymer particles.

Some typical applications of ABS plastics are domestic appliances like vacuum cleaners, luggage cases, safety helmets, toys, and furniture.

Cumene:

Almost all the world's supply of Cumene is now produced as an intermediate for phenol and acetone manufacture. Cumene is oxidized to Cumene hydroperoxide, which is then cleaved catalytically to phenol and acetone. The Cumene projects are being driven by a shift to zeolite catalyst-based technology, which promises higher yields, reduced production cost and possibilities for debottlenecking leading to an increase of one-third or more in the existing capacity.

Some refinery units still produce Cumene for use as an antiknock constituent of gasoline but it is doubtful whether new plants would be constructed for this purpose. Cumene may be prepared commercially by alkylating benzene with propylene.

2.4 Kuwait's Share in the Petrochemical Market

The State of Kuwait is a unique combination of size, resources, and population. With the second largest petroleum reserves in the world, it has the option of flooding the petroleum market and controlling world petroleum supply to a large extent. However, it has chosen the course of producing much less oil than its capacity, thus conserving the petroleum reserves, but at the same time, limiting income from oil. Developments in the world oil market in the early 1980s have added another concern that was less important during the decade of the 1970s. This awareness centres on the fact that oil depletion occurs not only through lessening recoverable oil reserves, but also through changes in revenue generated. Namely, the urgency felt by an oil producing country to diversify its economics stems not only from how much crude oil is left, but more from how much oil revenue is generated (Al-Sabban 1983). In other words, the value of oil is not only in its existence but also in its utilization into other valuable products. The best course for Kuwait to follow is to establish itself as a "Centre of Excellence" (Farouq Ali 1983), not only in the Middle East, but worldwide. This refers to the whole spectrum of activities: oil production using the

most advanced technology, meaningful research on increasing oil production from the existing reservoirs, using oil to produce petrochemicals, and developing high technology industries.

Kuwait petrochemical industries are mainly export oriented because of the small, though growing regional markets. With the implementation of the Gulf Cooperation Council (GCC) economic agreement, different GCC petrochemicals will be freely traded within the region, the remainder will be marketed internationally. Kuwait, however, has had little experience in marketing petrochemicals. Some observers (Al-Sabban 1983) believe that GCC countries including Kuwait will have great difficulty in marketing their products, for world overcapacity in petrochemicals production is expected to characterize the market. In addition, there is an increasing possibility that the industrial world will impose trade barriers to limit foreign competition. But because of the insistence of Kuwait to go ahead with its petrochemical plans, western industrialists have reassessed their previous analyses to reflect some fear of the potential Kuwait and GCC petrochemical development.

The involvement of large multinational chemical companies in Kuwait's joint-venture petrochemical projects may assist in the marketing aspect, which was the main reason for inviting the participation of these companies. In simple words, industrialized countries cannot just demand oil from Kuwait and then close the door on its petrochemicals. Al-Sharrah (2000) indicated that Kuwait should increase its share in the petrochemical market to 4 percent to get good economical utilization of the industry and its products.

2.5 Conclusion

Kuwait's petrochemical industry efforts to follow Health, Safety and Environment regulations should continue as its benefits were observed worldwide. Also, Kuwait should direct its development to play an increasingly important role in the petrochemical industry. Its role should be both in Kuwait, as a supplier of petrochemical intermediates and finished products, and in other parts of the world, probably as a participant in the petrochemicals market.

Kuwait has made a promising start in manufacturing, marketing and joint ventures in the field of some petrochemicals. Studies are currently underway for the establishment of one or more large complexes for basic petrochemical intermediates. It is essential for Kuwait to continue its development of the petrochemical industry and to promote further research into new products.

Chapter 3

Petrochemical Industry

3.1 The Structure of the Petrochemical Industry

The petrochemical industry, as the name implies, is based upon the production of chemicals from petroleum. However, there is more to the industry than just petroleum products. The petrochemical industry also deals with chemicals manufactured from the by-products of petroleum refining, such as natural gas, natural gas liquids, and tar.

The structure of the petrochemical industry is extremely complex, involving thousands of chemicals and processes. It is severely cross-linked, with products of one process being the feedstocks of many others. For most chemicals, the production route from feedstock to final products is not unique, but includes many possible alternatives. As complicated as it may seem, however, this structure is comprehensible, at least in general form.

At the beginning of the production chain are the raw feedstocks: petroleum, natural gas, and tar. From these are produced a relatively small number of important building blocks. These include primarily, but not exclusively, the lower olefins and aromatics, such as ethylene, propylene, butylenes, butadiene, benzene, toluene, and xylene. These building blocks are then converted into a complex array of thousands of intermediate chemicals. Some of these intermediates have commercial value in and of themselves, and others are purely intermediates. The final products of the petrochemical industry are generally not consumed directly by the public, but are used by other industries to manufacture consumer goods. To give some idea of the scale of complexity of the industry, a small portion is shown Figure 3.1.

Figure 3.1 is actually a small extraction of much larger and more complete flow diagrams found in Stanford Research Institute (SRI) reports. Note in Figure 3.1, that certain chemicals, Acetaldehyde and Acetic acid for example, appear in more

than one place in the flowchart. This reflects the multitude of production routes available for most chemicals. In the actual industry, many chemicals are products of more than one method, depending upon local conditions, corporate policies, and desired by-products (Bell 1990). There are also additional methods available, which have either become obsolete and are no longer used, or which have never been used commercially but could become important as technology, supplies and other factors change. Such versatility, adaptability, and dynamic nature are three of the important features of the modern petrochemical industry. Stobaugh (1988) outlined the important characteristics of the petrochemical industry in a simple but yet comprehensive way. The characteristics are shown in Table 3.1.

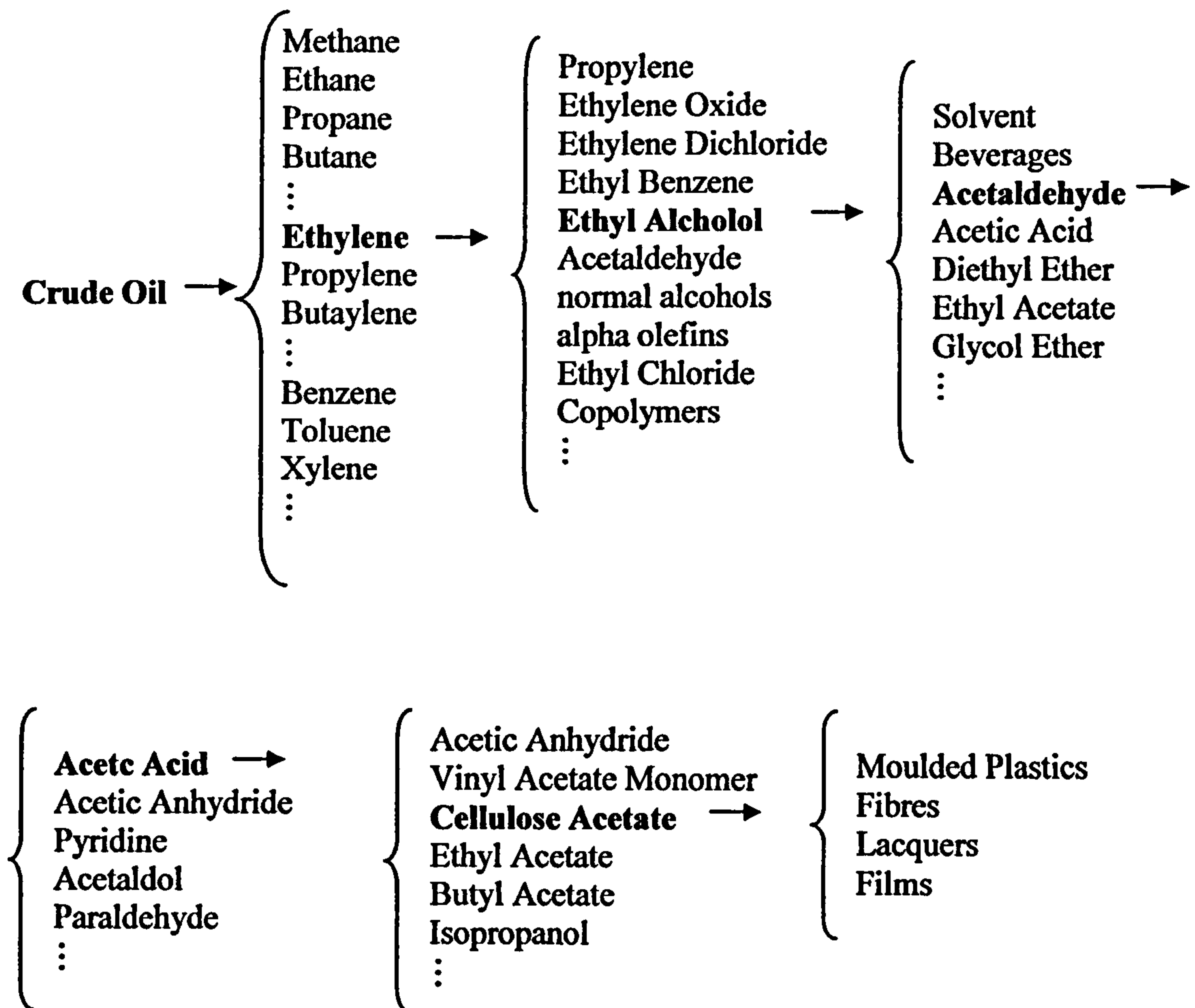


Figure 3.1: One Route from Crude Oil to Products

Table 3.1: Important Characteristics of the Petrochemical Industry (Stobaugh 1988)

<i>Supply</i>	
Raw material	Petroleum products from crude oil and natural gas
Technology	Some batch, but mostly continuous process facilities that are highly automated and capital-intensive, with large economies of scale
Work force	Proportion of engineers and scientists to workers greater than the average in manufacturing
Value/weight	Cost of transporting a petrochemical typically small compared with its price
Research and innovation	One of the leading spenders on research and development and output of innovations compared with other industries
Efficiency and progress	High rate of productivity growth compared with other industries
<i>Demand</i>	
Nature of end products	A liquid or solid that can be further processed in one or more steps into final products most often made from plastics, synthesis fibres, or synthetic rubbers
Price elasticity	Low for specialties, and high for commodities – with specialty status most often occurring in early years of a product's life and commodity status most often occurring in later years
Substitutes	Final products made from petrochemicals competing in many separate markets, sometimes with one another and sometimes with products made from such natural materials as wood, leather, silk, cotton, wool, rubber, steel, aluminium, glass, and paper
Rate of growth	High during early years of product's life and low during later years

Fortunately, the petrochemical industry has a built-in flexibility, which will allow it to adapt to its ever-changing environment. There are several possible methods for producing most petrochemicals. Therefore, when one production route becomes prohibitively expensive, or otherwise untenable, the industry can switch to a different route. The different processes, which make up the industry, are all interrelated, by the products and by-products of one process being the feedstocks for other processes. Therefore a model is needed to plan orderly development of the petrochemical industry in light of its ever-changing environment, and to see how changes in one sector will affect the rest of the global industry.

3.2 Petrochemical Industry Modelling

Mathematical models of the petrochemical industry have the objective of defining the technical structure within which the petrochemical industry must function. The structure is formed by the large but linked number of chemicals that are available on a commercial scale and by the rigid feedstock, by-products, and energy requirements of these chemicals. The products of one segment of the industry become the feedstock for another segment; thereby defining a network of material and energy flows that constrain business activities.

Petrochemical companies seeking to upgrade their hydrocarbon raw materials have integrated forward into the petrochemical industry towards fibres, elastomers, plastics, and other consumer products. Rubber, textile, and steel companies, seeing synthetic material as competition for their traditional market, have integrated backward towards the production of synthetic polymers.

Chemical companies are increasingly concerned with the development of planning techniques for their process operation. The incentive for doing so derives from the interaction of several factors. Recognizing the potential benefit of new resources when these are used in conjunction with an existing process is the first factor. Another major factor is the dynamic nature of the economic environment. Companies must assess the potential impact of important changes in the external environment on their business. Included, are changes regarding demand, prices,

technology, capital, markets and competition. Hence, due to technology obsolescence, the increasing competition, and the fluctuating prices and demand for chemicals, there is an increasing need for quantitative techniques to plan the selection of a new process, the expansion and shutdown of an existing process, and the production of chemicals.

Many models have been proposed to plan the petrochemical industry in the form of optimization and non-optimization models. Optimization models include linear, integer or non-linear programming under deterministic or uncertainty approaches. The non-optimization models, that are not common, include relatively new methods, for example, a graphical representation called structural simulation (Chavez et al. 1991) and black and white Petri-nets (Harhalakis et al. 1993). Linear Programming and Mixed Integer Linear Programming models will be presented below together with a discussion of variables uncertainty; these models have importance and wide use in modelling the petrochemical industry.

3.2.1 Linear Programming Models

It is required to select the optimal technology paths for the production of a given amount of chemicals. For this, it is assumed that a set of feedstocks is locally available in a limited quantity. Also, several alternative processes technologically are accessible for transforming the feedstock into final products. These technologies are characterized by technical coefficients of consumption of raw materials, chemicals, utilities, labour, by-products production, investment cost for different plant sizes and operation and maintenance costs. These technologies introduce intermediate chemicals, which are produced and consumed in the system.

The pioneering work of Stadtherr and Rudd (1976, 1978) defined the intermediate chemicals as a network and formulated the behaviour of the petrochemical industry as a system of linear equations. Figure 3.2 shows the overall perception of the Linear Programming (LP) model (Fathi-Afshar et al. 1981). The petrochemical industry is viewed as a system of M chemical transformations (processes) that produce or consume N chemicals. Let F_i be the amount of chemical i

used as a primary feedstock; let Q_i be the amount of chemical i emerging as a final product; and let X_j be the total amount of the main chemical produced from process j . If the chemical i is produced by process j , let o_{ij} be the amount of i produced per unit X_j ; if i is consumed by j , let $-o_{ij}$ be the amount of i consumed per unit of X_j ; if neither an input or output of j , let $o_{ij} = 0$. The industry is also constrained by the supply of feedstocks S_i , the demand of products D_i and a limit on the capacity of each chemical transformation L_j , where the production of each process X_j is usually lower than the current capacity of similar plants.

It is worth mentioning that the term *process* used in this section and the following one refer to a production plant using main feedstocks to produce final products while in Chapter 6 the term *process* has a different implication; it is a section of a plant.

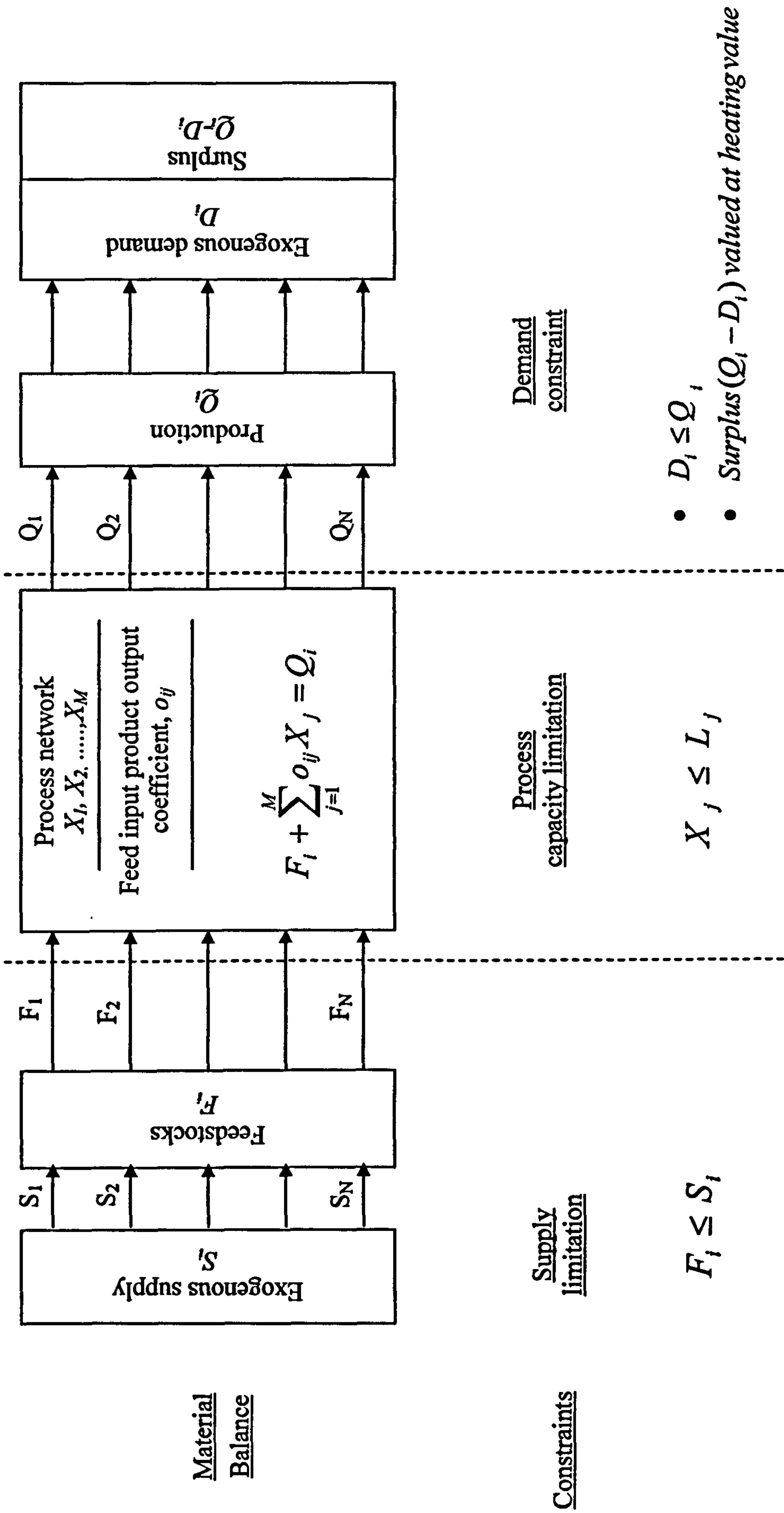


Figure 3.2: Linear Programming Model Structure (Fathi-Afshar et al. 1981)

The process capacity limitation constraint will impose the current industrial structure on the solution (Stadtherr and Rudd 1976); therefore, it can be neglected. Relaxing the capacity constraint was used in the models of Sophos et al. (1980), Sokic and Stevancevic (1983), Fathi-Afshar and Yang (1985), De Santiago et al. (1986) and Al-Fadli et al. (1988). Different applications of the LP model were studied to identify the optimal structure of the petrochemical industry. Some of these applications were optimal resource allocation (Stadtherr and Rudd 1978); the economic impact of new chemical technology (Fathi-Afshar and Rudd 1981); the impact of converting a petrochemical complex to a trigenerate petrochemical complex on the total CO₂ emission (Dijkema et al. 2003). Trigeneration represents a novel, functional view of the large-scale petrochemical industry; it not only provides petrochemicals but also acts as a large heat sink that enables a net CO₂ emission reduction.

The LP model showed its ability to identify the technological structure of the petrochemical industry that meets the needs of the economy, natural resources or environment as well as to test different development scenarios. However, the LP model must be applied with care since its result may recommend small production rates or the production of a single chemical using more than one technology. Using different technologies for one chemical was against investor strategy in some small countries. The studies of Al-Fadli et al. (1988) and Fathi-Afshar and Rudd (1981) for example, did not consider that the results of a model recommending the production of a chemical using more than one technology as a problem, because they modelled the Kingdom of Saudi Arabia and the United States respectively (large countries with large petrochemical industries).

3.2.2 Mixed Integer Linear Programming Models

Mixed Integer Programming deals with the solution of mathematical programming problems in which some of the variables can assume non-negative integer values. If the objective and constraints are linear, the resulting model is called Mixed Integer Linear Programming (MILP) model.

A MILP model was proposed by Jimenez et al. (1982) and Jimenez and Rudd (1987) to study the Mexican petrochemical industry. The MILP model proposed selects a process to be installed if the production cost of its product reaches a favourable level with respect to the cost of importing the chemical. The MILP model permits the determination of the economic break-even point and it can be recursively used to study the impact of different development policies. Figure 3.3 shows a general structure of the MILP model (Jimenez et al. 1982). The model parameters are the same as the LP model described in the previous section with the addition of the imports I_i for chemicals and the binary variable Y_j that reflects the event of building ($Y_j=1$) or not building ($Y_j=0$) a plant.

The development of the petrochemical industry in the Kingdom of Saudi Arabia was also studied with a MILP model. Al-Amer et al. (1998) proposed a MILP model similar to Jimenez et al. (1982) model but with the modification that the constraint imposed on the process capacity:

$$0 \leq X_j \leq L_j Y_j$$

is replaced by:

$$B_j Y_j \leq X_j \leq K Y_j$$

where K is a valid upper limit on production rates applicable to all processes.

The above constraint states that if only process j is selected, the production level must be at least equal to the process minimum economic capacity B_j . Also, since the Kingdom of Saudi Arabia is a large petrochemical country, no imports of chemicals and no constraints on the supply of feedstocks were included in the model. The sensitivity analysis on the model indicated that it was quite insensitive with respect to the overwhelming majority of given parameters. Thus, the solution can tolerate a wide range of change in selling price, production costs, and supply deficit data. A newer MILP model for Saudi Arabia by AlFares and Al-Amer (2002) included feedstock constraints for some chemicals and expressed the production rate

X_j as a linear combination of low, medium and high production rates as defined by the industry common standards.

Al-Sharrah et al. (2001, 2002) used a MILP model similar to Al-Amer et al. (1998) with some modifications and applied it to plan the petrochemical industry of Kuwait. The main modifications were to include a constraint to limit the selection to one technology only to produce a chemical and to modify the demand constraint in line with the country's share of the petrochemical market.

Examples of other application of MILP models, in the process industry, include multi-period planning and optimal plant layout. Sahinidis et al. (1989) presented a MILP model for long-range planning presented by periods up to the fifth year. They planned a network of processes and chemicals consisting of existing as well as potentially new processes. Georgiadis et al. (1997) used a MILP model to find the optimal layout design in multi-purpose batch plants. They also presented some simple heuristic rules to aid in the solution of large-scale models. Heuristic rules mean rules of thumb to aid in getting the best model solution.

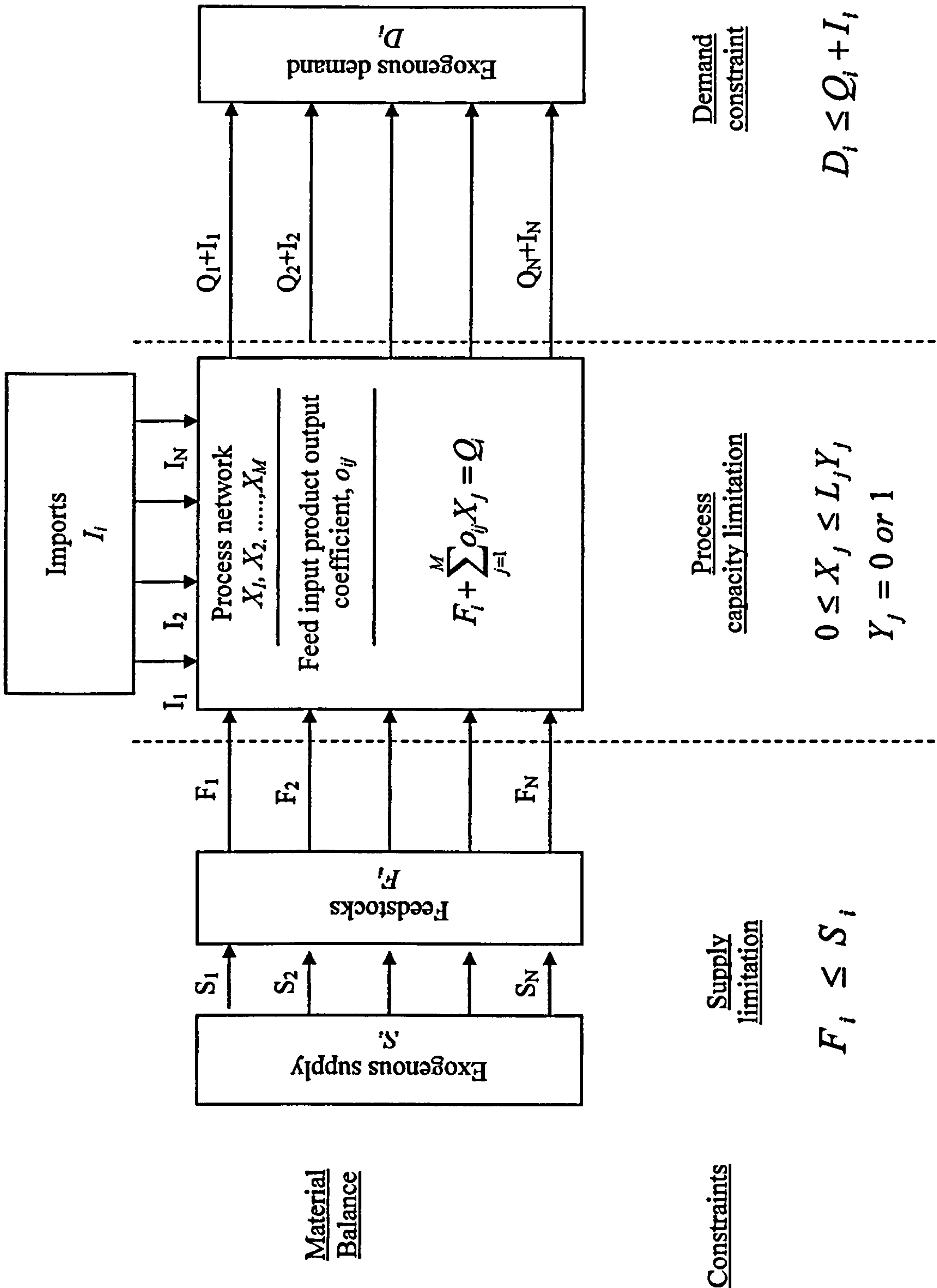


Figure 3.3: Mixed Integer Programming Model Structure (Jimenez et al. 1982)

3.2.3 Objective Functions

An objective function specifies the direction of improvement of a criterion, i.e., maximize or minimize the criterion. A criterion is a measure of effectiveness of performance, which forms a basis for decision-making. Examples of a criterion are cost, profit, return on investment, or any measure of effectiveness that guides the decision making process; note that cost and profit are examples of two conflicting criteria. The objective function(s) considered within a petrochemical model vary extensively in the literature. Researchers have selected a single objective function or multiple objective functions with different aspects

3.2.3.1 Single Objective Function

For the single objective function, Rudd (1975), Al-Fadli et al. (1988), and Fathi-Afshar et al. (1981) selected the minimization of the total production cost. Other studies, Stokic and Stevancevic (1983), and Stadtherr and Rudd (1976, 1978), selected minimizing feedstock consumption.

3.2.3.2 Multiple Objective Functions

The notion of Multiple Objectives (MO) in planning the petrochemical industry is used extensively due to the number of objectives decision-makers aim to achieve; most important of which are: profit, cost, environmental concerns and safety. MO programming deals with optimization problems with two or more objective functions. It differs from the classical Single Objective (SO) optimization only in the number of respective objective functions. In SO function problems, the goal is to identify a feasible solution that gives the best value of the objective function. However, for MO problems, the notion of optimality must be dropped because a solution which minimizes (or maximizes) one objective function will not in general minimize (or maximize) any other objective. In other words, what is optimum in terms of one objective is usually non-optimum for another.

As most optimization problems are MO by nature, there are many methods available to tackle these kinds of problems. Generally, a MO optimization problem can be handled in four different ways depending on when the decision-maker articulates his or her preferences for the different objectives; this could be never, before, during or after the optimization procedure (Anderson 2001). Each of the mentioned ways has different possible solution methods. The MO optimization problem has a vector (set) of solutions instead of a single solution. Determining the best outcome requires the ordering and preferencing of one solution over another. Optimal MO solutions are defined in terms of these sets by conditions called Pareto optimality conditions. A feasible solution to a MO optimization problem is a Pareto optimal if there exists no other feasible solution that will yield an improvement in one objective without causing degradation in at least one other. The Pareto optimal set is usually an infinite set. The decision-maker, therefore, in most cases has to choose the desired solution from the set.

There is an abundance of ways in which MO optimization can be solved; some of them are presented below for the objectives $f_1, f_2 \dots f_V$.

Weighted Objective method

In this method the MO problem with V objectives f is converted to a single objective problem by using a weighted sum of the original multiple objectives. The equivalent optimization problem is then given by:

$$\min \sum_{m=1}^V w_m f_m \quad (3.1)$$

And is subject to the model constraints. The w_m is the weighting coefficient satisfying the following conditions

$$0 \leq w_m \leq 1 \quad \text{and} \quad \sum_{m=1}^V w_m = 1 \quad (3.2)$$

A complete set of Pareto solutions can be obtained by varying the weighting coefficients. The final solution is then chosen by the decision-maker.

Trade-off Method (ε -constraint)

In this method, a trade-off among the objectives is specified by the decision-maker. The original problem is converted to a new problem in which one objective is minimized subject to constraints that limit the value of the remaining objectives together with the original model constraints. Mathematically the problem has the following form:

$$\min f_r(x) \tag{3.3}$$

Subject to

$$f_m(x) \leq \varepsilon_m \quad m = 1, V; m \neq r \tag{3.4}$$

Where ε_m is the limiting value of f_m desired by the decision-maker. By varying the values of ε_m , a complete set of Pareto optimal solutions can be obtained.

Goal programming

Goal programming is a common technique used for the solution of MO optimization problems. In this approach, the objectives are thought of as goals with targets or threshold values that are desired. However, these constraints are often not strict but are usually allowed to vary within a close range of the desired value. This is accomplished by using deviational variables. The goals are assigned some priority or weight to signify their importance relative to each other. The goal criterion can be one of the following: greater than or equal to, less than or equal to, equal to, or a range. Consider a MO optimization problem with only two objective functions f_1 and f_2 . Assume that the first goal is that f_1 be less than or equal to z_1 , and the second goal is that f_2 be equal to z_2 . Then the goal programming problem can be written as

$$\min (w_1^+ d_1^+ + w_2^+ d_2^+ + w_2^- d_2^-) \quad (3.5)$$

Subject to

$$f_1(x) - d_1^+ \leq z_1 \quad (3.6)$$

$$f_2(x) - d_2^+ + d_2^- = z_2 \quad (3.7)$$

Plus all the original model constraints. The w 's in the objective function are the penalty weights corresponding to each additional variable d , which specifies the undesired deviation in the achievement of each goal. This formulation can be solved by any SO optimization algorithm.

The distance-based method (Lp norm)

This method is based on minimization of the relative distance from the candidate solution to the best values of the objective functions that were found from single objective solutions. The objective function can be formulated as the following:

$$\min \left[\sum_{m=1}^v \left(\frac{f_m - f_m^*}{f_m^*} \right)^p \right]^{\frac{1}{p}} \quad (3.8)$$

The exponent p gives different ways of calculating the distance and its value ranges from one to infinity. The most frequently used values for p are 1 for simple formulation, 2 for Euclidean distance, and infinity for Tchebycheff norm.

This method, when used with other methods of MO optimization, can generate multiple points on the Pareto front. The most used form is the weighted Lp norm method and the objective function will have the form:

$$\min \left[\sum_{m=1}^V w_m \left(\frac{f_m - f_m^*}{f_m^*} \right)^p \right]^{\frac{1}{p}} \quad (3.9)$$

For this method, the computational difficulty increases when the value of p is increased, the function becomes more non-linear and sometimes with very high numerical values.

Analytical Hierarchy Process (AHP)

The AHP is a method that is able to consider subjective and judgmental information and can be used when the system can be formulated as a MO linear model, except for some qualitative relationships (that is, some relationships between the decision variables and the objectives may be difficult to specify directly). This kind of decision problem and the corresponding model is called qualitative. The AHP solves the problem by the following steps. Firstly, the AHP quantifies the qualitative relations. Secondly, the AHP is used to support the search procedure in the context of MO programming. The methods developed for solving MO problems typically comprise two phases. First, the decision maker is required to give some information concerning his/her preference structure over the MO and then, using preference information the algorithm seeks a solution or a set of solutions for the decision-makers evaluation. These phases are repeated iteratively until the most preferred solution is found. A detailed application of the AHP on solving MO linear models was performed by Korhonen and Wallenius (1999).

The different solution methods discussed thus far all require additional input from the decision-maker, which is often subjective. Therefore, MO optimization is as much an art as it is a science. Choosing a method to solve a MO problem depends on the nature of the system and on when the decision-maker articulates his preferences concerning the different objectives. For the algorithms presented above: the weighted objective method needs input from the decision-maker before or after optimization; the goal programming

and ϵ -constraint methods need input before optimization; the AHP needs input by the decision-maker during the optimization procedure.

MO analysis in modelling the petrochemical industry has been considered with objectives of maximization of the thermodynamic availability change (a measure of ideal performance), minimization of entropy creation (lost work), and minimization of feedstock consumption in the studies of Sophos et al. (1980), and minimizing cost and gross toxicity in the studies of Fathi-Afshar and Yang (1985). Song et al. (2002) considered maximization of total profit and minimization of environmental impact. To reach a trade-off between different objective functions, Sophos et al. (1980) used the weighted objective method and Fathi-Afshar and Yang (1985) used both the weighted objective and the ϵ -constraint methods, Song et al. (2002) used the ϵ -constraint method.

3.2.4 Deterministic Models

Deterministic models for the industry assume that all parameters included in the model, for example prices and demand, are known with possible certainty; either by taking current values or by studies prior to planning, to estimate or to forecast these variables. All the models presented in Sections 3.2.1, 3.2.2 and 3.2.3 were deterministic.

3.2.5 Models with Uncertainty

Decision-makers often have to make a decision in the presence of uncertainty. Decision problems are often formulated as optimization problems, and thus, in many situations, decision-makers wish to solve optimization problems which depend on parameters that are unknown. Typically, it is quite difficult to formulate and solve such problems, both conceptually and numerically. The difficulty starts at the conceptual stage of the modelling. In the formulation of optimization problems, one usually attempts to find a good trade-off between realism of the optimization model, which usually affects the usefulness and quality of the obtained decision, and the tractability of the problem, so that it could be solved analytically or numerically. Although the uncertainty is rigorously

defined, in practice it can range in detail from a few scenarios (possible outcomes of the data) to specific and precise joint probability distribution.

It is important to distinguish between data uncertainty and variability; variability represents inherent heterogeneity or diversity in well-characterized data. Fundamentally, a property of natural variability is usually not reducible through further measurement or study. Uncertainty, on the other hand, represents partial ignorance or lack of perfect information about poorly characterized models. Another mathematical term used for uncertainty in modelling and programming is stochastic. Stochastic programs are mathematical programs where some of the data incorporated into the objective or constraints is uncertain.

Several approaches have been suggested to formulate and solve optimization problems under uncertainty based on the way uncertainty is handled as well as in the design objective. The literature has provided two main approaches for evaluating and accounting for uncertainty in model parameters: sensitivity analysis and probabilistic programming. The former is too simple to account for uncertainties in more than one parameter at a time, while the latter requires detailed statistical properties of the parameter variations.

Many models were proposed for the chemical and petrochemical industry that included uncertainty in formulating the model rather than considering uncertainty as a final stage of the solution using sensitivity analysis. Systems modelled were batch plants, small operations or process networks. Uncertain system parameters, which may include operating temperature, reaction constants and yields, were studied by Friedman and Reklaitis (1975), Grossmann and Sargent (1978), and Rooney and Biegler (2000). The models of Ahmed and Sahinidis (1998) only considered uncertain demand. With the uncertain demand, Ierapetritou et al. (1994) included supply and process yield, and Bernardo et al. (1999) included supply and prices.

Probabilistic programming has evolved around two types of models:

- i) The two-stage programming.
- ii) The chance-constrained programming.

These models will be discussed in the next two sections.

3.2.5.1 Two-Stage Programming

This approach requires that one decision is made now and then to minimize the expected cost (or utilities) of the consequences of that decision. This paradigm is called the recourse model. A set of constraints describes the links between the first stage decision and the second stage decision. It is undesirable to make an arbitrary correction (recourse) to the first stage decision; it is desirable that the best such correction is made.

Recourse models can be extended in a number of ways. One of the most common ways is to include more stages. With a multi-stage problem, one decision is made now, wait for some uncertainty to be resolved (realized), and then make another decision based on what has happened. The objective, usually, is to minimize the expected costs of all decisions taken.

Solving a recourse problem is generally more difficult than the deterministic version. The hardest part is to evaluate the expected costs of each stage (except the first). In effect, it is attempted to perform high-dimensional numerical integration on the solution to mathematical programs. The two-stage programming can be solved in many different ways the most common being discretization, parametric, decomposition and robust.

Discretization

When the uncertain variable is discretely distributed, the problem can be written as a large deterministic problem. The expectations of the uncertainties can be written as a finite sum, and each constraint can be duplicated for each realization of the uncertain variable. The resulting deterministic equivalent problem can, in principle, be solved using

a general-purpose optimization package. Halemane and Grossmann (1983) used discretization with a non-linear model in the design problem of a chemical plant under uncertain design parameters with the objective of minimum cost.

Parametric Approach

The theory of parametric programming aims to provide basic tools for the analysis of the effect of parameter change on the optimal solution by defining a parametric profile of this solution as a function of uncertainty. The main driving force for solving an optimization problem parametrically is to avoid the unnecessary repetition of solution of the problem for different values of the uncertain parameter. Instead, the parametric solution provides explicit functions representing the optimal solution and optimal objective value for all the values of the uncertain parameters for which an optimal solution exists in a given range.

The parametric approach differs in its structure and complexity according to the model to be solved. Usually it starts by solving parametrically an (inner) optimization problem in terms of the uncertain parameter and the first stage decision. The next stage is different for different models.

Ierapetritou et al. (1994) used the parametric approach to plan a chemical complex with a LP model under demand uncertainty and with maximum profit objective. They used an iterative procedure between a master problem and subproblems with an economic risk function as a conversion indicator. Acevedo and Pistikopoulos (1996) used a similar procedure and tested the approach on synthesis/planning and heat exchanger network design. The model was mixed integer non-linear programming under uncertain demand and with a profit objective.

Decomposition Approach

In this algorithm, the two-stage stochastic model, for example a MILP model is solved iteratively through a sequence of LP subproblems and a MILP master problem,

with the former providing lower bounds to the expected objective function and the latter providing upper bounds. At the first stage, the selection of operational decisions (process, plant capacities, etc.) is performed, and then at the second stage the operating levels (production, purchases, sales, etc.) are determined. Hence, the master problem involves all the first-stage decisions, and the subproblem involves the remaining variables.

Shah and Pantelides (1992) used the decomposition approach to optimize the operation of a multi-purpose batch plant of three products and four scenarios. The model was a MILP model under uncertain demand with the objective of minimum capital cost of equipments. Liu and Sahinidis (1996) recommend the use of the decomposition algorithm to optimize process planning. They used the algorithm to optimize a plan for 10 processes, 6 chemicals, 4 time periods, 24 random parameters, and 5^{24} scenarios. Their model was a MILP model under uncertain demand and supply with the net present value objective. Bhatia and Biegler (1997) used instances of uncertain parameters to construct planning scenarios that are addressed through multi-period formulation of a batch plant. The dynamic processing under uncertainty was addressed in their work via a closed loop state feedback correction strategy. Large models were handled with up to 3774 equations and 3319 variables. The model was a non-linear model under uncertain process parameters and with a profit objective.

Robust Approach

A potential limitation of the two-stage approach described above is that it only accounts for the expected cost of the second stage recourse without any conditions on the variability of these costs. It is likely that, under high risk situations, a design with a low expected second stage cost might run into a specific realization of the uncertain parameters for which the actual recourse cost is unacceptably large. The importance of controlling variability of the cost as opposed to just optimizing its first moment is well recognized in management applications. To handle the tradeoff associated with the expected cost and its variability in stochastic programs, Mulvey et al. (1995) proposed

the concept of robustness. A decision is termed to be robust if the actual cost of the realized scenario remains close to the optimal expected cost for all scenarios.

Ahmed and Sahinidis (1998) used the robust approach to optimize four processing networks, one of which has 100 scenarios. The model was LP under uncertain demand and with a cost objective.

3.2.5.2 Chance-Constrained Programming

In some cases, it may be more appropriate to try to find a decision, which ensures that a set of constraints will hold with a certain probability. An example is a processing plant that experiences uncertain random demands, and wishes to find the cheapest way to satisfy its demand with a high probability. Thus, these models allow for the possibility that the constraint may, in unusual circumstances, be violated and only insists that it be satisfied most of the time.

The probability constraint or the chance-constraint can, under reasonable hypothesis, be transferred to its equivalent deterministic equivalent depending on the uncertainty. For a constraint of the form $g(x)=ax-b$, uncertainty in the constraints coefficient (a) are treated differently to the uncertainty in the constraints term (b).

For the uncertainties in the constraints term (b), Petkov and Maranas (1997) proposed a stochastic model for a multi-period planning and scheduling of multi-product plants under demand uncertainty. The stochastic model involves the maximization of the expected profit subjected to the satisfaction of a single or multiple product demands. The stochastic elements of the model are expressed with equivalent deterministic forms using the concepts of normally distributed random variables. The model was a mixed integer non-linear programming model.

For the uncertainties in the constraints coefficient (a) Friedman and Reklaitis (1975) considered all the fluctuations in the coefficient to include more constraints, the

nature of the models did not change but the size could double. They modelled a refinery scheduling problem and the model was LP with a profit objective.

Combining uncertainty and MO in models is considered to be the “most difficult” of all models and very little research has been done in this area (Al-Refai 1993). Few studies were found in this area, one study by Roderer et al. (2002) used the two concepts of uncertainty and MO to model investment planning in the process industry under uncertain prices and demand. In this work, the single objective of net present value is treated as multiobjective using decomposition; this formulation was solved by the weighted Tchebycheff sum approach. Overall, Roderer et al. (2002) work was a multiobjective MILP model derived by decomposition of a stochastic MILP model and considering multi-period planning through the concept of scenarios. Another work by Bonfill et al. (2004) used two objectives of expected profit and financial risk for scheduling batch plants under uncertain demand; the two objectives were combined by the weighting method.

3.3 Sustainability

Health, Safety and Environmental (HSE) issues are a concern for all industries, but particularly for the petrochemical industry. The consumers, employees, shareholders, legislators and the communities for which the industry operates are all becoming increasingly aware of HSE issues and demand ever-higher standards. The concept of Sustainability or Sustainable Development takes these issues into consideration together with other important needs. This section introduces the concept of Sustainability with reference to its definition, indicators, and application to the petrochemical industry.

3.3.1 Overview

To sustain means “to maintain; to keep in existence; keep going; prolong” (Webster’s New World College Dictionary 2001). If applied only in this sense, sustainability does not make much sense for human society. Human society cannot be maintained in the same state, whatever that state should be; therefore, other definitions

are used. One of the most commonly cited definitions stresses the economic aspect by defining sustainable development as “economic development that meets the needs of the present generation without compromising the ability of future generations to meet their own needs” (Engel and Engel 1990).

Sustainable development has become a widely recognized goal for human society ever since deteriorating environmental conditions in many parts of the world indicate that sustainability may be at stake. In previous times, sustainability of humankind was taken for granted and did not appear as an essential explicit goal. It certainly was an implicit goal: no human society has ever consciously promoted its own unsustainability. Global developments now focus attention on sustainability as an explicit goal. However, the concept has to be translated into the practical dimension of the real world to make it operational. It is important to be able to recognize the presence or absence of sustainability, or of threats to sustainability, in the system under our stewardship. Proper indicators are needed to provide this information, to tell where the system stands with respect to the goal of sustainability.

Finding an appropriate set of indicators of sustainable development for a community, a city, a country or even the world is not an easy task. It requires knowledge of what is important for the viability of the systems involved, and how that contributes to sustainable development. The number of representative indicators should be as small as possible, but as large as essential (Bossel 1999).

Sustainability is a dynamic concept; societies and their environments change, technologies and cultures change, values and aspirations change. A sustainable society must allow and sustain such changes. It must allow continuous viable and vigorous development, which is what sustainable development means. Despite the uncertainty of the direction of sustainable development, it is necessary to identify that direction and to define indicators that can provide essential and reliable information.

3.3.2 Sustainability in the Petrochemical Industry

Over the last 20 years, there has been a very rapid growth in environmentally related legislation affecting the petrochemical industry. The development of environmentalism in the industry has proceeded along two waves (Ulhoi 1998). The first wave was growing during the 1960s and peaked in 1972 when the Rome Club published its "Limit to Growth" report. Industry responded in a protesting and reactive way. Protection of the environment was seen by industry as an extra and unnecessary cost in production. However, regulation regimes were slowly introduced by public authorities in most parts of the western industrialized world based on "identify-and-repair" followed by a sanctioning approach towards the polluter. In the mid-1970s the "polluter-pays" principle was introduced and broadly accepted by most countries. The regulation was characterized by an expensive "end-of-pipe" pollution abatement arrangement.

The second wave was growing during the 1970s and began to take shape in the 1980s when the Executive Director of the United Nations Environment Program published a collection of his former speeches. During the late 1970s, he had persistently argued for a production philosophy that did not destroy the ecological basis to sustain economic development.

With the first environmental wave primarily based on nature's declining capacity to provide essential raw materials such as fossil energy, metals, etc., the second wave was primarily concerned with nature's capacity to absorb the waste from economic development. The effects of global warming and the destruction of the ozone layer dominated the debate during the 1980s.

However, this second wave crested in 1987 when the World's Commission on Environment and Development published its report and introduced the now well-known concept of Sustainable Development. At this point in historical development, environmental strategies increasingly left the former "identify-and-repair" approach and

adopted an “anticipate-and-prevent” approach. The issue is no longer growth or no growth, but what type of growth.

Sustainable Development is a concept that has to be translated by society (or industry) into interconnected economic, social and environmental goals, incorporating the long-term prospective of sustainability (Callens and van den Berghe 1998). Economic goals include, good economic indicators; social goals include salaries, work accidents, training, etc.; and environmental goals include, minimizing pollution, minimizing energy and water consumption, etc.

The quest for pollution prevention and increased pressure and demand for environmental well being and sustainable processes and products has created a new ethos in the process industry. Within the petrochemical industry, support for the concept of Sustainable Development is based on (Kohlhase 1994):

- Protecting and improving the quality of the environment.
- Prudent management of available resources including development of new, clean, and energy efficient technology.
- The transition towards a cleaner and more sustainable mix of energy sources and consumption patterns (including a switch from high carbon to low carbon fuels).

The highly complex nature of environmental effects makes it difficult to link environmental and design calculations with either sufficient scope or detail. Also, the balance of recourse use and benefit is an individual and social judgment and is clearly difficult to quantify (Sharrat 1999). Some studies used the sustainable concept in the design stage of a single process with relatively complex indicators. Young and Cabezas (1999) used the waste reduction algorithm (WAR) which is a tool to be used by design engineers to aid evaluating the environmentally friendliness of a process. This algorithm

determines the potential environmental impact of a chemical process and of the energy consumed within the process.

Steffens et al. (1999) used a multi-criteria function to represent the sustainable design. The work used two environmental impact indicators to rank flowsheets: life cycle analysis (LCA) and the sustainable process index (SPI). Life cycle analysis is a method to identify and quantify the environmental performance of a process from “cradle to grave”. Its main potential in environmental decision-making lies in providing a quantitative basis for assessing potential improvement in environmental performance of a system throughout the life cycle. Figure 3.4 shows a simplified scheme of a product life cycle. This life cycle is an environmental cycle because it is mainly related to the wastes in the product life. The SPI does not focus on the impact of pollutant streams leaving the system but, instead, evaluates the sustainability of the whole system, the basic units used by the SPI being the amount of area which is required to embed a process sustainability into the environment. The total area is made up of the area for raw materials production, the area required to provide process energy, the area for process installations, the area for staff, and the area required to accommodate products and by-products (including wastes).

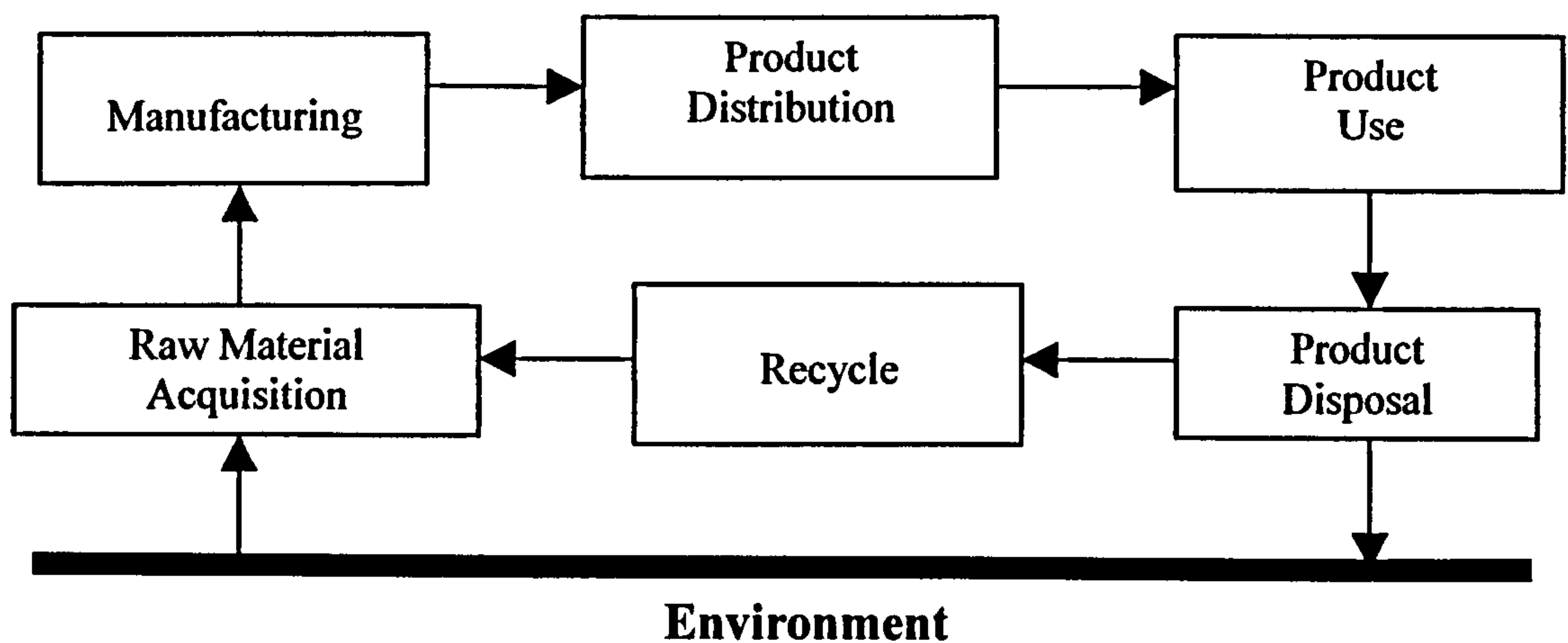


Figure 3.4: The Product Environmental Life Cycle Diagram

Environmental life cycle assessment was also used in the studies of Azapagic and Clift (1999). The life cycle was represented as a multiple objective linear programming model with the objective functions of economic performance, environmental impact, and total production. The system considered in the studies produces five boron products, and the final disposal phase of the products was not considered making this essentially a “cradle to gate” study. A life cycle “cradle to gate” analysis was done also for the assessment of two alternatives producing dimethylcarbonate in the studies of Aresta and Galatola (1999).

Another trend in Sustainable Development studies is the purely qualitative form, where the evaluation is done by questionnaires. A good example is the Green Management Assessment Tool (GMAT), which is a questionnaire on sustainable development, related to different levels of integration of environmental management systems into general business processes (see Eagan and Joeres 1997).

It is noticed that an industry can measure environmental performance in a number of different ways that range from compliance with existing internal standards and applicable regulations, to the amount of emissions, to eco-efficiency, to environmental cost. However, the industry must be allowed to preserve its profitability, otherwise investment will not occur and environmental protection will be eroded. Al-Sharrah et al. (2001) used a sustainability index as an objective for a MILP model; the index was a combination of health and economic indices.

In this work and thesis, the economics, represented by added-value, and the safety, represented by a chemical plant accident risk index, are used to represent the sustainability of the planned petrochemical industry.

3.4 Manufacturing Strategy and Products Selection Tools

Manufacturing strategy is an area of growing concern in most industries. It is simply an effective use of resources for a strong competitive position in the market. For

any manufacturing firm to stay competitive in the more globally oriented market of today, the understanding of strategic, tactical and operational issues concerning the link between markets, products and production is fundamental (Olhager and Wikner 2000).

Nowadays, there is a shift in strategic thinking arising from the increasing importance of technology and innovation to the overall strategy of the industry. These two aspects of the industry's activity can no longer be treated as a tactical issue. The resource development and environmental interactions are increasingly dependent on the availability of innovative products, processes and services. Therefore, to achieve its corporate and business objectives, the industry needs to have an innovation and technology strategy, and to integrate these into its corporate and business strategies. Quezada et al. (1999) outlined performance indicators to obtain an overall picture of the company business at a strategic level:

- Net sales.
- Sales index: net sales in relation to a reference value of 100.
- Capital intensity: investment divided by added-value
- Added-value = net sales – cost of purchases.
- Productivity: added-value per employee.
- Relative market share: market participation in relation to three main competitors.
- Market growth.
- Frequency of innovation: sales of products with less than three years in the market.
- Vertical integration: added-value divided by sales.
- Direction of the change of the previous indicators.

Usually, the main step in developing a strategy is to prepare a list of all the products that are in the portfolio of the industry for which a strategy is being prepared. It is then necessary to identify the development and competitive advantage the industry is able to achieve through these products using a strategic tool.

One strategic tool used in planning and product selection is the Bill Of Material (BOM) (Olhager and Wikner 2000). Normally, the end product is broken down into a number of intermediate products and additives. This creates a list of items, each with its own Bill Of Material (BOM), representing the items needed to produce an item. Therefore, any production planning should be accompanied by BOMs for successful operations. In strategic planning, the striving for a flatter BOM or, in other words, a shorter internal supply chain and simpler products, increasingly is an objective.

The changing market and increased product variety resulted in the proposal of another important strategic tool in the manufacturing systems, which is flexibility. Flexibility can support the industry strategies as a competitive weapon. Persentili and Alptekin (2000) quantified flexibility as being inversely related to the Sensitivity To Change (STC). The lower the sensitivity of the product to the globally changing environment, the higher the flexibility. Changes affecting products may include price, demand, environmental constrains, feedstock availability, etc. The original formulation of STC has two components, which are the penalty for change and the probability of change.

Another strategic tool used in planning and products selection is the Boston Consulting Group (BCG) Business Portfolio Matrix, as shown in Figure 3.5. Although developed for a multi-divisional firm, it can be used in a firm with a multi-product portfolio; the contribution of the product to the competitive position of the firm being similar to that of the business.

The BCG matrix is a simple four-square grid. One axis is the “Relative Competitive Position” usually measured by market share, and the other “Business Growth Rate” expressed as a percentage of increase in sales. Businesses are placed in the quarters according to an assessment of their performance. In the BCG matrix shown in

Figure 3.5, the size of the circle is proportional to the size of the business involved or the production rate of an industrial plant.

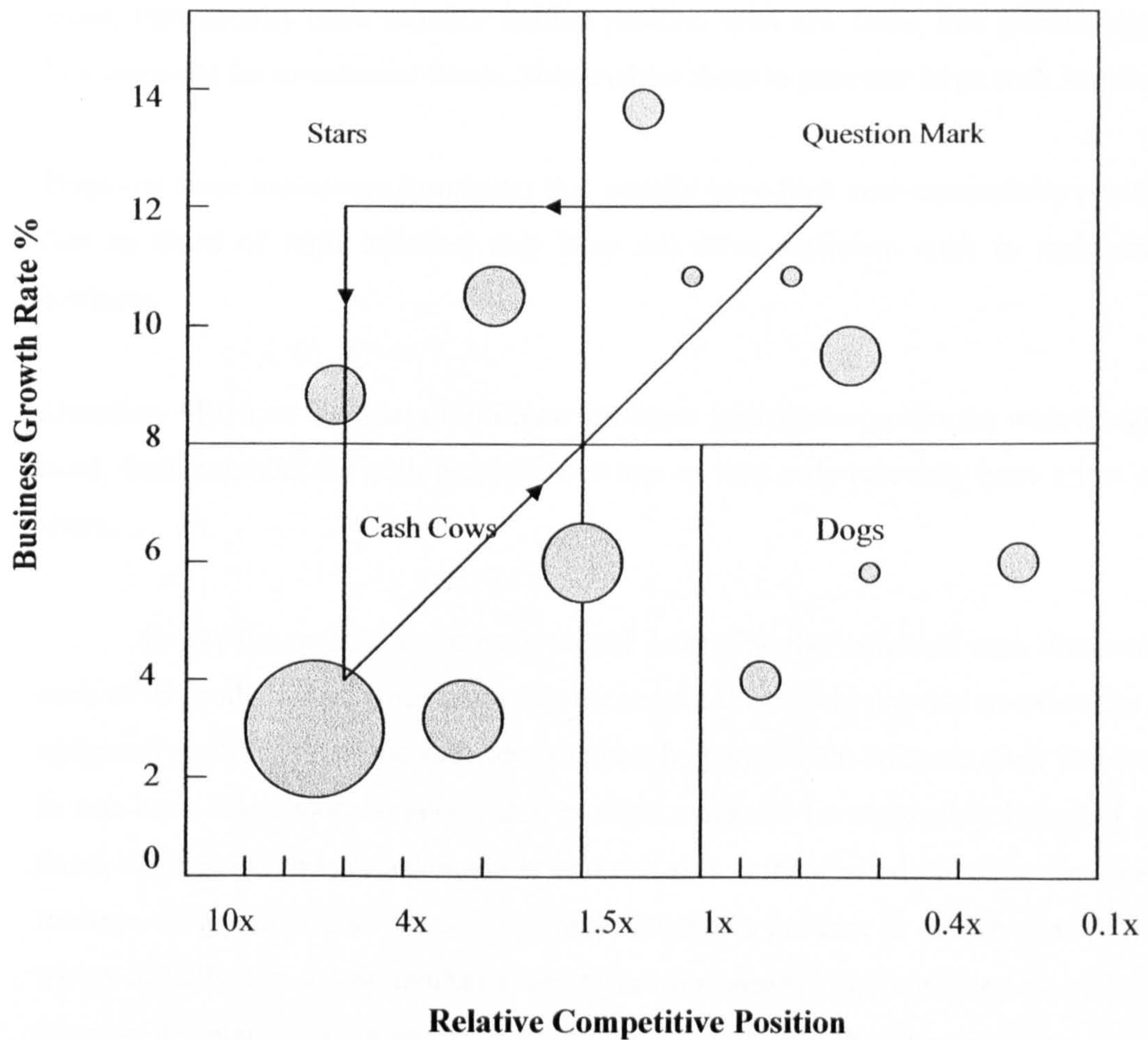


Figure 3.5: The BCG Business Portfolio Matrix

The names given to each quarter are supposed to reflect the nature of the business.

Stars are those businesses (products) that are growing rapidly and have high investment needs.

Cash Cows are those businesses (products), which have low growth and high market share; they usually have superior market position with low costs, low growth rates, and low demands for investment funds. This enables them to generate large cash surpluses.

Dogs are those businesses (products) that usually have high cost-competitive position, so that in times of high inflation they may not have sufficient cash to maintain their business.

Question Mark or Problem Children are those businesses (products) with a high cash need; their potential for cash generation is low as they only currently have a low market share.

To use the matrix, a company would determine the values of each dimension for each of its products and when placed in the matrix this would provide an overview of the company portfolio. It would indicate whether the parts of the business were concentrated in one area. The theory suggests that portfolios should be reasonably balanced among *Stars*, *Cash cows* and *Question marks* and that this is the desired direction for continued success and profitability. A company may develop a product in a high-growth market, which initially has a low market share (*Question mark*). The company should plan to increase the market share and thus move the product into the *Star* category. While the product remains a *Star* it is unlikely to release cash, given that the market is still growing rapidly, as the cash generated and maybe more, will be required for new plants to satisfy the increases in demand. As the market growth rate slows down, less cash is required for reinvestment and thus the product automatically becomes a *Cash cow*, the cash being released rather than used for reinvestment. As the growth slows even further, the theory enables revitalization to the *Question mark* stage and so the cycle begins again. *Dogs* are

low market-share products in a declining industry, and so the firm should exit from these businesses unless there is a special reason for not doing so.

If there are too many *Stars*, a cash crisis may result; if too many *Cash cows*, future profitability may be in jeopardy, and too many *Question marks* may affect current profitability.

Use of the BCG portfolio enables the scope and competitive advantage of each product to be established, and the strategy for each business to be identified. However, such two-by-two matrices need to be used with caution:

- They are too simplistic. The business world contains not only highs and lows, but middle positions as well.
- Growth rates are inadequate as a descriptor for industry attractiveness. Some industries with high growth rates may never be successful, because supply always outstrips demand.
- A market share is an inadequate descriptor of the overall competitive position, because it is so heavily dependent upon a definition of a market.

However, the portfolio matrix as such can be a useful analytical device for organizing ideas about the industry products. Al-Sharrah et al. (2002) used this BCG portfolio matrix concept as a constraint for planning the petrochemical industry in Kuwait. All products in the optimum selected petrochemical network have to be well distributed between *Cash cows*, *Stars*, and *Question marks* with very few *Dogs*.

Another strategic tool, which has the matrix form, is the General Electric (GE) / McKinsey matrix. This matrix, shown in Figure 3.6, was developed in 1971 and was designed to overcome the shortfalls that companies were encountering with the BCG matrix. This matrix is known as the industry attractiveness – business strength matrix or the nine-box matrix. To use the matrix, a company would determine the values of each dimension for each of its products and when placed in the matrix this would provide an

overview of the company portfolio. It would indicate which parts of the business were located in unfavourable boxes.

In the GE / McKinsey matrix, “Business Strength” is plotted on the vertical axis; the “Industry Attractiveness” on the horizontal axis and the size of the circle represents the size of the industry with a shaded wedge representing the firm’s current share of the industry. A market or industry is considered to be attractive if its potential for providing a significant growth and return on investment is judged to be high. Different strategists and consultants have devised different sets of variables for industry or market attractiveness; typical factors that affect market attractiveness are market size, market growth rate and market profitability. The other matrix dimension, business strength, is a factor that implies among others, high present or future cash flow, high relative profit margins and high product quality.

The matrix is divided into nine cells: the three cells at the top left hand side of the matrix are the most attractive and require a policy of investment for growth, the three cells running diagonally from left to right have a medium attractiveness and the management of businesses within this category should be more cautious and finally, the three cells at the bottom right hand side are the least attractive, and management should follow a policy of business rejection unless the relative strengths can be improved.

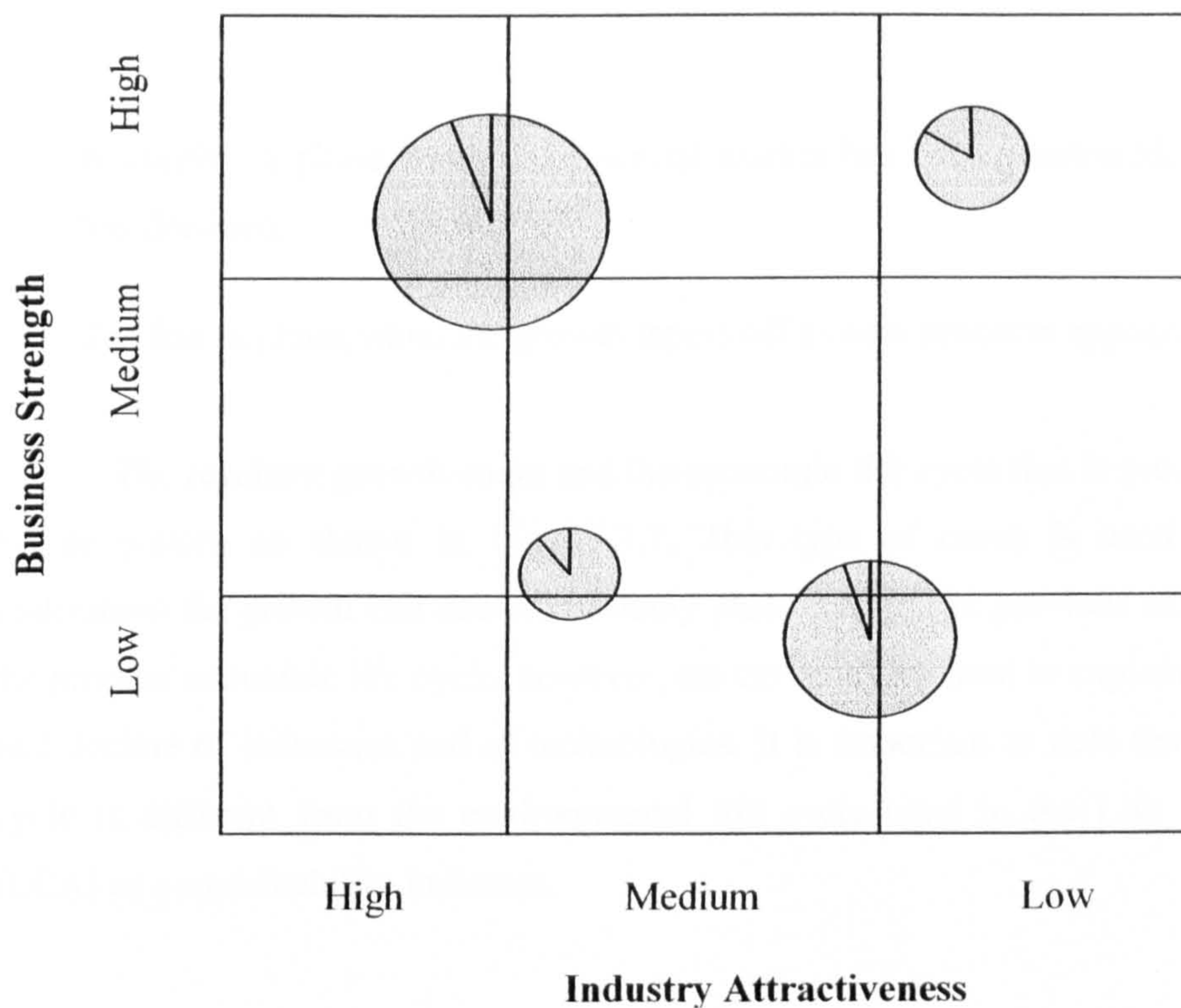


Figure 3.6: The GE / McKinsey Matrix

It should be noted that the BCG and the GE / McKinsey matrices are *static*. In preparing a portfolio analysis it is necessary to take into account that all products, processes and services have their own economic life cycles; that is, one must evaluate their dynamic behaviour over time. This notion is explicit in the economic life cycle concept, the basic hypothesis of which is that a phenomenon under investigation passes through a number of stages. These are:

- **Introduction:** a phase that is marked by slow growth, which reflects the difficulty of overcoming buyer inertia.
- **Growth:** a phase where the buyers rush into the market once the product has been proven to be successful.

- **Maturity:** a phase when the potential market has been penetrated, and growth has declined.
- **Decline:** a phase when the growth tapers off as new products appear.

The resultant growth curve and the economic life cycle that is produced follow an S-type pattern as shown in Figure 3.7. This type of curve is used extensively to understand the growth and decline of many phenomena. The previous example has been the product economic life cycle; however, the curve is also used to explain similar growth and decline of industries and of technologies. It is important to note that this economic cycle is different from the environmental life cycle used in the Life Cycle Analysis (LCA) as a sustainability indicator.

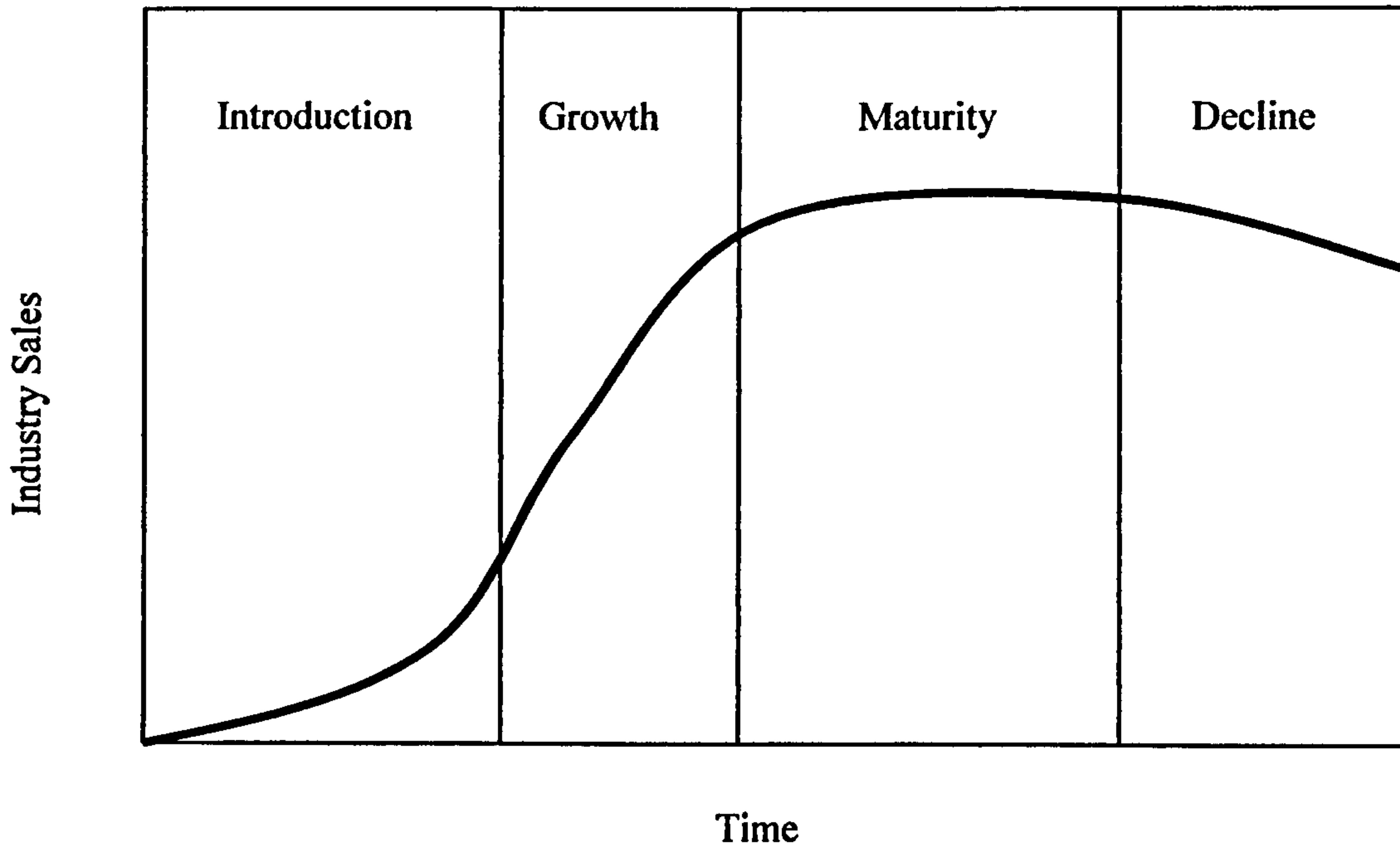


Figure 3.7: Growth Curve and Economic Life Cycle

Again, the economic life cycle diagram needs to be used with caution, keeping in mind the following qualifications:

- The duration of each stage varies from industry to industry, and the current stage occupied by an industry is often not clear.
- Not every industry or product goes through each stage. Often some stages will be skipped, or the duration in each stage is so short as to be non-existent.
- Companies can influence the shape of the curve by product innovation or market positioning; the strategic aim must be to control the shape of the curve.
- The nature of the competition can change at each stage, and will be different for each industry.

Consequently, care must be used when applying the curve to any situation. Such tools are for understanding behaviour of the product or the industry economic life cycle, and not a determinant of that behaviour. In addition, the use of strategic tools in the formulation of a technology strategy is principally to give an indication of the existing range of the company's products and services together with their relative contributions to the company's sales and growth.

In Chapter 6, the final results of planning are checked with the GE / McKinsey matrix, using present value, growth rate and production data.

3.5 Conclusion

An important characteristic of the petrochemical industry is its flexibility. For the production of many petrochemicals, there are two or more process available, each transformation involving different combination of feedstocks and co-products. Therefore, the petrochemical industry is a large network of several hundreds of chemicals and processes. Consequently, a model is very useful for petrochemical planning for production planning and transformation routes to help in eliminating inefficient

operation. Modelling is done with the application of basic engineering and mathematical rules like material balance and conservation of flow in a network. Likewise, the model illustrates basic economic principles.

Most models can be classified as Linear Programming models and Mixed Integer Linear Programming models, each combined with different objective functions single or multiple. Objectives of petrochemical models are strongly related to the Sustainability concept. Objectives take different forms under two main categories, the first one is Health, Safety and Environment protection and the second one is economic gain.

Chapter 4

Economic Planning For the Petrochemical Industry

The petrochemical industry is a dynamic industry and can be seen as a network of chemicals from basic feedstock to final chemicals. The aim of this chapter is to identify and model trends in chemicals and oil prices and to introduce them to the petrochemical industry planning process using forecasting. The dynamics of oil prices can be considered as a significant disturbance to the petrochemical industry and this work should be viewed as a preliminary effort in incorporating dynamic disturbances in the planning exercise. The implication of such disturbances on the economic viability of the planned industries will be discussed. In addition, this work presents a procedure to make forecasts for oil and chemical prices. An application to the planned development of the Kuwait petrochemical industry will be performed.

4.1 Economics and the Petrochemical Industry

The Chairman of Kuwait's Petrochemical Industries Company (PIC), Al-Shuwaiyeb, indicated that the world sales of petrochemicals continue to increase and, for the year 2004, it reached \$ 0.5 trillion, which counts for 5.8% of the world trade exchange (Al-Shuwaiyeb 2004). With relatively low raw material prices and adequate feedstock supplies, the general short-term outlook is for a strong performance and more penetration of diverse markets in the economy.

The petrochemical sector plays an important role in the industries of developed countries. This role in industrial modernization has been linked to progress in the manufacturing sector and the ability to promote exports (Vergara 1991). Relatively low and stable feedstock prices and continuous growth in demand have contributed to profitability of petrochemicals manufacture. Also, the appetites of oil companies to join the petrochemical industry field have grown rapidly for the following reasons:

- 1- Little profit from petroleum refining for fuel production.
- 2- The increasing rate of consumption of petrochemicals (14% increase per year) as compared with fuels (3 to 4 %).
- 3- Availability of new materials needed for petrochemical manufacturing such as naphtha, butane, propane, tail gases, aromatics and hydrogen from catalytic reforming of gasoline.
- 4- High profit resulting from petrochemical sales.
- 5- The continued expansion in this industry by the development of new products.

In spite of all the above mentioned favourable factors for the development of petrochemical industries, Kuwait projects should be chosen extremely carefully on their own economic merits, coordinated with similar projects in the neighbouring countries and areas. They should be based more on stable predicted internal market developments than on the more sophisticated and changeable export market, which is out of the economic and political influence of the Arab countries (Reis 1971).

For Kuwait, financing of the required investments in the petrochemical industries is possible with the important resource of oil income. However, technological help, training of local labour and marketing (with transportation) are also necessary. Therefore, joint ventures with foreign companies will be required.

4.2 Planning with Economic Disturbances

The petrochemical industry is dynamic and is affected by different types of disturbances. The economic environment in which a chemical plant operates is a dynamic rather than a static one, and it undergoes continuous change. During the life of the plant, the demand and prices for its product will change, as will all the factors that determine its profitability, e.g., labour, raw material, and utilities costs. Many of these factors can be included in a complete economic evaluation of a proposed plant.

Reasons for the dynamics of the chemical industries are not difficult to find. One of the most important reasons is the continual replacement of conventional materials, often of agricultural origin, by materials of synthetic origin, such as synthetic fibres, plastics, and synthetic rubbers. Another strong factor is the high demand for fertilizers and pesticides, required to raise and maintain high agricultural productivity. Rising standards of health care have resulted in increased demand for pharmaceuticals. These factors are also fed by a spirit of innovation, characteristic of this industry that has resulted in a constant stream of new or improved products.

Dynamic inputs to a system are termed disturbances. For the petrochemical industry, this includes many factors such as prices and demand. The dynamic disturbances in this industry are usually characterized by cycles with long-range duration (decades) and/or short-range duration (years).

4.2.1 Long-Range Disturbances

Since the onset of the 20th century, students of the world economy have been drawing attention to certain long-term regularities in the behaviour of the leading economies. The first to make this argument in a sustained manner was Nikolai Kondratieff, a Russian economist writing in the 1920s. Statistical work on the behaviour of prices, and some output series, for the United States and Britain since the 1790s, led him to conclude that the existence of long waves was very probable. Thereafter, this has been named after him (Kondratieff wave or simply K-wave). Looking at the cause of this long-wave, different approaches can be found in the literature ranging from pure exogenous causality, for example, solar activity and/or astronomical configurations, to a pure endogenous process of a biological or social nature (Devezas 1999).

Kondratieff saw the capitalist world economy as evolving and self-correcting and, by implication, he denied the notion of an approaching collapse of capitalism that was common among Marxist economists. Kondratieff expressed the belief that the dynamics of free market economics are not linear and continually progress upward in a cyclical

manner. He acknowledged that each cycle advanced and developed the economy further and brought it to a new height. The cyclical economic growth or K-wave is related to the innovation in products. Therefore, each wave is associated with a new technological environment in which new products replace old ones.

Kondratieff taught and believed in the intermediate 7-11 years cycle that many economists believe in today. However, Kondratieff taught that reducing the system to this small cycle only was simplistic and that a broader long-wave scope should be superimposed onto the development of the system. He also recognized the necessity for flexibility in the system and believed that the long cycles fluctuate between 45 and 60 years. Table 4.1 shows an outline for K-waves recognized by economists and the corresponding dominant forces during each wave (Alatiqi and Notley 1998).

Table 4.1: K-waves Dates and Forces (Alatiqi and Notley 1998)

K-Wave	1st Wave 1785-1843	2nd Wave 1843-1894	3rd Wave 1894-1941	4th Wave 1941-xxxx
Industry	Textile	Railroads	Automobiles	Electrification
Material	Cotton	Iron	Steel	Plastic
Energy	Water	Wood	Coal	Oil
Communication	Overland	Telegraph	Telephone	Electronics
National Economy	France and Britain	Britain	Germany	United States

The foundation of Kondratieff's theory, and the element considered to be one of the most important aspects of his research, is the cycles impact on the rise and fall of prices. The movement of prices is key to understanding the K-wave and the effect that the

K-wave has on investment and planning. Raw material and commodity prices in the recent decades have closely followed the outline Kondratieff laid out for the rise and fall of the cycle (Barker 1995).

Kondratieff was not the only person to notice long-term cycles within the economy. In 1939, the great economist Joseph Schumpeter, the author of the concept “Creative Destruction”, hypothesized that technology runs in fifty-year waves. Schumpeter noticed that bursts of technical transformation coincides with upturns in economic activity (Dewey and Dalein 1987). He assumed that they were the causes of that activity, new technology drives the economic growth, and the more the innovation in technology, the greater is the chance of damage to the economy, especially through loss of jobs. Kondratieff found cycles in industrial production, and Schumpeter found them in technical application. Then, in the 1970s, Jay Forrester and his team of computer modellers at the Sloan School of Management at Massachusetts Institute of Technology (MIT) came up with a persuasive long-wave theory. It was an application of system dynamics created during the mid-1950s. Forrester (1958) disapproved with the approach taken by operations research in the 1950s, where methods are applied to isolate company problems. He suggested that the success of industrial companies depends on the interaction between many flows of information, some of which are global (Forrester 1961). In his paper (Forrester 1977), he showed that economic models for capital goods: metals, machines, chemicals, concrete, etc. can generate long-wave cycles about 50 years in length.

Forrester’s work has inspired a group of researchers at MIT to follow him; most notable is John Sterman, who showed how interaction between multiple time scales in a non-linear model can lead to long-waves cycles about 50 years in length, on top of short-waves cycles (Sterman 1985, 1990, 1992). The debate continues concerning the existence of the long wave itself. Although some analysts may simply argue that a pattern is being forcibly created, there is strong supportive evidence from, Sterman’s work using modelling methodologies, that the long wave is reality.

Another similar approach to explain the K-wave is the “Learning Dynamics of Succeeding Generations” (Devezas 1999). This approach, shown in Figure 4.1, explains the conceptual framework that generations follow and it is mainly successive processes of technological substitution or “Succeeding Technosphere”.

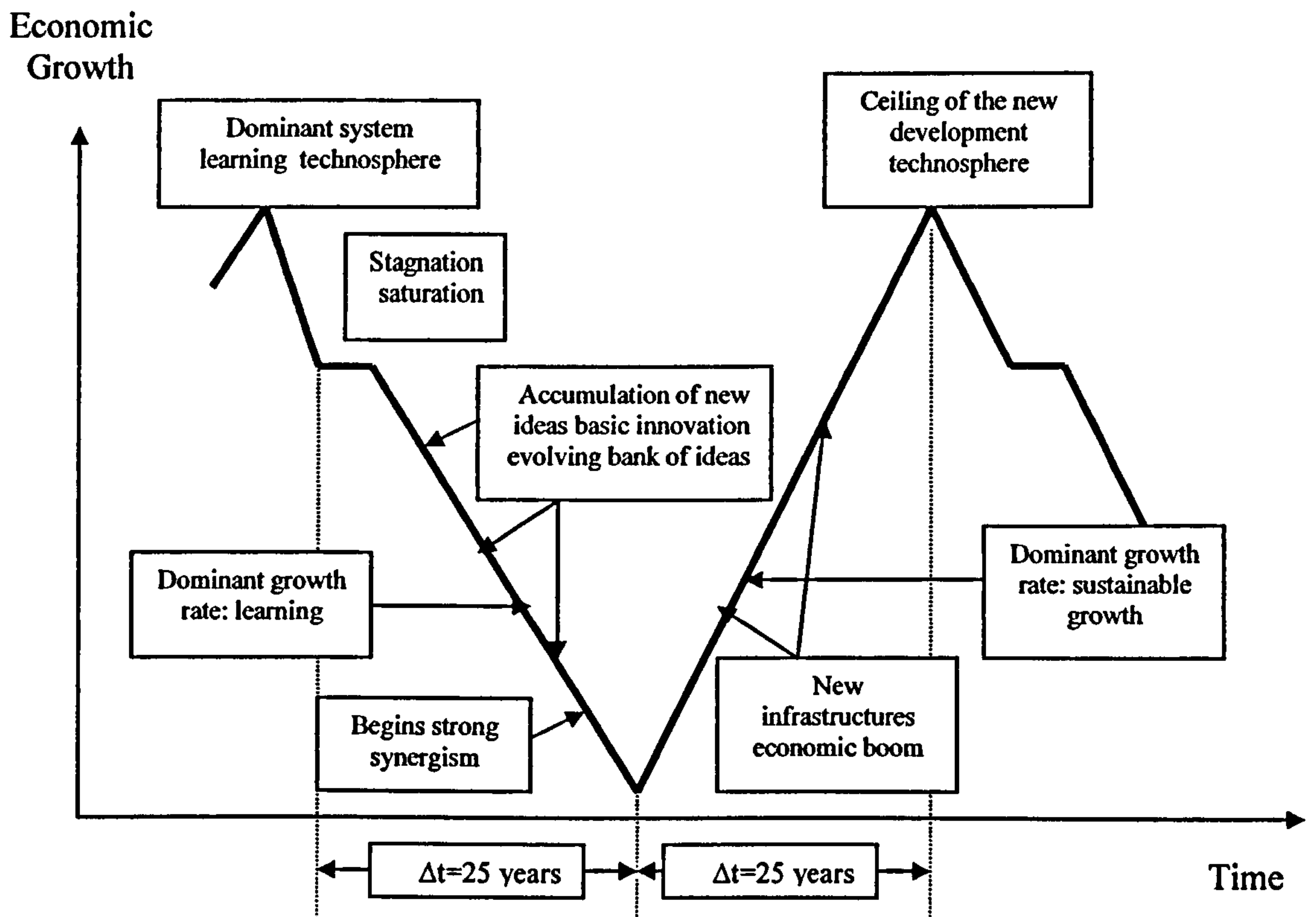


Figure 4.1: Learning Dynamics of Succeeding Generations (Devezas 1999)

Significance of the long wave

History of the long wave has been discussed since its discovery by Kondratieff. This long history, however, did not transfer the long wave to the main stream of the investment community. Many economists and financial planners pass over its implications and it is not likely that the debate over its validity will end soon. For example, the current long wave implies declining stock market prices from 1998 to 2010. That means indices like Dow Jones Industrial will be at best near their current level by 2010. Prominent writers pass over this prediction and forecast at least 100% appreciation for the same period (Dent 1998). On the petrochemical industry side, there is little evidence that major consulting houses paid the slightest attention to the long wave. When the capital long wave top was realized in Asian markets in 1998, coinciding with an oil price bottom, planners revised down their demand expectations and Asia was treated as an anomaly (Teleki 1999). Recovery of demand was predicted for base chemicals and oil prices were predicted to remain weak (Adams 1999). Other prominent forecasters predicted declining prices for oil from 2000 until 2003 in different scenarios around and below 20 \$/bbl (125 \$/m³) (Cambridge Energy Research Association 2000). In fact, as already known, oil prices remained strong from 1999 until 2006. Finally, a caution is in place; the cyclic phenomena is neither new nor its discussion novel.

K-waves are not exactly about history repeating. Instead, they are about the dangers and rewards of going there (Zwick 1998). It is clear that there is a risk of ignoring and/or abandoning a viable economic opportunity, which the understanding of the long wave should help avert. Market analysts know that the cycles of human progress are based on a psychology which takes a long time to manifest and will not accrue in a strict periodic rhythm (Slatyer 2002).

Although long wave understanding is essential, studying its effect was rare especially in the petrochemical industry. Even the concept of long-range planning was mis-represented, Sahinidis et al. (1989) considered 5 years as a long-range planning period and Ierapetritou et al. (1994) considered weeks and few months as short to

medium-term planning periods which means a few years can be considered as a long-term period.

Long-term cycles are key factors in analyzing or modelling the economic activity of large international industries such as the petrochemical industry and understanding them is essential for sound investment decisions (Alatqi and Notley 1998). Yimoyines (1995) explained this by recognizing that the petrochemical industry is characterized by large plants that take several years to be built. Finally, the plants come on stream together, creating oversupply and thus the bottom of the cycle. Sedriks (1999) stated that the petrochemical industry has become commoditized and subjected to severe cycling in its profitability due to cycling in demand (linked to business cycle) and capacity expansion (linked to construction cycle).

Applications and uses of long cycles can be found for interest rates (Notley 1994), commodities prices (Murphy 1986), stocks and bond forecasting (Pring 1991).

Implications for Kuwait Petrochemical Industry

Through the incorporation of cyclic analysis, various difficulties that were encountered in the Kuwaiti petrochemical industry were explained. A most notable example is the Equate Chemicals Company, a Joint venture of Petrochemicals Industry Company (PIC) with Dow Chemicals, which commenced production in 1997 for ethylene, polyethylene, and ethylene glycol. With a four months delay in startup, prices were at the bottom of the business cycle. In 1998, the Asian crisis hit the markets and products prices were substantially below forecast. To add insult to injury, technical problems were encountered at the same time and interruptions in operations took place. In the mean time, PIC and Equate sponsored a conference on "Petrochemicals in Kuwait Investment Opportunities" in October 1998. At this conference, a critical analysis of the Asian crises from the perspective of the long wave was presented. It was suggested that the crises were not isolated but part of the unfolding of a bigger picture (Alatqi and Notley 1998). Further, it was suggested to incorporate cyclic disturbances in feasibility

studies and forecasting. Weak prices continued for the first half of 1999 and operating income continued below target. As a result, the parent company of Equate required an injection of additional capital. A cyclic study was performed by an international consultant who forecasted prices into 2010. The realization of the cyclical nature of the chemicals business lead the Supreme Oil Council in Kuwait to support the additional capital and the continuation of support for the project. Operations soon recovered to target potential and beyond and, by August 2001, phase 2 of the Olefin complex (2000 million USD capital) was approved. In addition, a much delayed and debated aromatics complex of 1400 million USD capital was also approved (Alatiqi 2001). The understanding of the short, intermediate and long wave phenomena contributed much to the continued support for petrochemical projects in Kuwait despite the tough challenges. In March 2003, Dow Chemicals signed a strategic partnership with Petrochemicals Industry Company (the Parent of Equate) for the realization of the expansion. The proposed processes in this work rely heavily on the raw materials provided by the olefin and aromatics complexes and, with further understanding of the cyclic economic disturbances, confidence in the proposed products should increase and investors should stay committed.

4.2.2 Short-Range Disturbances

Energy prices, mainly oil prices, affect all industries and they are determined by the capacity use of OPEC members and other producers. The capacity use, however, is influenced by the simultaneous actions and interactions of numerous variables that affect supply, demand and producers actions. Figure 4.2 shows a representative diagram of variables affecting oil price and consequently causing short-term disturbances to the petrochemical industry (Stanford Research Institute 1992).

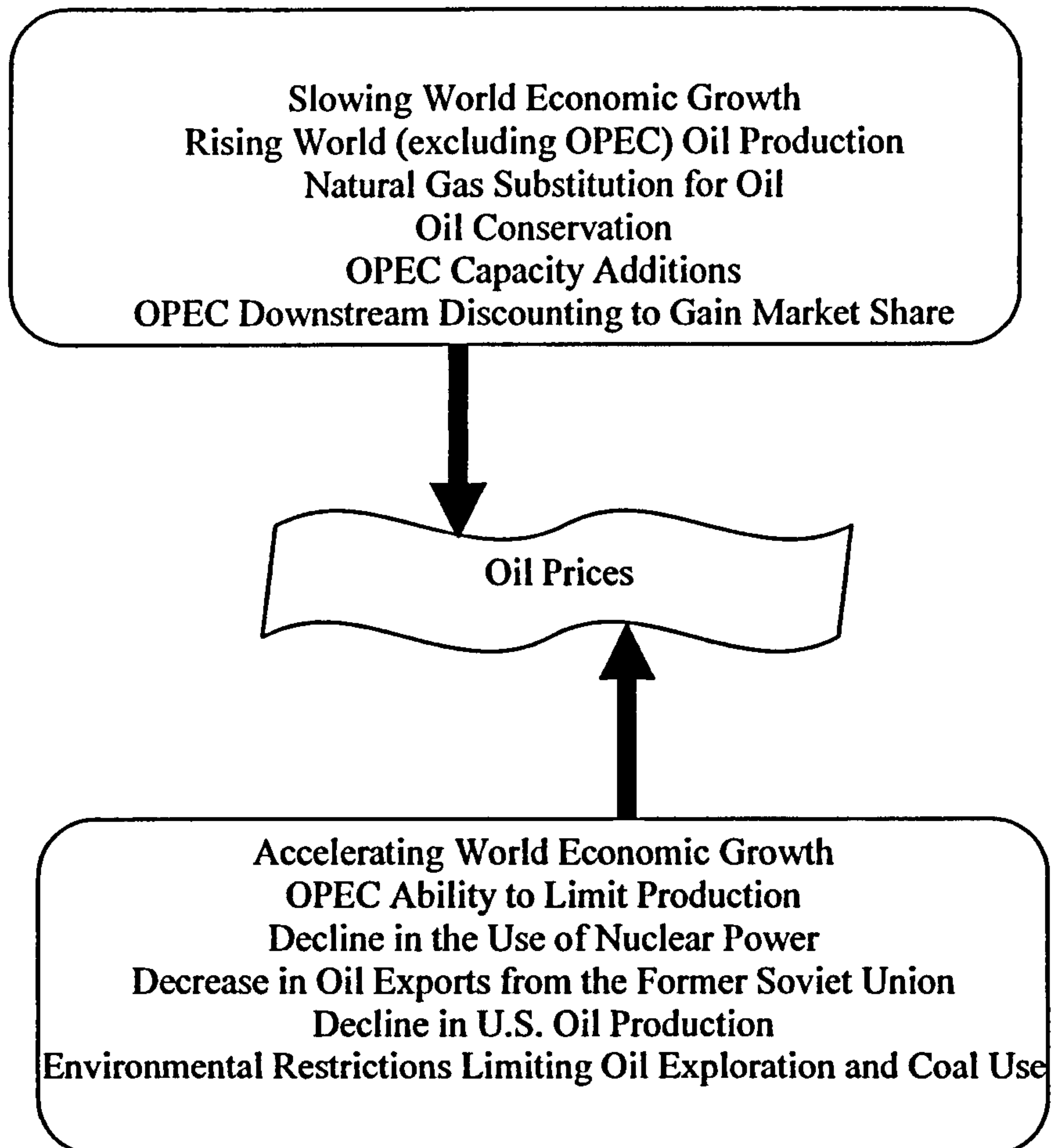


Figure 4.2: Variables Determining Oil Prices in Short-Range

Short-term disturbances occur also in the form of cycles. A famous short-cycle is the “Kitchin” 3½ to 4 year cycle. It is also closely related to the business cycle that affects business activities, interest rates and wholesale and retail prices. A wide variety of linear and nonlinear techniques have been employed to model short-cycles features. Simpson et al. (2001) forecasted the UK quarterly index of production using a model of

the business cycle. He adopted both linear and non-linear approaches. Kontolemis (2001) also analyzed the US business cycle and identified the cycle turning points using four time-series indicators. Turning point means the cycle upward or downward peaks, these are key points in economic analysis because they separate a rising economy from a falling one.

4.3 Forecasting as an Economic Tool

Forecasting of future prices of oil and petrochemicals are a major input to all aspects of production and market planning in the petrochemical industry. The two classes of forecasting techniques are: qualitative, which use either experts, sales people, or customers to make forecasts; and quantitative, most of which use historic data to make the forecasts.

4.3.1 Qualitative Techniques

Qualitative forecasts are usually based upon individual, subjective estimates drawn from personal experience and intuition, combined with the opinions of experts and market surveys. There are formal procedures for obtaining such forecasts, which range from considering the estimates of sales personnel to the application of Delphi-type methods (iterative questionnaires to identify the opinion of expert forecasters and to secure a common agreement among them on a specific forecast). These procedures may rely in part on marketing tests, customer surveys, sales force estimates, and historical data, but the process by which the information is used to obtain a forecast is highly subjective. The objective of qualitative forecasting methods is to bring together in a logical and systematic way all the information and judgment, which relate to the variable being estimated. These methods are usually used when data are scarce, for example, when a product is first introduced into a market. Thus, these techniques are frequently used in new-technology areas, where demand for the product is difficult to estimate.

4.3.2 Quantitative Techniques

There are two basic types of models in the quantitative category: time-series models and causal models.

4.3.2.1 Time-Series Models

These models use past time-ordered sequences of observations of the forecasted variable. In this type of analysis, only the time-series history of the variable being forecasted is used in order to develop a model for predicting future values. Then, forecasts are made by extrapolating the fitted model. The extrapolation is based on the assumption that the future will continue on the same basis as the past.

One of the useful tools in analyzing time-series data of a cyclical nature is the Fourier analysis; it is based on the concept that a series can be approximated by a sum of sinusoids, each at a different frequency. It has been used in its basic form to study oil short cycles. For example, the cyclic behaviour of the quarterly average of the non-OPEC supply in the studies of Jazayeri and Yahyai (2002), and it is identified in a form called “Dynamic Harmonic Regression” as useful to investigate periodic phenomena for forecasting (Young et al. 1999). Ierapetritou et al. (2002) also used a time-series model to generate necessary scenarios for future power prices.

4.3.2.2 Causal models

These models relate statistically the time-series of interest (dependent variable) to one or more other time-series (independent variables) over the same time period. If these other variables are correlated with the variable of interest and there appears to be logical cause for this correlation, then a statistical model describing this relationship can be constructed. Knowing the value of the correlated variable (independent variable), the model is used to forecast the dependent variable. There are two types of causal models, regression models and econometric models.

Regression models:

This approach attempts to quantitatively relate a chemical demand (dependent variable), for instance, to the causal forces (independent variables), which determine the chemical demand. Thus, regression is a mathematical procedure that takes account of the relationship of the dependent variable and the independent variable(s). Therefore, regression is more powerful than subjective estimation because it enables the forecaster to measure explicitly the apparent association between variables over time, thus eliminating most of the guesswork. If, for example, there is statistical association between the demand and the oil prices then this relationship becomes the basis for the forecasts.

Econometric models:

Whereas regression involves a single equation, econometric models can include any number of simultaneous multiple regression equations. The term econometric model is used to denote systems of linear multiple regression equations, each including several interdependent variables. The best starting point for understanding the basics of econometric forecasting is regression. Regression analysis assumes that all of the independent variables included in the regression equation are determined by outside factors, that is, they are exogenous to the system. In econometric models, however, such an assumption is often unrealistic. To illustrate this point, one can assume that the demand for a chemical is a function of the Gross Domestic Product (GDP), chemical price and oil price. In regression, all three independent variables are assumed to be exogenously determined; they are not influenced by the level of demand itself or by each other. This is a fair assumption as far as GDP is concerned, which is not influenced directly by the demand for a single chemical. However, for the chemical price there is unlikely to be a similar absence of influence. If the per-unit cost (and thus price) decreases as sales volume increase (and vice versa), different levels of sales will result in different per-unit costs (and thus prices).

Price forecasting in petrochemical planning may include tens of interdependencies and variables. An example is the price forecast elements considered by Chem Systems (1985). These elements include production elements (crude oil price forecast, feedstock cost trend, alternative feedstock economics, production costs and technology trends) and profitability elements (current price, general macroeconomic forecast, specific petrochemical business area trends and opinions of petrochemical purchasers and sellers).

The main idea behind econometric modelling is that everything in the real world depends on everything else. The world is becoming more aware of this interdependence, but the concept is very difficult to deal with at an operational level. The practical question is, of course, where to stop considering these interdependencies. Figure 4.3 shows an econometric model used by Probe Economics, Inc. (2005) as a forecast tool for petrochemicals prices. This model shows some of the main interdependencies in the petrochemical industry.

In an econometric model, one is faced with many tasks similar to those in regression models. These tasks include (Makridakis and Wheelwright 1989):

1. Determine which variables to include in each equation (specification).
2. Determine the functional form (that is, linear, exponential, logarithmic, etc.) of each equation.
3. Estimating, in a simultaneous manner, the parameters of the equations.
4. Testing the statistical significance of the results.
5. Checking the validity of the assumption involved.

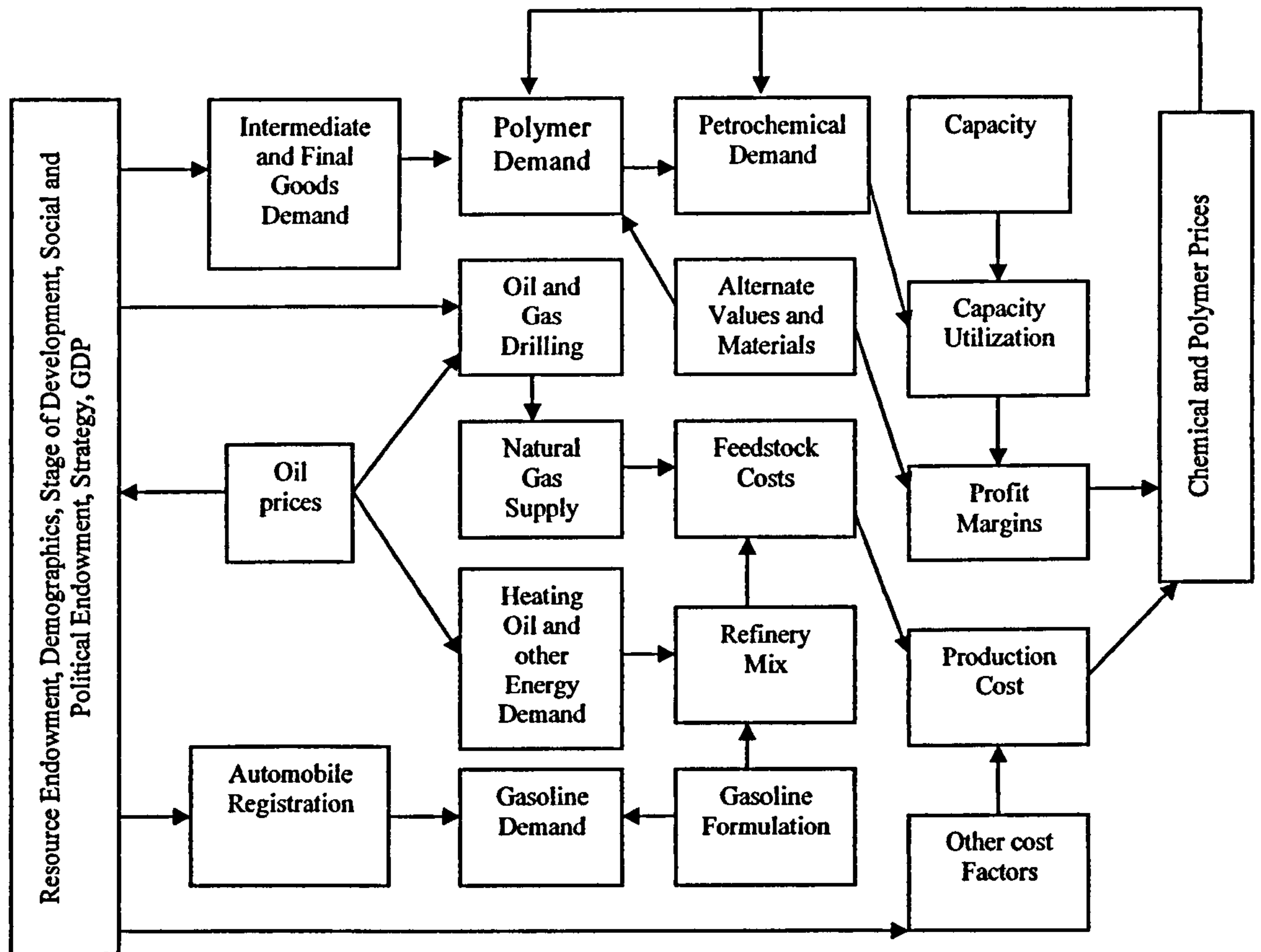


Figure 4.3: Petrochemical Econometric Model (Probe Economics 2005)

An obvious limitation to the use of causal models in general and econometric analysis in particular, is the requirement of an extensive investigation of many explanatory variables. This process is usually time-consuming and costly. The other limitation is that only explanatory variables whose values are known can be used, in the derived model, to forecast the dependent variable.

Forms of models that can be used as causal models are transfer functions and polynomials. The Second Order Plus Dead Time (SOPDT) transfer function model is used extensively in system identification and it can be used as a forecasting model. Another useful model, used extensively in forecasting, is a polynomial form of a transfer function. It is explicitly defined as a polynomial between the input u (independent variable) and the output y (dependent variable) at any time t . The current output $y(t)$ (dependent variable) is a function of previous na outputs and previous nb inputs delayed by nk together with some noise $e(t)$. The model is named Auto-Regression with exogenous variable (ARX) model (Ljung 1999) and is presented as:

$$y(t) + a_1y(t-1) + \dots + a_{na}y(t-na) = b_1u(t-nk) + b_2u(t-nk-1) + \dots + b_{nb}u(t-nk-nb) + e(t) \quad (4.1)$$

Nogales et al. (2002) used ARX and a transfer function causal model to forecast the next-day electricity prices. They used the electricity demand as the independent variable.

4.3.3 Types of Patterns in Time-Series Data

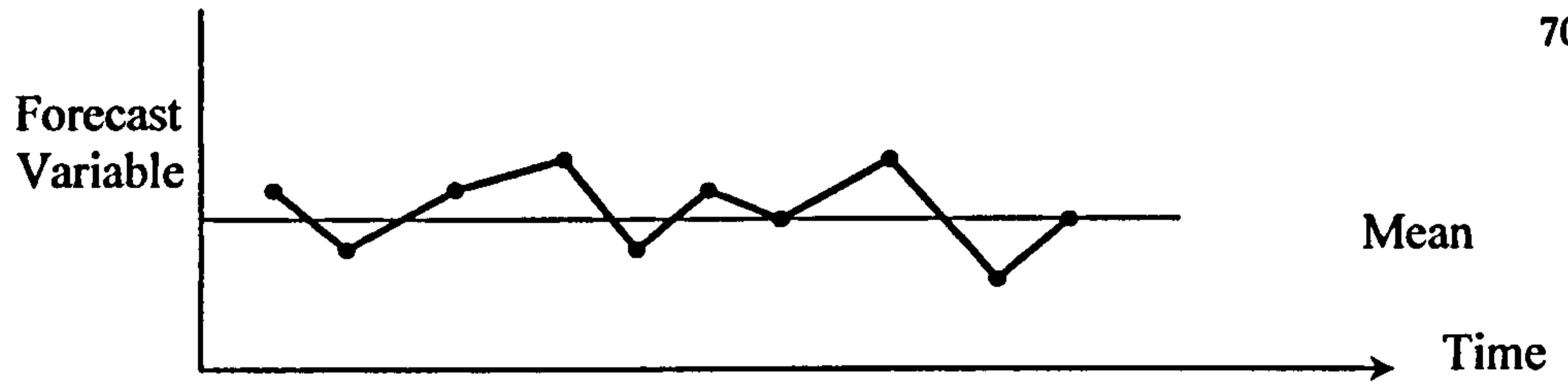
There are four types of patterns usually seen in data series in relation to forecasting: horizontal, seasonal, cyclical, and trend. A horizontal pattern exists when there is no trend in the data. When such a pattern exists, the series generally is referred to as stationary, that is, it does not tend to increase or decrease over time in any systematic way. Thus, it is just as likely that the next value of the series will be above the mean value as it is that it will be below it. Figure 4.4-a, shows a typical horizontal pattern for a variable. The kind of situations that generally exhibit a horizontal pattern would include products with stable sales or the demand of a chemical over fairly short time periods. The element of time is generally an important one in considering horizontal patterns, since in the short run, even patterns that may exhibit a defined trend over several years might be assumed to be horizontal patterns for short-term forecasting.

A seasonal pattern exists when a series fluctuates according to some seasonal factor. The season may be the month or the four seasons of the year, but they could also be the hours of the day, the days of the week, or the days in a month. Seasonal patterns exist for a number of different reasons, varying from the way in which an industry has chosen to handle certain operations (internally caused seasons) to external factors such as the weather. Figure 4.4-b illustrates a pattern in which the seasons correspond to the four calendar quarters of spring, summer, autumn, and winter.

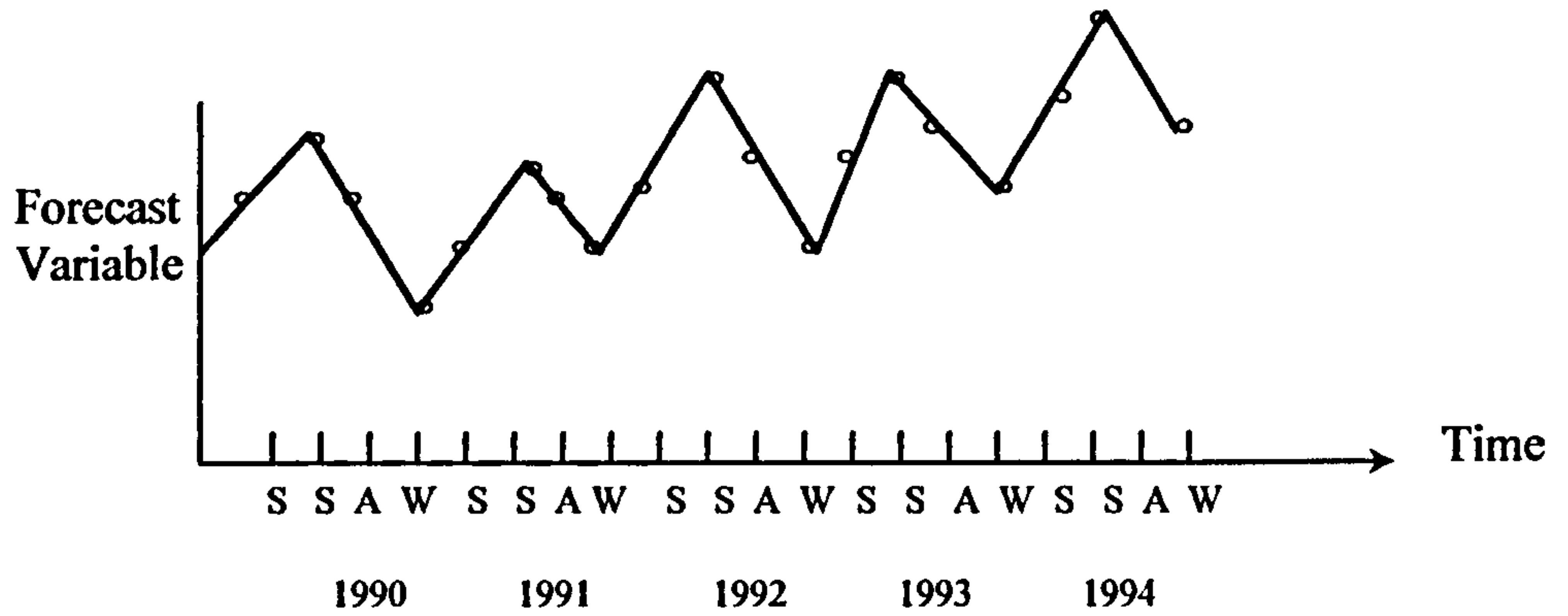
A cyclical pattern is similar to a seasonal pattern, but the length of a single cycle is generally longer than one year. Many series in the industry follow this pattern as discussed previously. Figure 4.4-c illustrates a cyclical pattern. The cyclical pattern is a difficult one to predict, because it does not repeat itself at constant intervals of time, and its duration is not uniform. The duration is usually approximately known from long-range data.

A trend pattern exists when there is a general increase or decrease in the value of the variable over time. The demand of many products that are related to the population, for example construction material and fuel, follow a trend pattern like that shown in Figure 4.4-d in their movements over time.

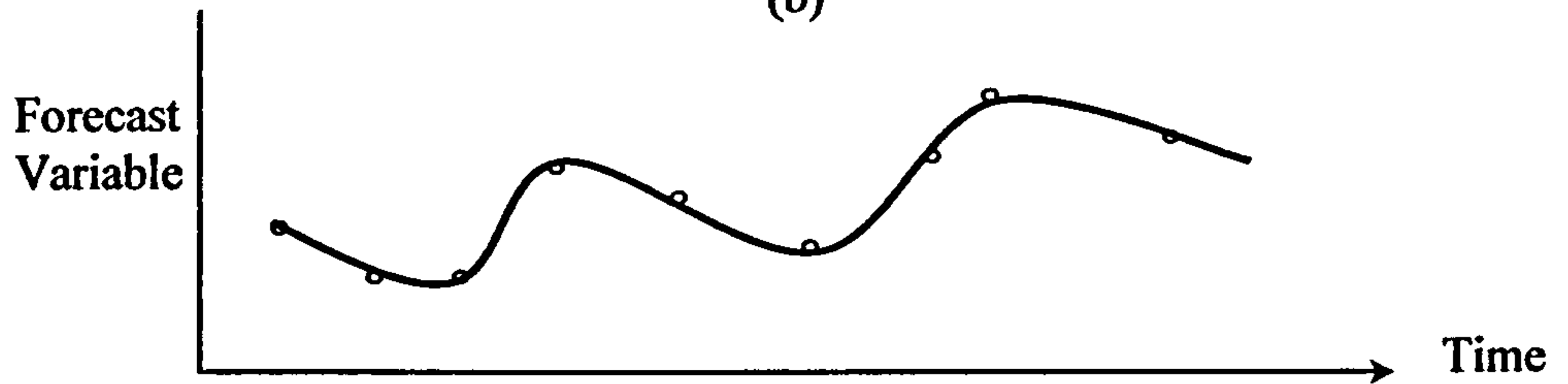
Although a number of other patterns can be found in specific series of data, the four previously discussed are the most important. They often can be found together or individually. In fact, some series actually combine a trend, a seasonal pattern, and a cyclical pattern in addition to the horizontal level, which is a part of all series.



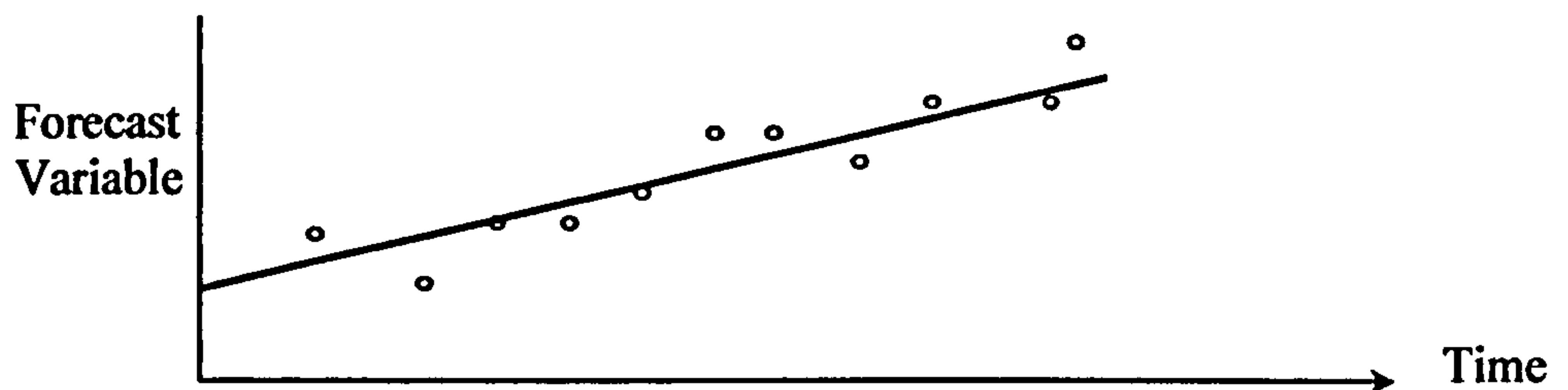
(a)



(b)



(c)



(d)

Figure 4.4: Patterns in Time-Series Data, (a) Horizontal, (b) Seasonal, (c) Cyclical, (d) Trend

4.4 Economical Analysis and Forecast for Oil and Chemical Prices

A price forecast for the final product chemicals is proposed for the development of the Kuwait petrochemical industry. It will be performed using the forecasting tools presented in Section 4.3. Also the oil price will be forecasted for use in causal forecast models. The final products are:

- Acrylonitrile Butadiene Styrene (ABS)
- Cumene
- Polystyrene, crystal grade (PS)
- Polyvinyl chloride (PVC)
- Vinyl acetate monomer (VAM)

Data needed for the prices of chemicals were taken mainly from the Stanford Research Institute (SRI) reports and the Chemical Market Reporter journal and they will be presented in \$/kg. Oil prices needed for the causal model were taken mainly from Jenkins (1989) and Platts Oilgram Price Report (2002). Prices of 1871-1899 were based on the prices of Pennsylvania crude; 1900-1944 were based on the prices of U.S average crude and 1945 and after were based on Arabian light crude. Oil prices will be presented in the industry and widely used units for oil prices, \$/bbl, however the SI units of \$/m³ will be quoted. Figure 4.5 shows the variations in oil prices since 1871, with the figure divided into two parts due to the high price-range difference. It is clear that long and short-range cycles characterize the price. Inspection of Figure 4.5 and price data of oil suggests a pattern of waves of period 55 years indicating a possible K-wave in oil prices. Peaks (tops) of these cycles occur in 1871, 1921 and 1980. Extrapolation of Figure 4.5 would indicate that the next low price should register near 2007.

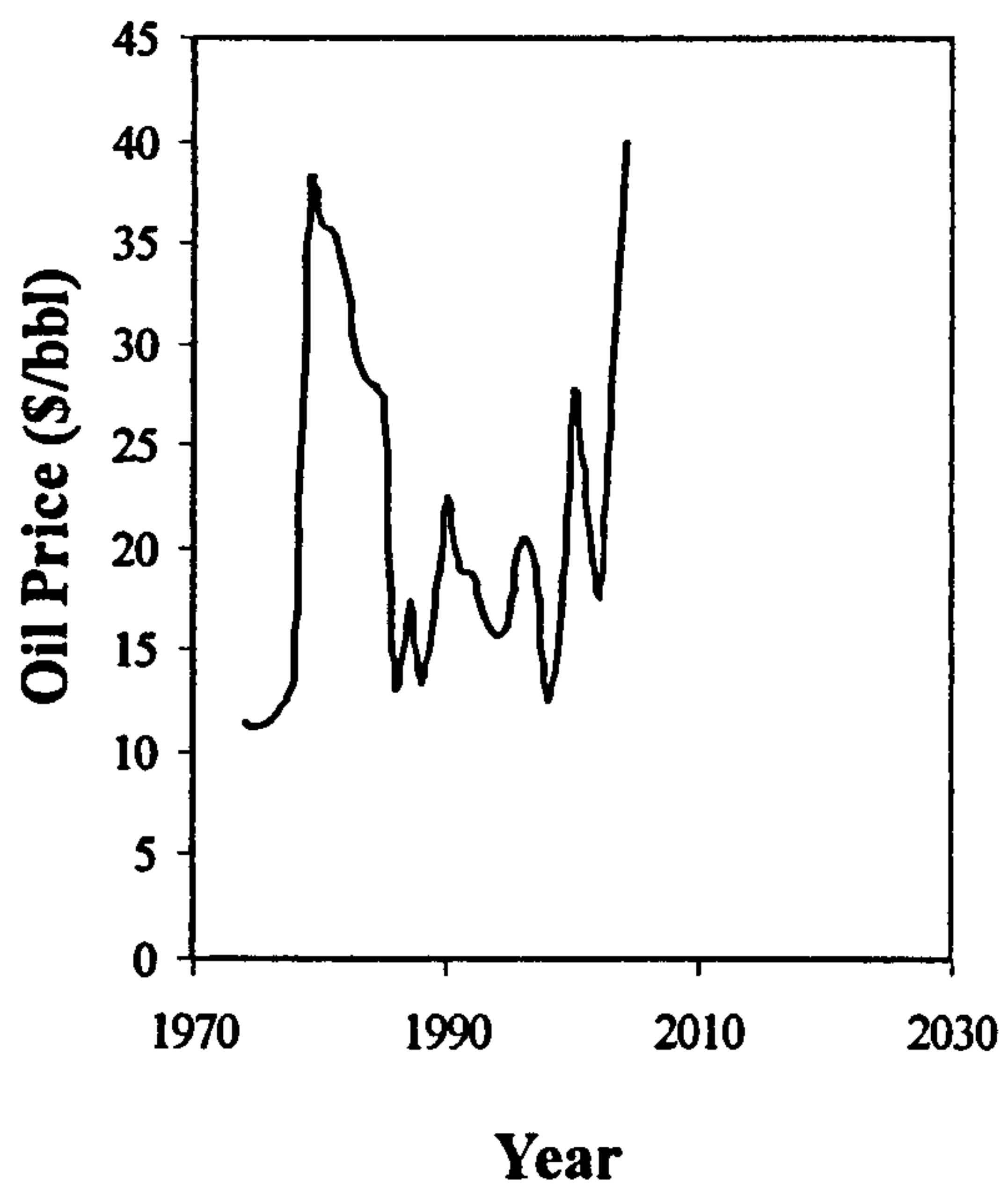
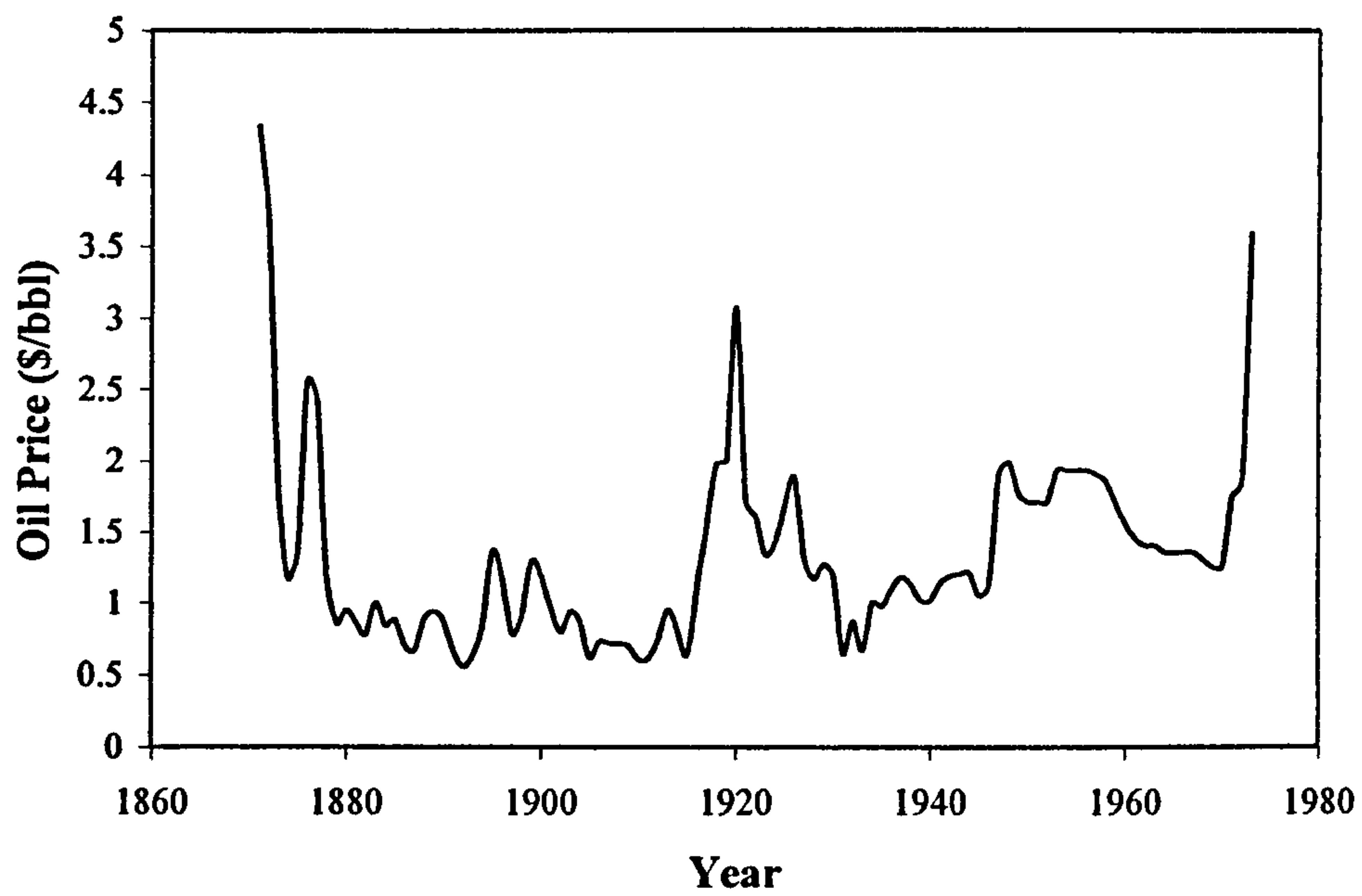


Figure 4.5: Historical Data of Oil Prices

Without doubt, economic factors and political events play an important role in the change of crude oil prices. However, it is believed that economic factors have the upper hand in determining long-term trends in oil prices, while political events related to the stability of the region take the lead in the short run. Indeed, a study of economic factors alone, without an attempt to understand the complexity of political events, is insufficient to explain and predict oil price trends in both the short and long terms. Some of the political events that affected oil price were (Bell Globemedia 2004 and Roubini and Setser 2004):

- **1876 Russian oil export starts:**

The first oil well was drilled in Russia in 1864. By 1876, commercial oil production began in Russia, followed shortly by oil export.

- **1920 Fears of U.S. shortage:**

U.S. Geological Survey (USGS) chief geologist David White estimated that the total oil remaining in the United States was 6.7 billion barrels promoting fears over dwindling U.S. oil supplies. At the same time, Russia's oil fields were nationalized.

- **1945 Post-war reconstruction:**

Following the Second World War, demand for oil increased in the United States but the price shock was offset as more foreign supplies of petroleum became available. As a result, post war prices remained low.

- **1956 Suez Crisis:**

Egyptian president, Gamal Abdul Nasser, nationalized the Suez Canal to fund the Aswan High Dam, interrupting the transportation of valuable crude oil through the canal.

- **1974 Arab Oil Embargo:**

On Oct. 6, 1973, the Egyptian forces attacked Israel as Syrian troops attacked the Golan Heights. Israel counter attacked and, with help from U.S., succeeded in reversing Arab

gains. A cease fire was negotiated by November. Arab oil exporting nations retaliated by imposing an oil embargo on the United States, and increased the price by 70 percent for countries who supported Israel. By the end of 1974, the crude price of oil had quadrupled.

- 1980 Iran/Iraq war:

The war reduced Iraq's crude oil production by 2.7 million barrels per day and Iran's production fell by 0.6 million barrels per day.

- 1986 Saudi netback Pricing :

In early 1986, Saudi Arabia discontinued selling its oil at official prices and switched to a market-based pricing system called netback pricing, which guaranteed purchases at set refining margin. As a result, Saudi Arabia regained control of a significant market share from OPEC and crude oil prices fell.

- 1990 Iraqi Invasion of Kuwait:

During the Iraqi occupation, Kuwait's oil-producing capacity was reduced to practically nothing. To make matters worse, Iraqi occupation forces set fire to or damaged 737 of Kuwait's oil wells as they retreated. It was not until 1993 that oil exports surpassed their pre-invasion levels.

- 1998 Asian Economic Crisis:

The rapid growth of Asian economics came to an end in 1998, resulting in the decline of Asian Pacific oil consumption for the first time since 1982. This decline combined with increased OPEC production levels, caused crude oil prices to fall.

- 2004 Asia and Middle East Situations:

The current high oil prices reflect both booming Asia demand (China alone is expected to account for roughly 40% of the increase in demand for oil in 2004) and geopolitical risk in the Middle East.

Some Comments on Current Oil Prices

In 2004, crude oil prices averaged 40 \$/bbl (252 \$/m³) with prices turning upwards throughout the year and well into 2005, reaching more than 50 \$/bbl (314 \$/m³). This price increase is different from predictions of long-term cycles in Figure 4.5, which predicts a bottom in year 2007. Several factors have contributed to this increase in crude oil prices in the near term, some of which are presented below:

1. Hurricane Katrina and, to much less extent, Hurricane Rita, have disrupted U.S. Gulf oil production and refinery operations in an environment of tight international supplies.
2. The geopolitical tension in major oil-producing countries including the continuing war in Iraq and the uncertain prospects for a return to normality in Iraq's oil sector. The potential unrest in Nigeria and Venezuela has also contributed to the volatility in the world oil market. This effect is commonly termed "War Premium" and it appeared previously during World War II as a recognizable peak in the K-wave. It is an artefact of war and is not considered a genuine result of long-wave behaviour (Kiel and Elliott 1999).
3. The volatility in the oil price would be less apparent if the oil prices were presented in a commodity based currency rather than the U.S. dollar. Such currencies have value being explained reasonably well by movements in commodity prices because they are currencies of countries that have a large share of primary commodities in their production and exports. Most important of these currencies are the Australian dollar, the Canadian dollar and the New Zealand dollar. The rise in the price of energy caused the Canadian dollar to depreciate relative to the U.S. dollar (Laidler and Aba 2001). Consequently, presenting oil prices in a commodity based currency would help to absorb the shock that different world events impart to the oil price when presented by U.S. dollars. However, presenting oil prices in U.S. dollars is more common and, hence, better understood in the industry. This was the main reason for selecting U.S. dollars as the currency in which to present prices in this thesis.

4. One source of uncertainty in the long wave is actions of governments. In all previous long wave downturns, the action of governments was a much small sector (Sterman 1990); now governments have expanded to control a considerable part of the economy. The actions of governments that were directed to create and/or prolong expansions in the economy have worsened many imbalances of the long wave (Sterman 1990). The use of governments policies to direct economic activity results in outcomes which many people find detrimental (Cleveland 2002). Although, actions of governments are inevitably required to prevent market crashes and company bankruptcies, they can cause high volatility in prices. Currently, oil prices are affected, to a large extent, by the actions of governments, causing an unusual price peak. The case of regulatory control by governments over crude oil prices during the 1970s provides an excellent example of how such activities disrupt the market. By attempting to soften the initial rise in oil prices caused by the Arab oil embargo, regulators actually compounded the problem (Cleveland 2002).

5. Stagnation of planning oil price; major oil companies plan their projects with a low oil price around half the current oil prices. This is caused by their disbelief in the ability of oil prices to remain high. Therefore, explorations of new oil fields or new oil sources could not be economically justified. This planning price increased only in Dec. 2004. This factor, along with the maturity of major oil fields, caused a low supply of oil.

6. World petroleum demand has grown at a robust rate in recent years, reflecting the continued increase in consumption in the U.S. and the dramatic increase in the requirements of the emerging Asian nations mainly China and India. However, this factor will not be given a high weight as a reason for this unusual increase in oil price because it is a factor that should always be expected for the whole growing world economy. It comes in the form of continually upward progressing price cycles

Incorporating the recent dramatic increase in oil price into the construction of a long-range oil price outlook is difficult and raises the following question: will oil prices decrease? The uncertainties associated with answering this question are significant if the above causes of the increases in oil price stay affecting the oil industry. It is not expected that the price will return, as before, because the K-wave cycle, that exists in the oil price will probably grow with the growing world economy.

It is well recognized that tension in the oil producing countries could give rise to serious disruption in oil production and trading patterns. On the other hand, market forces can play a significant role in restoring balance over an extended period. Expectations are that demand will remain strong as a result of population growth and human ingenuity while supply will remain low with the perceived scarcity of the oil resources. With time, high oil prices may deter consumption and encourage the emergence of significant competition from large marginal sources of oil, which currently are uneconomical to produce, and other sources of energy.

4.4.1 Chemical Price Forecast Based on Historical Data

Preparing a price forecast must be done for later use in a petrochemical model. Historical chemical price data were collected from the *Chemical Market Reporter* and a simple time-series forecast is applied; this model is basically a function with time that best fits the chemical price data. The first time-series forecast used was a simple third order polynomial of price with time. However, its results were very poor since it indicated some negative prices or very high prices when used in the forecast; this is shown in Figures 4.7-b to 4.11-b. The second time-series forecast used Fourier analysis and is applied with only one frequency together with a trend term. This form is suggested from the nature of the chemical prices collected. The results of the Fourier time-series are presented below as chemicals prices for the year t after 1978:

$$\begin{aligned} \text{ABS } (\$/\text{kg}) &= -3.4 \times 10^{-4} t + 32.984 \times 10^{-2} \cos(5.857 t) \\ &\quad + 15.047 \times 10^{-2} \sin(5.857 t) + 2.578 \end{aligned} \quad (4.2-a)$$

$$\begin{aligned} \text{Cumene } (\$/\text{kg}) &= 0.5 \times 10^{-4} t + 4.324 \times 10^{-2} \cos(5.500 t) \\ &\quad + 4.872 \times 10^{-2} \sin(5.500 t) + 0.377 \end{aligned} \quad (4.2-b)$$

$$\begin{aligned} \text{PS } (\$/\text{kg}) &= 0.2 \times 10^{-4} t + 7.561 \times 10^{-2} \cos(5.782 t) \\ &\quad + 13.854 \times 10^{-2} \sin(5.782 t) + 0.979 \end{aligned} \quad (4.2-c)$$

$$\begin{aligned} \text{PVC } (\$/\text{kg}) &= 2.7 \times 10^{-4} t - 12.061 \times 10^{-2} \cos(5.533 t) \\ &\quad - 0.273 \times 10^{-2} \sin(5.533 t) + 0.179 \end{aligned} \quad (4.2-d)$$

$$\begin{aligned} \text{VAM } (\$/\text{kg}) &= 3.8 \times 10^{-4} t - 13.465 \times 10^{-2} \cos(6.011 t) \\ &\quad - 12.387 \times 10^{-2} \sin(6.011 t) + 0.139 \end{aligned} \quad (4.2-e)$$

The above equations can be directly used to forecast chemical prices for the planning horizon.

4.4.2 Chemical Price Forecast Based on Oil Price Forecast

For the causal model, a forecast of chemical prices (dependent variable) is done using oil price (independent variable). First the oil price is forecasted using Fourier time-series analysis but with two frequencies in order to capture short and long cycles noticed in oil prices. The analysis result is given in Equation 4.3 below, which can be used to calculate theoretical oil prices for the year t after 1978:

$$\begin{aligned} \text{oil price } (\$/\text{bbl}) &= 0.0136 t + 9.4163 \cos(6.2 t) - 2.1974 \sin(6.2 t) \\ &\quad + 1.921 \cos(8.5372 t) - 0.7131 \sin(8.5372 t) \end{aligned} \quad (4.3)$$

A plot of actual and theoretical oil prices is given in Figure 4.6. The figure clearly shows the cyclic nature of the data. Figure 4.6 also shows the prediction of the oil price until 2030. For the petrochemical industry, the long-range horizon is considered as the time for building then running the plant through its expected life. This time is about 25 years. Therefore, all forecasts were done to the year 2030. These oil price predictions, based on Equation 4.3, suggest the next bottom in the oil price to be in the year 2006 at a

price of 16.88 \$/bbl (106.17 \$/m³). This is consistent with the predictions for Kuwait Export Crude (Kuwait Petroleum Corporation 2002) and Dubai crude (Cambridge Energy Research Association 2000); the bottom was at 2006 and at 17.2 \$/bbl (108.19 \$/m³) and 17.5 \$/bbl (110.07 \$/m³) respectively. However, this bottom is slightly earlier than the predictions of some analysts for the K-wave's next bottom. Notley (2002) and Barker (1995) modelled interest rates and have predicted the next bottom at 2010 and 2009 respectively. This indicated that interest rates are affected by oil prices and follow the same trends. It also indicates that oil prices lead interest rate in the long wave sense by 3 to 4 years, which is logical with the role of oil as a driver of inflation. Another prediction for oil price was 21 \$/bbl (132.09 \$/m³) by the year 2015 (Sedriks 1999), this value is close to 23.0 \$/bbl (144.67 \$/m³) that can be forecasted using Equation 4.3.

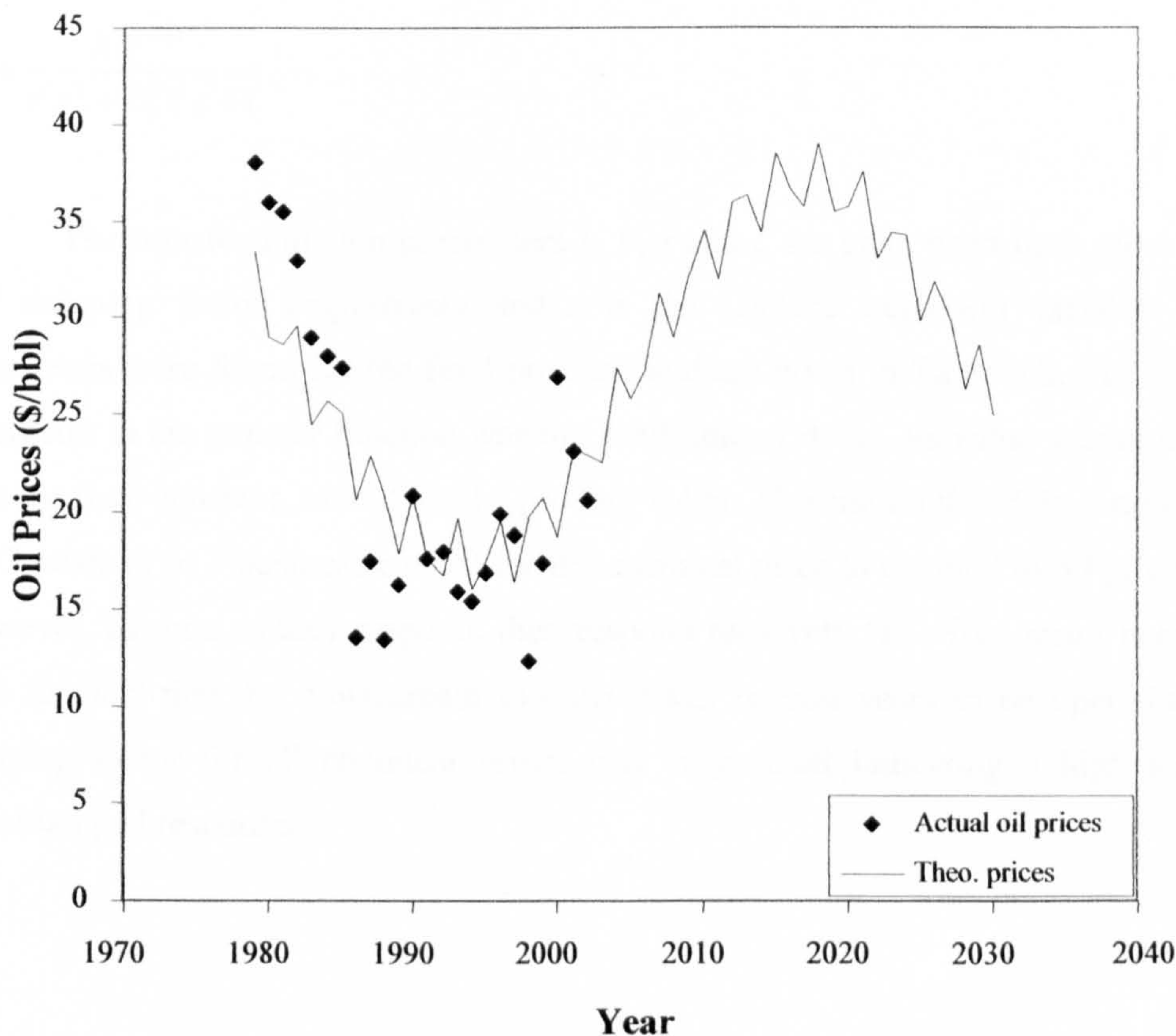


Figure 4.6: Actual and Theoretical Oil Prices

The current behaviour of oil prices may be quite different from that portrayed in the model projection due to factors explained previously in Section 4.4. It is strongly believed that oil prices will, eventually, decrease, if not soon then after reaching the peak of this current K-wave.

The second stage in causal forecasting is to find the causal model between the oil price and the chemical price.

4.4.2.1 Transfer Function Causal Model

The first causal model is represented by a transfer function relating the change in oil price as an input and the change in chemical price as an output. The transfer function G is found in the form of a Second Order Plus Dead Time SOPDT:

$$G = \frac{k e^{-\theta s}}{\tau^2 s^2 + 2\zeta\tau s + 1}$$

The transfer function parameters k , θ , τ and ζ are gain, dead time, time constant and damping factor respectively and s is the Laplace transform variable. Suitable parameters were found for the final products and are given in Table 4.2. The significant parameter in the transfer function was the dead time or delay. Its value was much higher than the time constant, except for the product VAM. This means that delays range from 4 to 13 years (1 to 3 business cycles) for the chemical price to respond to oil price change. However, as soon as they respond, they respond relatively fast. This result is consistent with the fact that the downstream industry takes several years to be operational. The damping factor for all chemical prices was very small indicating a high oscillatory underdamped response.

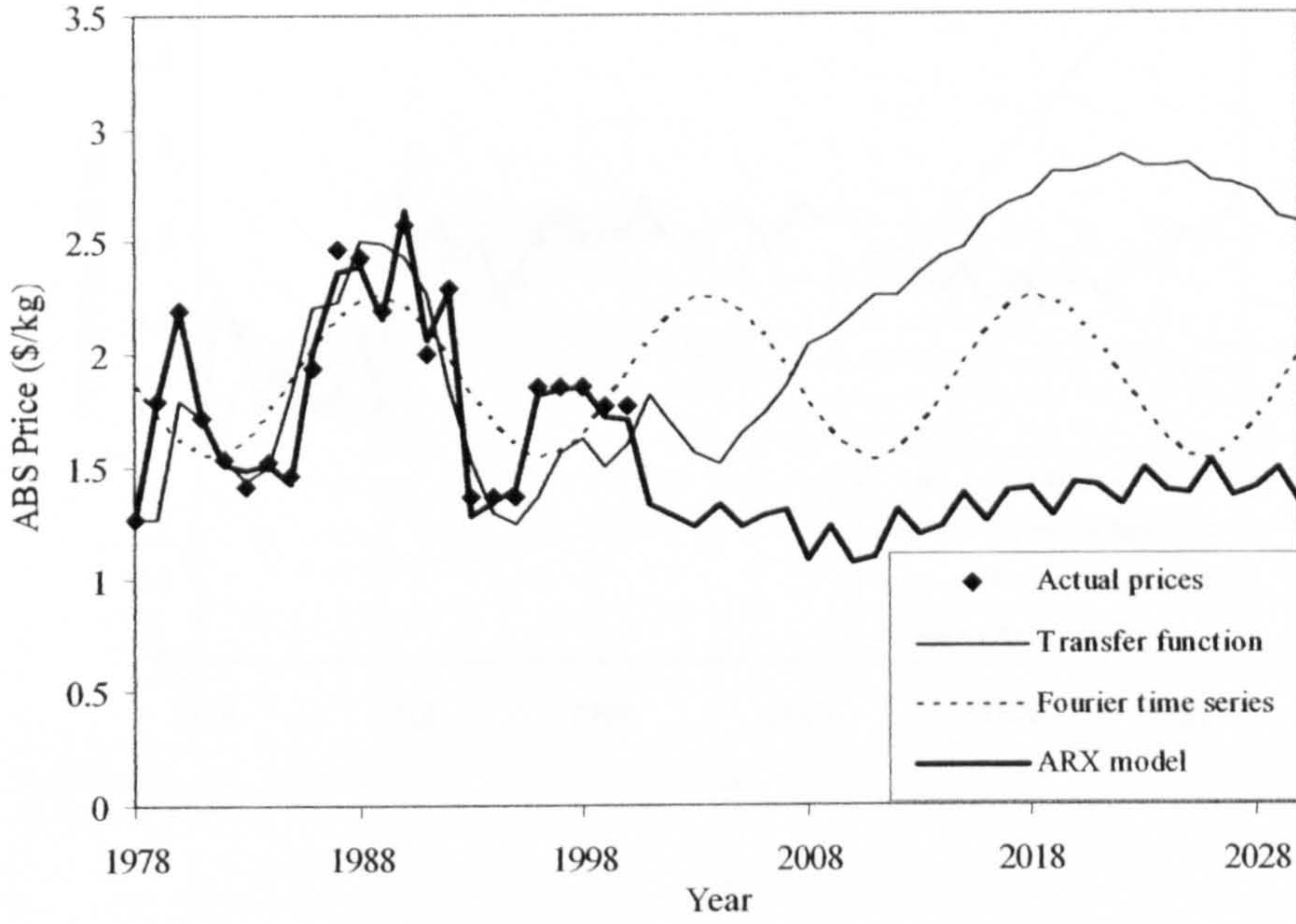
Table 4.2: SOPDT Transfer Function Parameters Relating Chemical Prices to Oil Prices.

	Gain k (\$/kg)/(\$/bbl)	Time constant τ (year)	Damping factor ζ	Dead Time θ (year)
ABS	6.9801e-2	0.1760	0.0316	5.8408
Cumene	2.4313e-2	0.0831	0.0193	4.0313
PS (C.G.)	3.5699e-2	0.0830	0.0177	6.7276
PVC	1.6729e-2	0.1498	0.0450	13.3748
VAM	4.6014e-2	0.1559	0.0064	0.0894

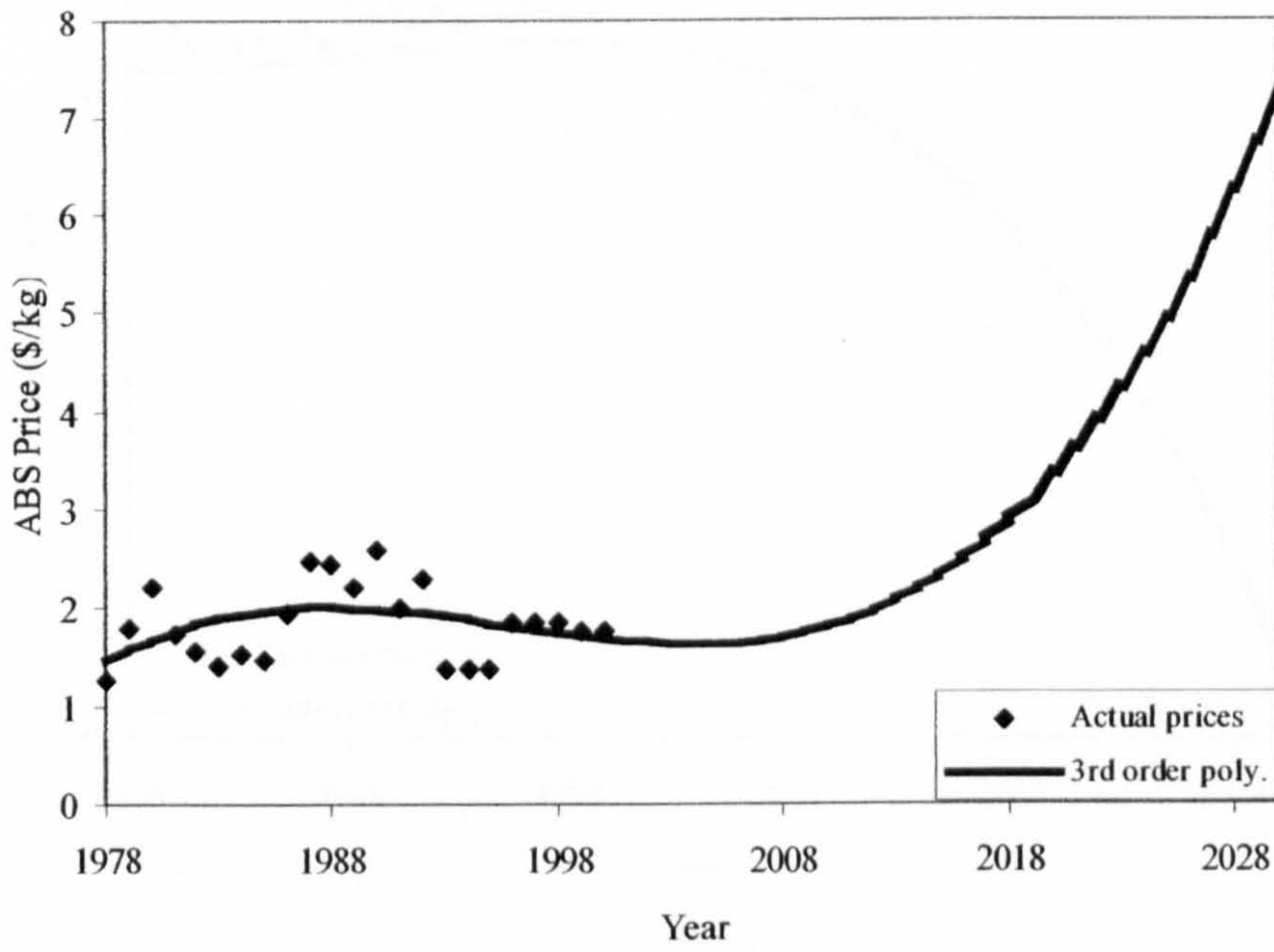
4.4.2.2 ARX Causal Model

An alternative to the transfer function model is the ARX model represented by Equation 4.1. ARX models for the chemical prices were found to be best in the order of 6 for na and nb and 2 for the delay nk . This was concluded after many trials of model order.

The third stage of causal forecasting is to use the forecasted oil price and the casual models, SOPDT and ARX, to forecast the products prices. All forecasting results for chemicals prices are presented in Figures 4.7 to 4.11. The forecast with third order polynomial (time-series forecast) is plotted in a separate graph because it has forecasted prices with a significant difference from the other forecasts.

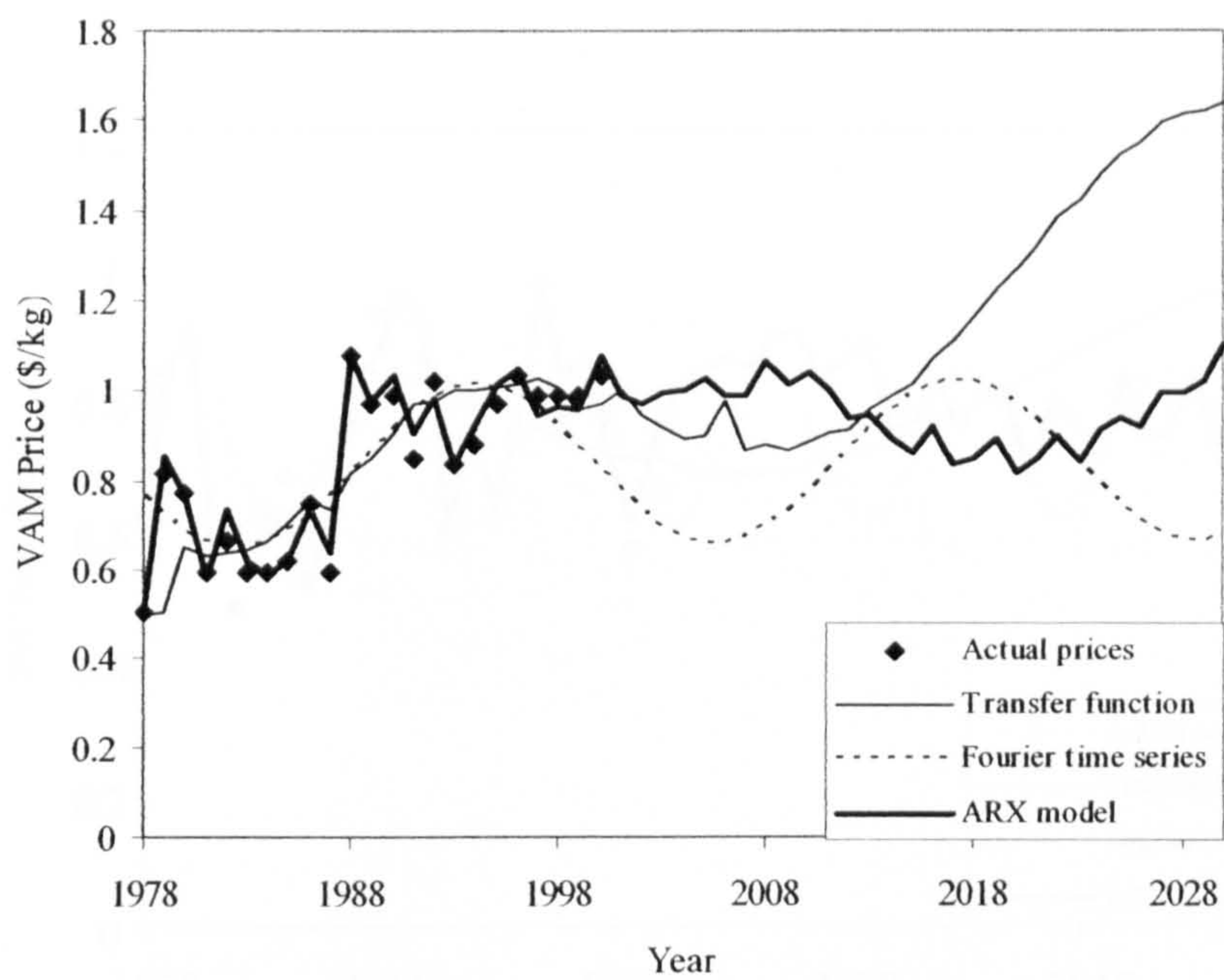


(a)

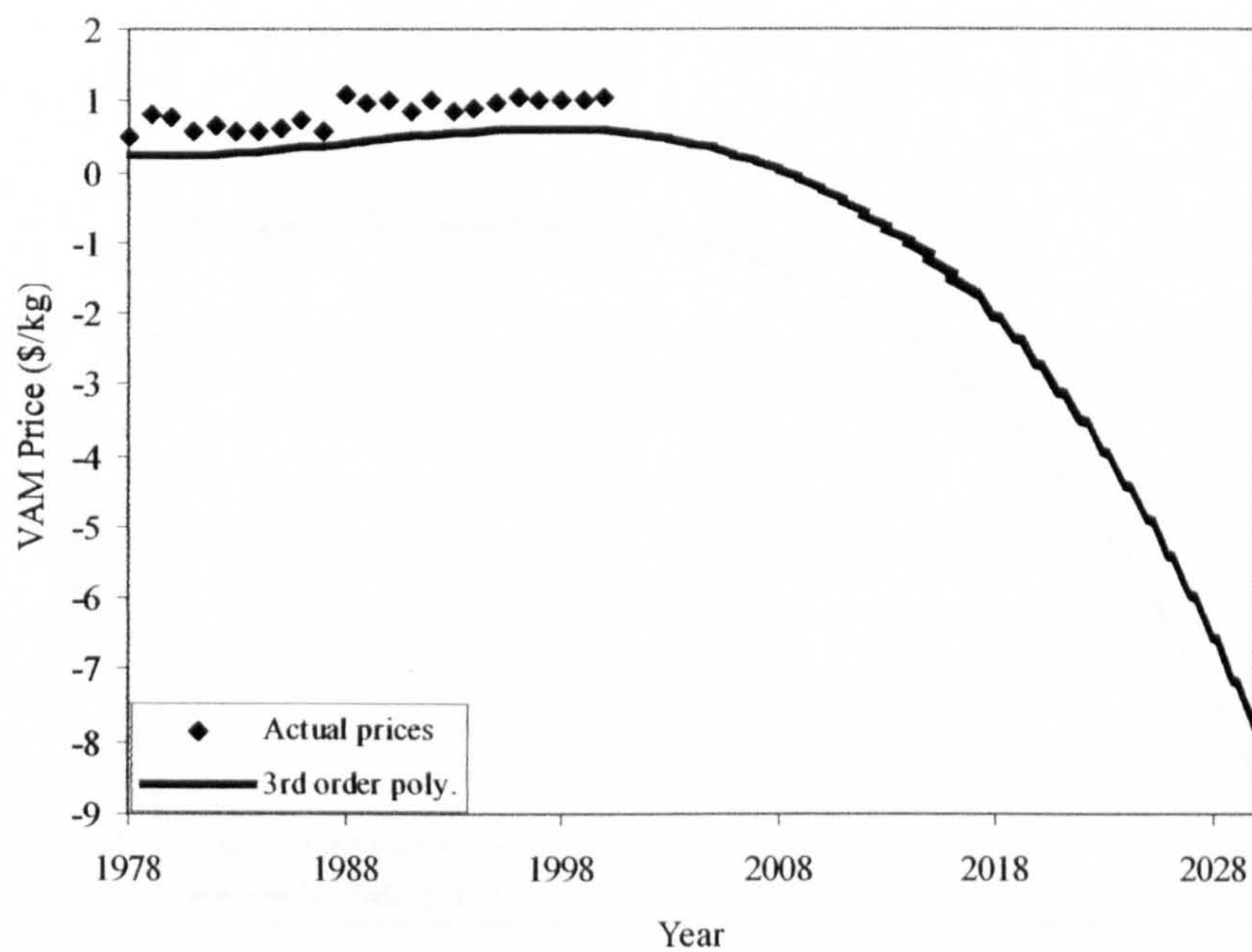


(b)

Figure 4.7: ABS Actual and Forecasted Prices

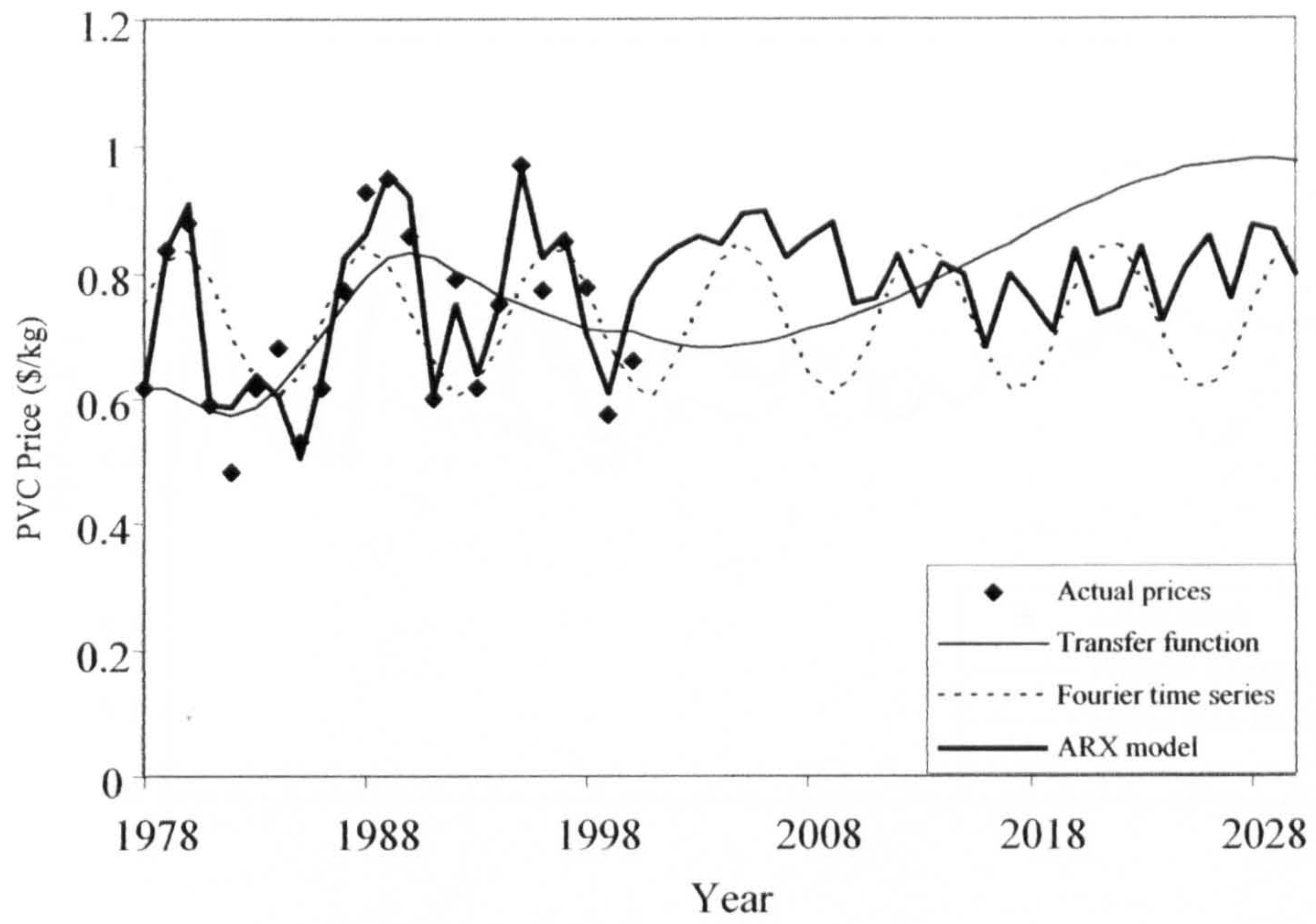


(a)

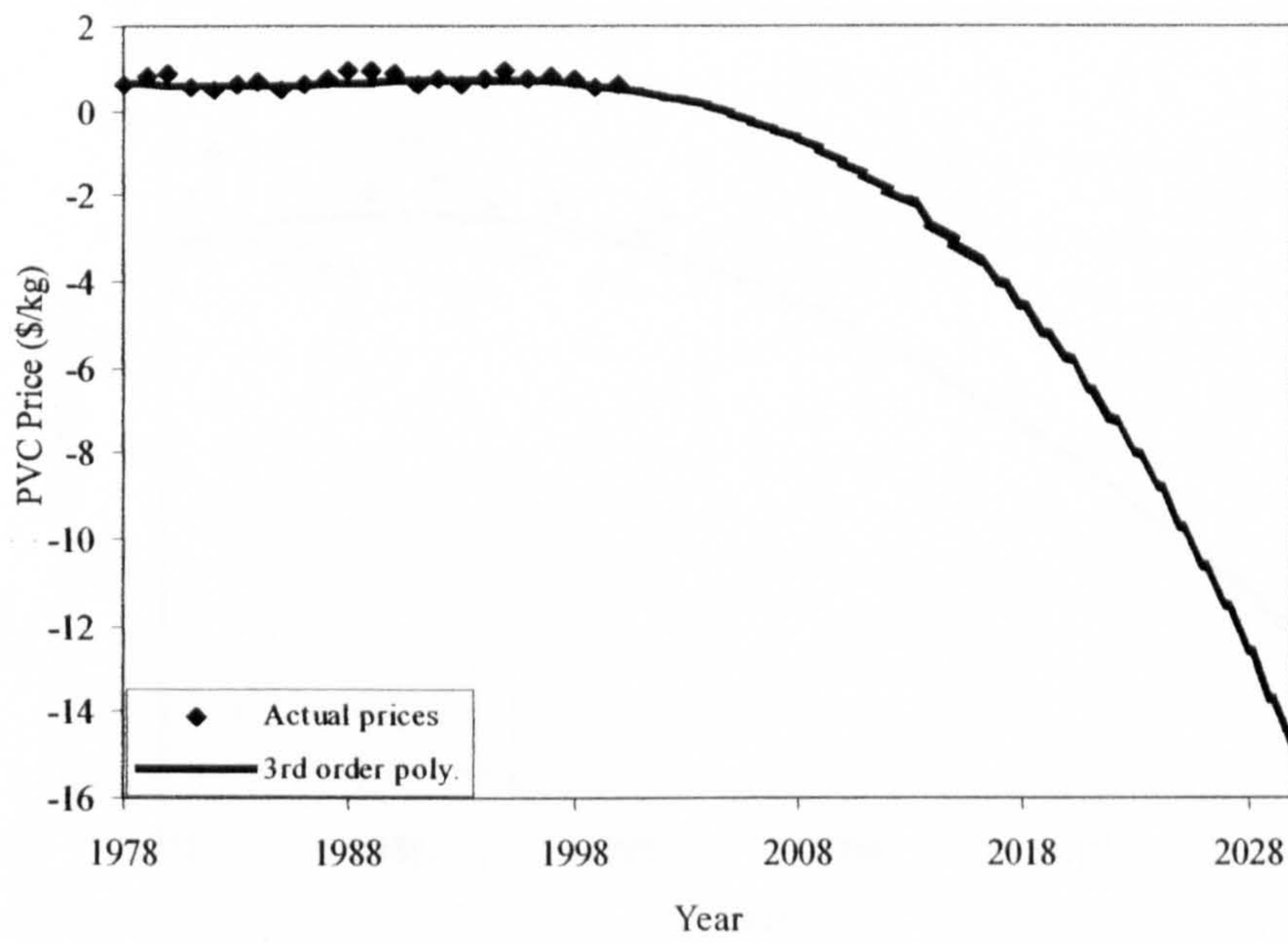


(b)

Figure 4.8: VAM Actual and Forecasted Prices

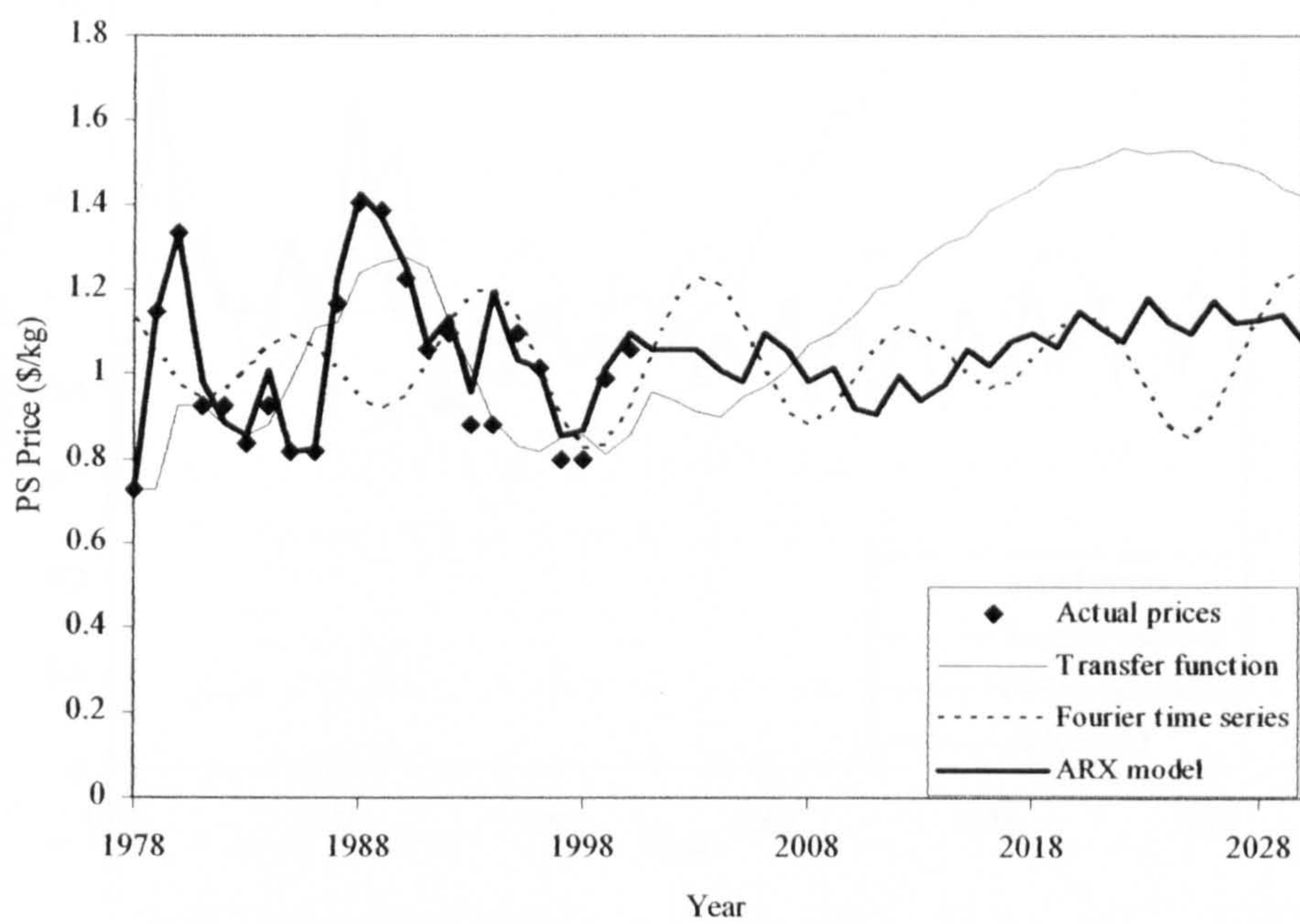


(a)

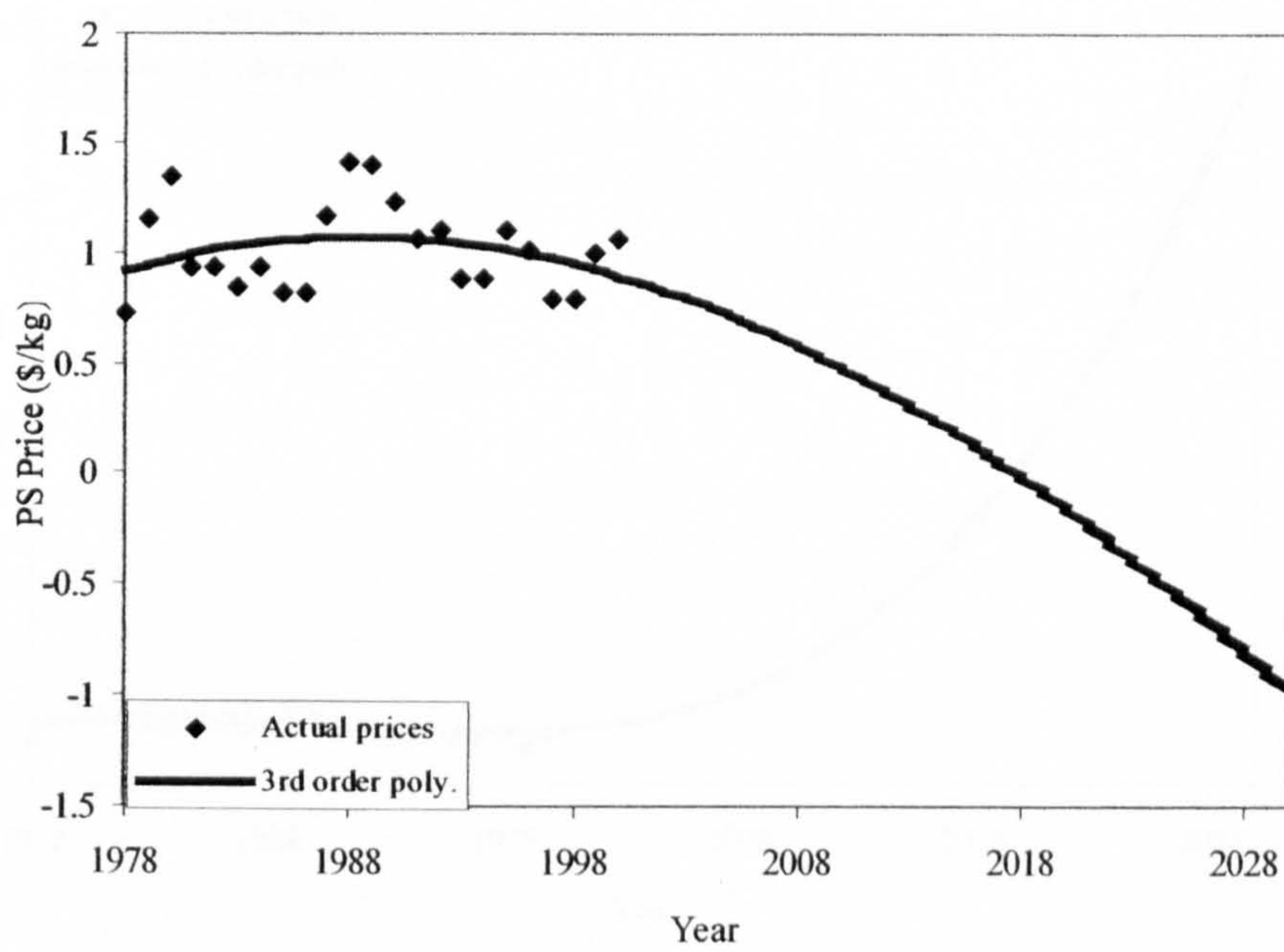


(b)

Figure 4.9: PVC Actual and Forecasted Prices

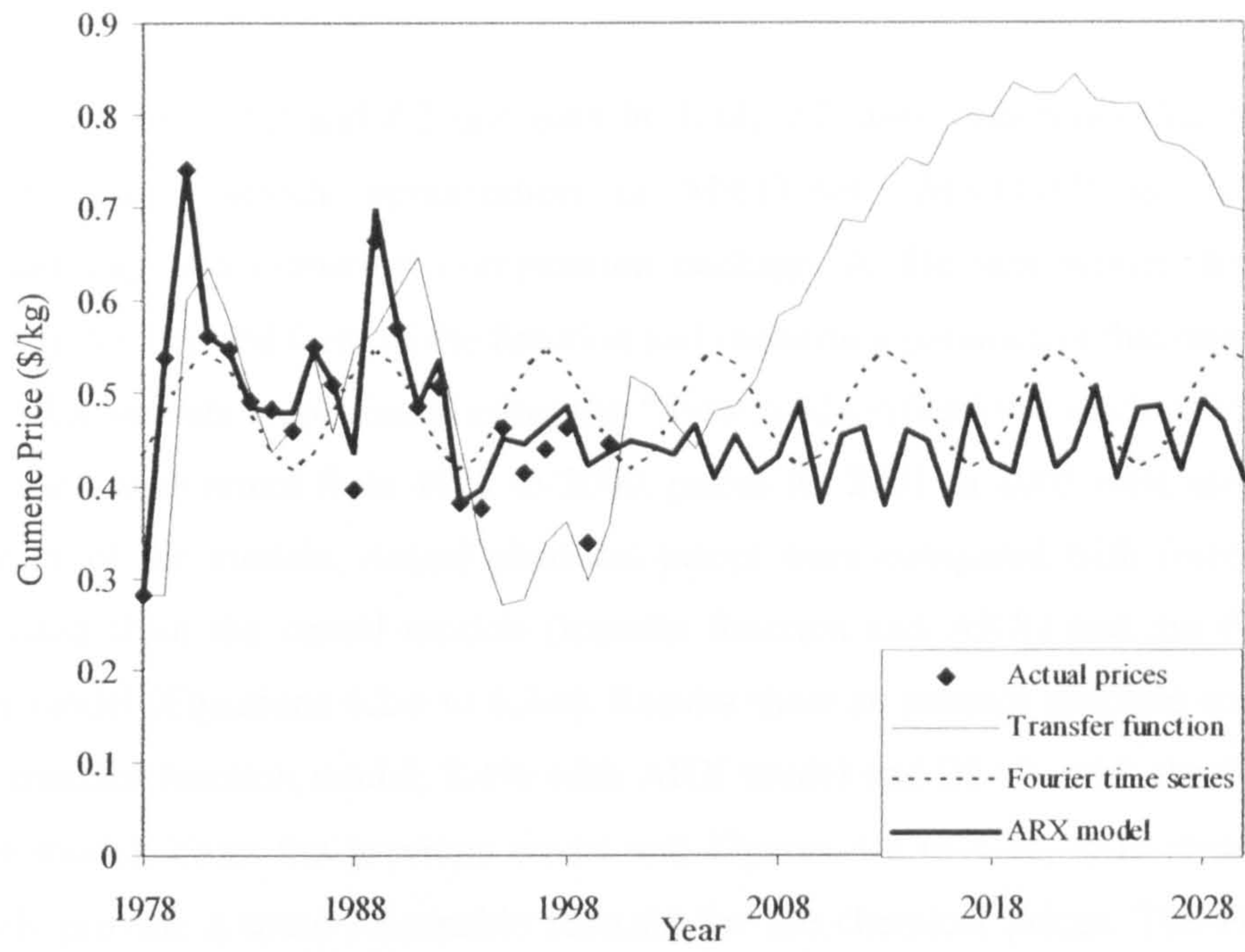


(a)

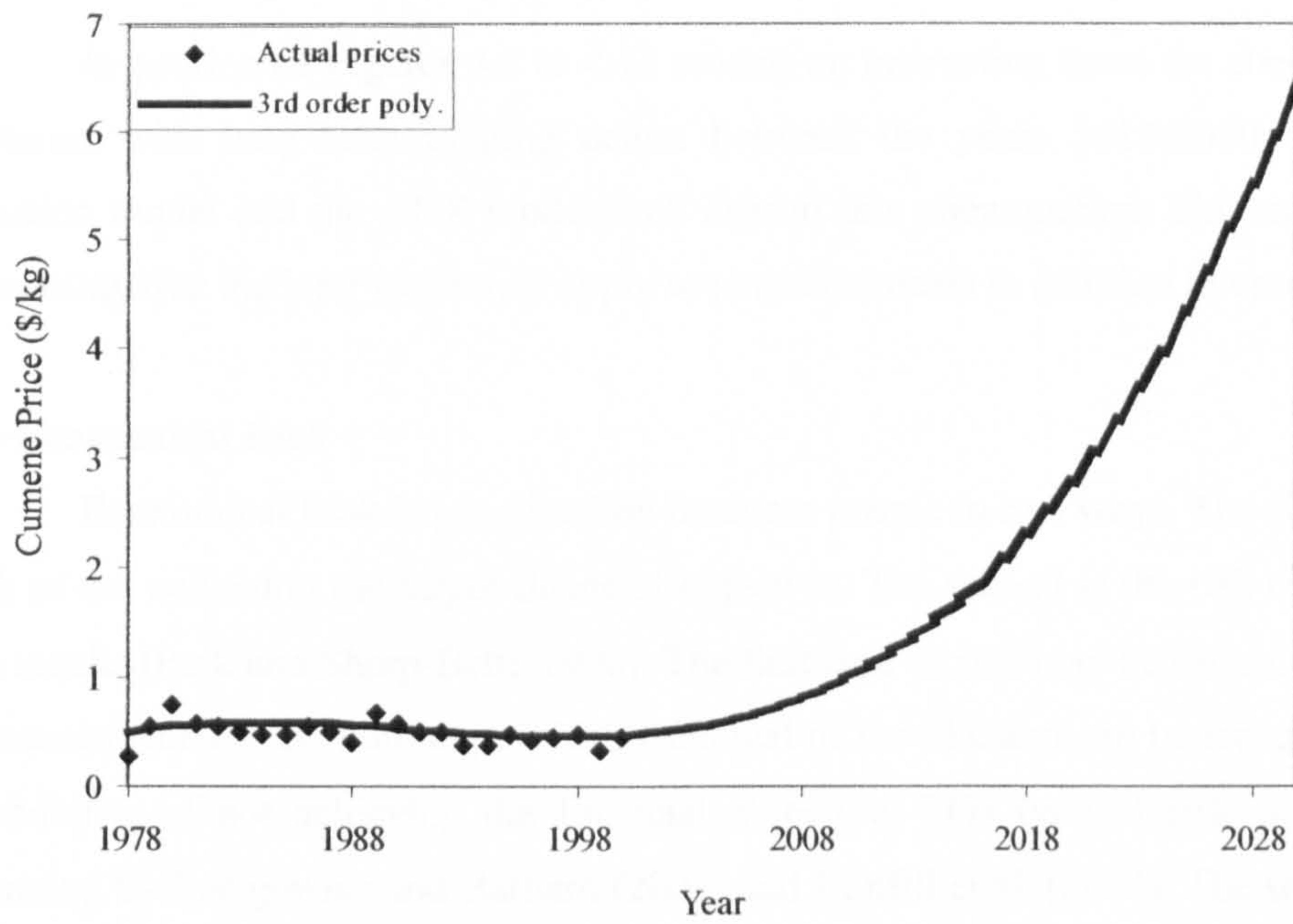


(b)

Figure 4.10: PS Actual and Forecasted Prices



(a)



(b)

Figure 4.11: Cumene Actual and Forecasted Prices.

Equations 4.2 and 4.3 and data in Table 4.2 were obtained using Nelder-Mead simplex direct search optimization in MATLAB. MATLAB is an interactive programming and numerical computation package. A file was written for MATLAB defining the required form of the function and requesting parameters that best fit the data. The ARX models were found using the "System Identification" toolbox in MATLAB. Data used were prices from 1978 to 2000, prices for 2001 to 2005 were used to test the accuracy of the models. Actual chemical prices were compared with forecasted prices calculated from the causal models (transfer function and ARX) and the Fourier time-series model (Equations 4.2-a to 4.2-e). Results show an average absolute error of 14.6% with transfer function model, 8.4% with ARX model and 30.0% with the Fourier time-series model. From the previous errors and Figures 4.7 to 4.11, it is clear that causal models provide a more reasonable forecast for the chemical prices. The Fourier time-series model gives pure cyclic behaviour with no trend and the simple polynomial fit gives an unrealistic forecast.

Inspection of Figures 4.7 to 4.11 reveals an interesting trend for chemicals prices patterns, with long term topping action between the years 2018-2030. The transfer function model and the ARX model both exhibit this phenomenon. This may imply the possibility that the long wave may apply to petrochemicals in addition to commodities.

4.5 Economical Risk

Economical Risk is perceived by business people in two ways. The first one is the risk of not achieving the target financial objective. The second is the risk of variation in the results (Park and Sharp-Bette 1990). The first type of risk may be caused by a number of causes whether economic, political, technical or the like and can be represented as the probability of not achieving the financial objective. This type of risk was used with planning by Bagajewicz and Barbaro (2003) and Bonfill et al. (2004). The second type of risk can be well handled by variance techniques such as the variance of Expected Monetary Value (EMV) (Bush and Johnson 1998), or risk adjusted return family of methods like Sharpe ratio (Jones 1998). Applequist et al. (2000) used a risk premium,

defined as the increase in expected return in exchange for a given amount of variance, to evaluate risk and uncertainty for chemical manufacturing plants.

The economical risk problem can be addressed from another angle, using historical accounts. The lack of appreciation of the long wave may result in a lot of disruption in the administration of project plans and strategic plans. Even the better understood and accepted cyclic phenomena typically cause disruptions in fund allocation and planning. It was noted by several observers that the chemical business cycles result in unfavourable investor response. During weak market periods, profits are low and investors refrain from allocating money in a new capacity. This inaction results in the demand increasing and the supply becoming stable. After a few years, shortage appears and prices rise and overshoot. Investors jump and provided money above the required demand. By the time the added capacity goes on-stream, prices go down again due to the competition. Thus the boom-bust and cyclic phenomena (Zinger 1999 and Yimoyines 1995).

Looking back to Figure 4.7, for example, this illustrates the potential risk of reacting to weak market conditions. The ARX model had the least numerical error and, if taken alone, investors may decide to abandon a plan of investing in ABS. Considering the transfer function model in the analysis would provide additional insight to the probable scenarios. In fact, recent trends suggest that prices would be stronger than what the ARX itself would have forecasted.

A paper containing the economical analysis and forecast of this chapter has been published in "*Industrial & Engineering Chemistry Research*" journal under the title "Modeling and Identification of Economic Disturbances in the Planning of Petrochemical Industry". The paper also, used the forecast with a MILP model to plan for the petrochemical industry. The paper is shown in Appendix C.

4.6 Conclusion

This chapter enhances our understanding of the nature of historical economic trends in the petrochemical industry by placing such trends within a framework of larger techno-economic cycles. Historical cycles are not completely predictable phenomena. No one would expect them to emerge with exact historical timing. However, the pattern of the long-range cycles, emerging and ending in 45 to 60 years cycles, strongly suggests underlying consistency in the dynamics of the petrochemical industry. Therefore, it is not possible for a heavy industry like the petrochemical industry to do without short- and long-range forecasting. A very simple and very general procedure for modelling disturbances in the petrochemical industry was proposed to forecast chemical prices and consequently good planning in the long-range. Modelling of disturbances was based on oil prices that clearly followed the well-known long- and short-range cycles. It was found that the oil prices follow the traditional K-wave theory with an average period of 55 years.

From the tested forecasting models, the causal models in the form of a Second Order Pulse Dead Time (SOPDT) and ARX models were shown to provide a reasonable forecast of future prices. These forecasts will be used with a petrochemical model to plan the developments in Kuwait's petrochemical industry.

Chapter 5

Safety in the Petrochemical Industry

In Chapter 4, economical planning was presented and applied to the petrochemical industry. In this chapter, safety related planning is presented in the form of a risk index. Minimizing the risk to people from plant accidents is an important objective for any industry. It is a goal, however, which is closely linked to the plant flowsheet and chemicals handled.

In this work, an objective is to incorporate safe production of petrochemicals into planning by identifying an industry structure that has minimum risk following the accidental release of chemicals.

5.1 Industrial Safety

Health, Safety and Environmental (HSE) issues are high up the agenda for all industries, but particularly for the petrochemical industry. The consumers, employees, shareholders, legislators and the communities for which the industry operates are all becoming increasingly aware of HSE issues and demand ever-higher standards. Over the last few decades, the petrochemical industry has reduced its harmful emissions significantly, by using environmental and technological developments together with an increased awareness of the safety aspects of plant operation. HSE legislation is being proposed and/or refined continuously aiming for a better living and working environment in the whole world. HSE issues are not easily resolved because of the enormity of the task and its components. However, identifying the nature of the safety problem and to which stages of planning it can be applied is an essential task.

Safety engineering has to protect the people and the environment, as far as possible, from the dangers that can arise from an industrial plant. On the other hand, the

application of safety engineering must avoid restricting production or increasing costs of these plants more than is necessary.

5.1.1 Chemical Related Safety

During the last 30 years, individual chemical plants have grown larger, often increasing 10 times in size, to take advantage of the economics of scale. A chemical plant today will typically produce 300,000 to 600,000 tonnes of products per year. Storage tanks at plants may hold as much as 50,000 m³ of product or raw material. The primary hazard in the chemical industry resides in the material, because materials are a hazard even if only in storage, with no processing or other activity being performed. The raw material, the intermediate, and the finished products present the primary independent hazard element (Ward 2002). A major factor, which has a decisive influence on the safety performance of the chemical industry, and production safety in particular, is the toxicity of the chemicals. Overlooking this increasingly important factor would be to ignore one of the major forces that shape the development of the industry. The issue of safely producing hazardous chemicals is as important as the economics of producing and selling them. Examples of hazardous substances prevailing within the petrochemical industry are:

- Gases (flammable, toxic, compressed).
- Liquids (flammable, toxic, acidic, alkaline, cryogenic).
- Solids (flammable, volatile).
- Viscous materials.
- Oxidizing, reactive and corrosive substances.

The hazardous effect of chemicals comes through three ways: fire, explosion and toxicity. The first essential step towards greater plant safety is being aware of the potentially dangerous properties of the substances, i.e. whether they are flammable, explosive or toxic.

Fire

Fire, or combustion, is a chemical reaction in which a substance combine with oxygen and heat is released (Lees 1980). To produce combustion, three conditions must coexist: flammable substance, oxygen, and a source of ignition. Determining the fire potential of a chemical substance is accomplished through its flammability characteristics; no single factor, however, defines a substance's flammability. When a flammability comparison is to be made between different substances, the following factors should be considered:

1. Flammability limits (or explosion limits)
2. Flash point
3. Autoignition temperature
4. Vapour pressure
5. Burning velocity
6. Ignition energy

The most important and widely used factors are the first three, i.e. flammability limits, flash point and autoignition temperature. Flammability limits of a gas define the concentration range of a gas-air mixture within which an ignition source can start a self-propagating reaction. Thus, a gas-air mixture below the lower explosive limit is too lean to burn, and the mixture above the upper explosive or flammable limit is too rich to burn. Within these lower and upper boundaries only, a gas or the vapour of a liquid will ignite or explode when it comes in contact with a source of ignition. Flammability of a liquid is also explained by the term flash point. The greater the flammability of the liquid, the lower its flash point. The flash point of a liquid is the lowest temperature at which the liquid releases vapour in a sufficient amount to form an ignitable mixture with air near its surface. Many common chemicals have flash points below ambient temperature. Liquids that have a flash point of $< 37.8^{\circ}\text{C}$ (100°F) are generally termed flammable liquids, and those with a flash point of $37.8\text{-}93.3^{\circ}\text{C}$ ($100\text{-}200^{\circ}\text{F}$) are called combustible liquids (Patnaik 1999). The flammability of a substance also depends on pressure, oxygen

enrichment, and process conditions, such as mechanical agitation. The autoignition temperature is the minimum temperature required to cause or initiate self-sustained combustion independent of the source of heat. In other words, a substance will ignite spontaneously when it reaches its autoignition temperature. Most fire hazards involve flammable liquids (Patnaik 1999). The flammable liquid does not burn itself, the vapours from the liquid burn. Thus, the flammability of a liquid depends also on the degree to which the liquid forms flammable vapours; in other words, its vapour pressure.

Products of an oxidation reaction involving fire are smoke, gases, heat, flame and pressure. Each of these products exerts specific effects on people and the environment. Smoke results from nonstoichiometric combustion of fuels (Tuhtar 1989) and its harmful effect comes from inhalation. Fire gases also, cause inhalation problems due to their toxicity, high temperature and often oxygen deficiency. During fires, enormous amounts of heat is liberated. This heat can have an effect on people ranging from simple discomfort to death. Most heat transfer in fires is by convection and radiation (Lees 1980) and with the temperature of the hot products in the range of 800 – 1200 °C. If the oxidation reaction in a fire causes an explosion, the overpressure of the explosion will have a significant destructive effect as presented in the next section.

Explosion

Explosion is a sudden and violent release of energy (Lees 1980). This energy could be physical energy, chemical energy and nuclear energy. The physical and chemical energies will be discussed due to their relevance to the process industries.

Physical energy may take the form of a sudden expansion of high pressure gases. An example is the rupture of high pressure vessel or pipe. Explosions caused by the sudden release of chemical energy are classified into two main types: deflagrating and detonating explosions (Noon 1995). In a deflagration explosion, the flammable mixture burns relatively slowly and, generally, causes damage by pushing things about because of the pressure difference. A detonating explosion is a violent chemical reaction with a very

high energy release, and a high peak explosion pressure. The great destruction from this type of explosions comes in the form of smashed and shattered material, due to the transmission of an intense shock wave through them. The shock wave speed in a detonation is supersonic and will strike an individual before the sound from the explosion has had the chance to arrive. Although a deflagration over pressure is significantly lower than a detonation, it can still cause damage as, generally, it is of longer duration.

Most chemical explosions involve a limited set of simple reactions, all of which involve oxidation. An explosion can be spontaneous or initiated by light, heat, friction, impact, or a catalyst. Explosions are not confined to closed systems; explosions may occur in an open area such as a process plant in which case the pressure wave will expand itself until the pressure gradient becomes insignificant.

The lower and higher explosive limits, discussed previously with flammability, and heat of combustion are the important factors when studying the explosive potential of a substance in terms of chemical energy.

Toxicity

Toxicity is defined as the ability of toxic (poisonous) substances, when absorbed by living tissues (either ingested or via the skin), to cause injury or destroy life. Injuries, caused by the toxic effects of chemicals, vary and occur both close to and distant from the point of release of these chemicals, especially when the correct precautions to chemical releases are ignored. The injuries include eye, skin, poisoning, asphyxia and respiratory system injuries.

The effect of toxic substances may be acute, chronic, systemic, or local. Acute toxicity is manifested from a single dose or one-time exposure within a short period of time, usually from a few minutes to several days. Chronic toxicity results from several exposures of small concentrations for long periods of times, usually greater than an 8-hour work shift; certain substances cause illness after several years. A systemic effect is

the toxic effect of a chemical at one area in the body, the chemical having entered the body at another point. When a substance affects the tissues at the point of contact or where it enters, it is termed a local effect.

Toxicology data are available for most chemicals. The most commonly used in the industry are LC_{50} , LD_{50} and TLV. Their definitions are:

LC_{50} Median Lethal Concentration 50 (Calculated concentration of a chemical in air exposure, which can cause the death of 50% of experimental animals in a specified period of time)

LD_{50} Median Lethal Dose 50 (Calculated dose of a chemical that is expected to cause the death of 50% of experimental animals when administered by any route other than inhalation)

TLV Threshold Limit Value (Concentration of a substance in the air to which workers can be exposed without adverse effect)

Most of the information used to predict the adverse effects of exposure to substances comes from animal testing or a test tube procedure using cells or tissues isolated from animals or humans. These types of studies allow the examination of potentially toxic substances while accounting for different exposure levels and genetic variability. Animals, including rodents, which are frequently used in toxicological testing, biologically resemble humans in many ways.

In the industrial context, TLVs are the most usable toxicity values, and their aim is to protect employees at work (Heikkila 1999). However, the threshold limit may give inaccurate relative toxicity of some chemicals, for example, the TLV for acrylonitrile is 2 ppm while for hydrogen peroxide is 1 ppm; so according to their TLV, hydrogen

peroxide is relatively more toxic than acrylonitrile which is not correct because acrylonitrile is one of the “top 100” hazardous substances listed by Sitting (1991).

Many flammable, explosive and toxic properties of chemicals were used in many hazard indices to rank units according to their hazardous effect on humans and the environment. These indices will be discussed in Section 5.4.

5.1.2 Equipment Related Safety

In a process, not only the substances but also the equipment or unit operations play an important role in safety. Equipment and units represent an inherent hazard, secondary to material, because the equipment acts on the materials and cannot be the cause of problems without the materials and operation.

Accident consequences due to equipment failure alone is mainly economic loss and an in-plant problem, while the equipment failure accompanied by a chemical release is an off-plant problem, mainly for human health and environmental damage. This means that the existence of a hazardous chemical within the equipment increases the consequences of accidents.

Failure rates, defined as equipment failure per unit time, are related, to some extent, to the safety of process items. However, failure information does not express safety directly, since not all failures are dangerous and not all accidents are due to failure of equipment (Heikkila 1999). All equipments have various forms of flaws. However, most of these flaws do not affect the operations. Only a few cause leakage and/or break down and only very few among these can cause large-scale accidents (Kim et al. 2002).

Equipment failure rates are related to many factors, most important of which are the operating conditions, the external environment and maintenance. Equipment may also be ranked according to the risk from its malfunction, whether that risk is based on inspection, spare parts, or maintenance. When a plant is inspected in its entirety, any

apparatus/installation areas of various units have the potential to cause problems. In this case, it is necessary to decide which parts need to be inspected and/or improved first.

5.2 Inherent Safety

Webster's dictionary (1996) defines *inherent* as: existing in someone or something as a permanent and inseparable element, quality or attribute. A chemical process is described as inherently safer if it reduces or eliminates one or more process hazards, and this is accomplished through changes that are permanent and inseparable from the basic process technology. An inherently safer design is one that avoids hazards instead of controlling them, particularly by removing or reducing the amount of hazardous material in the plant or the number of hazardous operations (Kletz 1996)

5.2.1 History of Inherent Safety

Following the Flixborough explosion in 1974, there was an increased interest in chemical process industry safety, from within the industry as well as from government regulatory organizations and the general public. Much of the focus of this interest was on controlling the hazard associated with the chemical process and the plant through improved procedures, additional safety interlocks and systems, and improved emergency response. Kletz (1978) proposed a different approach – change the process and the plant to eliminate the hazard completely or reduce its magnitude. If this could be accomplished, elaborate safety systems and procedures could be eliminated.

On December 14, 1977, Trevor Kletz, who was, at the time, safety advisor for ICI Petrochemical Division, presented the annual Jubilee Lecture to the Society of Chemical Industry in Widnes, England. His lecture, "What you don't have can't leak" was the first clear discussion of the concept of inherently safer chemical processes and plants (Kletz 1978). In 1984, Kletz collected many examples of inherently safer designs into a short book called "Cheaper, Safer Plants or Wealth and Safety at Work" (Kletz 1984) to emphasize his belief that inherently safer plants are usually cheaper than traditional designs. He described the various routes to inherently safer designs, namely:

- Intensification, using so little hazardous material that it will not matter if it all leaked out.
- Substitution, using a safer material instead.
- Attenuation, using a hazardous material in the least hazardous form.
- Limitation of the effects of failures, not by adding on protective equipment but by equipment design or by changing the conditions of use.

In 1985, Kletz brought the concept of inherent safety to North America through his paper “Inherently Safer Plants” (Kletz 1985). Thereafter, Dr. Kletz has continued to actively promote the concept of inherent safety throughout the world. Interest in inherently safer chemical processes and plants has grown over the years since 1978, and that growth has been particularly rapid in the 1990s (Kletz 1996) but slower than other advances in process safety like Hazard and Operability Study (HAZOP) and quantitative risk management (Kletz 2003).

Inherent safety for a chemical process represents a fundamentally different approach to safety in the chemical industry. The process designer and planner are challenged to identify ways to eliminate the hazard associated with the process, rather than to develop add-on barriers to protect people from the hazards of the manufacturing process and its materials. It is referred to a process that eliminates or minimizes hazards as “inherently safer” because the safety basis of the design is inherent in the process chemistry and operations, rather than coming from added safety equipment and procedures.

The inherent safety concept is only part of the broader one of Sustainable Development. Sustainable Development starts with the development of a product and covers all aspects of the product, from the source of raw materials, through

manufacturing to the use and the eventual disposal or recycling of the product at the end of its useful life; while inherent safety looks at manufacturing only. The objective of developing inherently safer processes can be considered as part of sustainability, but with enough importance to receive specific attention.

5.2.2 Applications of Inherent Safety

Inherently safer design has drawn the attention of many safety researchers in the chemical industry. In 1995 and 1996, there were more than 30 papers and presentations related to inherently safer chemical processes (Hendershot 1999). Although it is an attractive and cost-effective approach to hazard/risk management, inherent safety has not been used as widely as other techniques such as HAZOP and quantitative risk assessment. There are many reasons for this; key among them are: a lack of awareness; and the non-availability of systematic methodologies and tools (Khan and Amyotte 2002). Also, a lack of time for development, the fear of unforeseen problems, the influence of licensors and contractors, and the inability of the innovator to sell his or her ideas (Kletz 1999). Or perhaps the concept is too simple for people to grasp (Kletz 2003).

Despite all the difficulties in the inherent safety concept, it has been successfully applied. Many case examples include: applications in the development of hazard indices in the studies of Edwards and Lawrence (1993), Heikkila (1999) and Gentile et al. (2003); investigating less hazardous materials in the study of Amyotte et al. (2003); for better design options in the studies of Hendershot (2000), Khan and Amyotte (2002) and Zwetsloot and Ashford (2003); and for developing ideas for computer based tools in the studies of Rushton et al. (1994) and Etona (2001). Even if the concept was not explicitly stated, some designs introduce inherent safety to plants; an example is the optimal plant layout in the work of Georgiadis et al. (1997 and 1999). Plant layout design is used to best arrange equipment, for safety, before constructing the plant.

5.3 Risk and Risk Assessment

Another important and widely established term in the process industry is risk. The risk of an industrial process or a technical installation is defined in the process industries as the combination of the incident probability and the magnitude of the harmful effects. Thus, this term strongly refers to probabilistic assessment. Another definition is: risk is the time related, or location related likelihood of a hazard actually resulting in an undesired event which can impose acute and/or chronic effects. There are two main categories of risk: *risk to life* and *risk to plant and profit*.

Risk to life

This first category can be sub-divided into two main groups:

1. Ordinary Risks: these are common to all plants and arise principally from human activity on or around the plant e.g.
 - Falling off structures.
 - Tripping over obstacles.
 - Impact by falling objects.
 - Contact with moving parts of equipment.
2. Process Risk: these vary from plant to plant, the main classes of process risk being
 - Fire or explosion due to release of flammable material.
 - Emission of toxic or corrosive materials.
 - Discharge of hot scalding fluids.
 - Discharge of cold sub-zero fluids.
 - Projectiles arising from equipment rupture or fragmentation due to overpressure.
 - Asphyxiation risks.

Risk to plant and profit

These risks are concerned with damage to the plant or with plant unavailability for other reasons and can be classified into two main groups:

1. Risk due to incidents, where there is also risk to life: the main risks falling into this category are the same as for *process risks* previously mentioned which lead either to plant unavailability in their own right (e.g. equipment rupture, fire or explosion) or to a plant shutdown pending an enquiry (e.g. toxic release or other dangerous incidents). *Ordinary risks* to life previously mentioned also may call for a plant shutdown pending investigations.
2. Risks due to incidents where there is no risk to life: the risks falling into this category are purely operational risks e.g. equipment breakdown or unavailability, blockage of equipment or pipe work and fouling of equipment.

Risk is a concept that is used in the chemical industry by practicing chemical engineers. The term risk is multifaceted and is used in many disciplines such as finance, raw material supply, plant design and process change, and site selection. The term risk used in these disciplines can be discussed qualitatively or quantitatively. This section will focus on the basic concept of risk to human health and risk assessment as applied to the manufacturing processing or use of chemicals, and the impact of exposure to these chemicals on human beings.

The chemical process industries already use a wide range of process analysis tools to identify, quantify and control risks and problems in plant operation, safety and environmental performance. Broadly, two separate sets of tools exist for the identification and quantification of abnormal situations and they are in the form of qualitative and quantitative risk tools.

5.3.1 Qualitative Risk Assessment

Experience

Experience forms the most basic source for the qualitative risk assessment methods. Most plant engineers and managers with detailed knowledge of their plant and materials can rapidly identify the major hazards in their area. Incidents that have occurred will be recorded, and hazard data collected from similar plants worldwide will also be

available. Designers of new plants will obtain data from other plants, from material properties and from laboratory scale experiments. In many production facilities in the process industries, such experience exists and can be rapidly used to identify the major hazards. Some means of channelling this experience and recording results is essential if a thorough study is to be made.

Safety Audits

Safety audits provide a means of harnessing experience to form a qualitative risk procedure. The term safety audit implies the inspection of a production facility by a team of experienced safety assessors to determine whether operating procedures and design conditions are being adhered to. The involvement of process personnel in this activity is essential if unrevealed hazards are to be identified. The team will also investigate past incidents and near misses (accidents that could have caused injuries) and consider the methods of handling emergencies and abnormal conditions. The report of a safety audit team usually identifies the major hazards and many minor hazards for the area audited and provides a useful record for future use.

Checklist

Another qualitative risk assessment method, which is widely used in the industry, is the checklist. Checklists are essentially simple and empirical. They are generally used to check compliance with good design and operating practices. Many companies tend to devise their own checklists for specific areas of design and operation.

The use of checklists has many drawbacks, as analysts tend to ignore items not included in the list, or to tick items systematically without careful consideration. Checklists should be designed to stimulate thought and enquiry. Questions should preferably be open rather than in a form which requires “Yes/No” answers. Therefore, for a checklist to be comprehensive, it may have to contain many questions, and yet more questions are added as experience reveals more problems. Checklists can therefore be cumbersome, and the analyst may be misled into believing that all aspects which ought to

be questioned have been covered without confirming that it is so. By their nature, checklists provide no quantitative measures. Thus, they do not allow relative ranking either of hazards or of the effectiveness of designed protection against risk. This is another drawback in complex systems having multiple hazards.

Hazard and Operability Studies (HAZOP)

A HAZOP study is a predictive safety analysis technique for identifying hazards and potential operability problems, in simple or complex equipment, processes or plants. A team of experts uses key words to prompt recognition of a deviation from normal operating conditions that could have adverse effects on safety, the environment, operability or performance. This method relies on the expertise of the persons performing the analysis. HAZOP is described as a technique of imaginative anticipation of hazards and operating problems. It is now widely used in the chemical (especially petrochemical) industry. There are many publications describing experiences applying the technique and suggesting improvements; practical examples can also be found. HAZOP involves a vessel to vessel and pipe to pipe review of a plant. For each vessel and pipe, the possible disturbances and their potential consequences are identified. HAZOP is based on guide words such as no, more, less, reverse, which should be asked for every pipe and vessel. These words are applied to flow, temperature, pressure, liquid level, composition, and any other variables affecting the process. The intention of the guide words is to simulate an imaginative accident and the team should combine knowledge from different domains to explain and react to this accident.

HAZOP is generally carried out by a small team of industrial specialists, directed by an experienced group-leader. The study is of the brain-storming type and could be very time consuming. Therefore, only those deviations, which would lead to hazardous outcomes, are recorded for future action. The HAZOP team normally consists of about six people, representing a number of interest groups. For a standard HAZOP of a new plant design, these include:

The *plant design engineer* whose primary role in the meetings is to explain their design. Where changes are considered necessary, the designer's role may also include advising the meeting about cost/benefit trade-offs of various options; they will also eventually be responsible for producing revised designs to satisfy the meeting recommendations.

The *Commissioning or installation engineer* is expected to help resolve practical issues relating to the siting, structure and construction of the plant. With experience of the problems of startup and initial operation of new plant, they also have a key role in suggesting possible problems in the proposed control and safety systems.

The *Operators and maintenance engineer* may have either a questioning or an explanatory role in the meetings, exploring whether the proposed design meets operating requirements, and what provision has been made for the safe management of unusual circumstances such as shutdown and maintenance.

One or more *independent experts*, who have a broad knowledge of process chemistry and engineering but who have not previously been closely involved with the project. Their main role in the HAZOP meetings is to suggest and explore possible deviations from the intended behaviour of the plant, and to apply their experience to identify and suggest alternatives to any undesirable features of the design.

The study meetings are chaired by the HAZOP *leader*, who has overall responsibility for the conduct of the analysis. This responsibility normally extends to the selection of team members and the practical administration of organizing the study meetings; it also includes ensuring that the necessary follow-up work, such as answering queries or ensuring that recommendations are implemented after the meeting. The discussion and conclusions of the meeting are documented by the *recorder* or secretary. The person selected for this role must have sufficient understanding of process chemistry so that they can follow and accurately minute the discussion.

HAZOP can be used at different stages of process design but in a restricted mode. A complete HAZOP study requires final process planning with flowsheets and P&IDs.

5.3.2 Quantitative and Semi-Quantitative Risk Assessment

The level of risk for some industries can be judged from experience or relevant accident statistics. However, there are some cases where this may not be feasible or realistic, e.g. for new processes of unprecedented size, new concepts of design, modification to an existing plant or when design standards have been improved. In such cases, there is a need for additional techniques to assess the level of risk to individuals, property, environment and society. These techniques can range from relatively simple quantitative methods of hazard identification to advanced quantitative methods for risk assessment, in which numerical values of risk are derived.

Modern quantitative methods of risk assessment emerged in the mid-1970s, and they have been applied to a wide variety of regulatory issues, including pesticides, food additives, ambient air, indoor air and other environmental media. Quantitative risk assessment is only appropriate where it is both reasonable and practicable, reasonable in that the cost of doing it is not high compared to the value of solving the problem, and practicable in terms of the availability of information and data (Carter et al. 2003).

In the past, risk characterizations have frequently consisted of brief descriptions of potential adverse effects and affected populations, along with a single estimate of the level of risk. This estimate would summarize whether humans would experience any of the various forms of toxicity or other effects associated with the risk agent. More recently, however, this short form approach to risk characterizing has been criticized (American Chemical Society 1998). It is now generally acknowledged that characterizations need to provide deeper insights into how risk estimates and findings are generated and should more clearly discuss the uncertainties and limitations in empirical data on which the risk assessment is based.

Risk analysis of engineered systems usually involves detailed engineering evaluations of systems design and operations. The prospect of failure is often analyzed with the help of probabilistic or scenario tools. The considerations involved include historical operation and accident experience, vulnerabilities to human errors and failure rates of key components such as valves, pipes, and dials. As with health risk assessment, these inputs are based on a mix of hard data, modelled simulations, and expert judgments.

Risk analysis on a theoretical basis with a full-scope analysis is difficult for the chemical industry. The variety of chemical installations would require too much effort for such a procedure (Hille 2002). Nevertheless, the question remains as to whether procedures of risk evaluation are available that, maybe, are not entirely comprehensive but, consequently, are much easier to apply and will still yield useful results for risk comparisons. Such a tool could be extremely valuable tool for risk comparison between different installations in the sense of a vulnerability analysis and to achieve the same prevention level within the plant.

Relatively new quantitative risk assessment tools are found in the literature. They modify and combine risk assessment tools under the basic definition of risk. Yoon et al. (2000) defined a risk matrix from the multiplication of frequency and severity matrices. The proposed method describes accidents frequency and severity in a matrix form: the frequency is composed of an n by m matrix whose elements are the number of accidents for each n unit in the plant and with m severity degree (fire, explosion, etc.). The severity is defined as m by 1 matrix, which is composed of a weighting factor for each severity. Another quantitative risk assessment is the risk curve developed used by Cuny and Lejeune (2003). The curve plots the probability of the undesired event versus severity defined as days off work. This curve was found from statistical methods performed on data of undesired events.

For semi-quantitative risk assessment, Khan and Abbasi (1998b, 2001) developed and applied the Optimal Risk Analysis tool (ORA). ORA involves four steps: i) hazard

identification and screening, ii) hazard assessment (both qualitative and probabilistic), iii) quantification of hazards or consequence analysis, and iv) risk assessment. Another semi-quantitative and widely used method that can bridge the gap between purely qualitative and fully quantitative approaches is the risk matrix. This risk matrix, which is different to the quantitative risk matrix of Yoon et al. (2000), enables the likelihood (frequency) and consequences (severity) of major accidents to be combined in a single diagram. Table 5.1 is an illustrative risk matrix from Carter et al. (2003).

Table 5.1: Illustrative Risk Matrix (Carter et al. 2003)

Outcome Likelihood	Single fatality	2-10 fatality	11-50 fatality	50-100 fatality	100+ fatality
Likely $> 10^{-2}$ per year	Intolerable	Intolerable	Intolerable	Intolerable	Intolerable
Unlikely $10^{-2}-10^{-4}$	Intolerable If $>10^{-3}$	Intolerable If $>10^{-3}$	Intolerable	Intolerable	Intolerable
Very Unlikely $10^{-4}-10^{-6}$	Tolerable	Tolerable	Tolerable	Tolerable	Intolerable
Remote $10^{-6}-10^{-8}$	Acceptable	Acceptable	Tolerable	Tolerable	Tolerable

If all the possible events in the plant were located in this matrix, an overall view of the plant risk is recognized.

5.3.3 Probability and Frequency for Risk Assessment

Estimating a probability number for an event is based on an extensive study and data collection for that event including the failure of all its components and consequences. Probability as an essential part of risk assessment is used in the fields of

occupational risk as the probability of accidents or any undesired event. The studies in this field began when insurance companies started to use science, psychology and statistics for their evaluations

The German author Marbe, in 1926, worked on the psychology of accidents and, based on the data of a large insurance company, he was able to show that the probability that a given person will have an accident varies directly with the number of accidents he has already had within a given time. Furthermore, based on data from the German railways, he was able to show that the probability that a given worker will cause damage will likewise vary directly with the number of times he has already caused damage within a certain period of time in the past. This gives the possibility to show that those people who frequently suffer accidents are the same ones who repeatedly cause them. This finding became known as “Marbe’s Law”: a given individual’s probability of having an accident is calculated based on the number of accidents he has already had. This was one of the first times in the study of accidents when a conclusion employed the term *probability* and, furthermore, related probability to an observed frequency.

Although “Marbe’s Law” was developed for human performance, it can be applied to other events and fields, including plant accidents and chemical releases. This concept of relating probability to frequency was used extensively because probability was not directly available for many events, especially if these events were complicated, multi-staged or new. Cuny and Lejeune (2003) supported this and indicated that estimating the probability is more problematic; the frequency approach is the most tangible. They estimated probability using its relative frequency and the assessment was statistical.

5.4 Hazard Indices

The selection of appropriate measures of environmental or safety performance for a process will depend on the nature of the environmental concerns, the type and quantity of information available and the degree of accuracy required in the representation. Several hazard analysis indices have been developed, some of them are internationally

known and proven, and some have been used and developed inside companies. Data required for each index is different and the results produced may vary. The different hazard indices are suitable for different stages of process development, design and operation. Some can be applied at a very early stage of planning and require an overall knowledge of the system under consideration, and some must be applied to existing units with full knowledge of all aspects of the unit. Some hazard indices are presented below.

5.4.1 Comprehensive and Detailed Indices

Detailed Indices, that consider many aspects of the unit under consideration, have been proposed from time to time for hazard identification. Noteworthy among them are the Dow fire and explosion index, Dow chemical exposure index and the Mond fire, explosion and toxicity index.

Dow Fire and Explosion Hazard Index (Dow F&EI)

This Dow index aims primarily at identifying fire, explosion and chemical reactivity hazards during a plant design and to identify equipment that would be likely to contribute to the creation of an incident. A number of aspects are explored in deriving the Dow F&EI, these are combined into three factors – material, general process and special process factors. Of these, the material factor is dominant.

The Dow F&EI is calculated as follows. First, a material factor (MF) is obtained. Then two penalty factors (F1 and F2), one for general process hazards and one for special process hazards, respectively, are determined. Next, the process unit hazards factor (F3), which is the product of F1 and F2, is calculated. The Dow F&EI is obtained as the product of MF and F3.

The material factor is a measure of the inherent rate of potential energy released due to fire and explosion produced by combustion and a chemical reaction. Thus, a measure of flammability, and the reactivity of materials are used to determine the

material factor; that is normally selected from tables in the Dow F&EI Guide. It falls in the range 1-40. General process hazards are a sum of the penalties due to the type of reaction/process, type of chemical handled in the process unit, and drainage and spill control of chemical. The special process hazard covers a wide range of process parameters, e.g. process temperatures, pressure levels, sizes of inventory of flammable materials, potential for corrosion/erosion, and how near the process operates to the flammable range.

Dow (1994) specified certain requirements that must be met before the Dow F&EI can be applied to the process. An accurate plot plan of the manufacturing unit and the process flowsheet must be available. The minimum inventory of the base material must not be less than 2,268 kg. If these requirements are not met, the hazard involved in a chemical process can be over-estimated by the index.

Dow Chemical Exposure Index (Dow CEI)

The Dow chemical company developed this index to complement the Dow F&EI in the assessment of hazards associated with the release of toxic materials. This index is a measure of the relative acute toxicity risks to people within chemical plants and neighbouring communities. It may be used for initial process hazard analysis and in emergency response planning. The purpose of the earlier Dow CEI was to provide a simple empirical rating of an acute toxic hazard from chemicals that was quantitative in nature, but allowed a comparison between substances (Marshall and Mundt 1995)

The information needed for the calculation of the Dow CEI includes physical and chemical properties of the material, a simplified process flowsheet, showing vessels and major pipe work with inventories, and an accurate plan of the plant and its surrounding.

Dow CEI depends on two key parameters, the quantity of the material and the maximum concentration below which no adverse effect on humans will develop.

However, in detail, it identifies five elements that influence the impact from any potential release. These are:

1. Toxicity of the substance described by a material factor.
2. Quantity of material becoming airborne.
3. Distance to area with hazard concentration and needing special attention.
4. Molecular weight of the substance.
5. Process variables influencing the magnitude or potential for release.

Each of these elements was characterized by scale numbers, typically ranging from 0 to 4 or 5 with the higher number representing a potentially greater hazard. The Dow CEI was determined by evaluating each of the factors for the chemical of concern then multiplying the numbers to arrive at a value that was the Dow CEI.

Mond Index

Members of the Explosion Hazard Section of ICI Mond Division (ICI Mond Division 1993) developed the Mond Index from the Dow Fire and Explosion Index Hazard Classification Guide, principally for the chemical industry of ICI, following the Flixborough disaster. The main purpose of the Mond index is to extend the applicability of the F&EI to include a wider range of processes. It includes a consideration of toxicity hazards that was not accounted for in the Dow F&EI at that time. It expands the Dow Index to include a wider consideration of continuous and batch processes in the storage and loading/unloading areas and materials such as oxidative and other explosive materials, which are not considered fully in the Dow F&EI Classification Guide. Similar to the Dow F&EI, the application of the Mond Index highlights features of plant having a significant fire and explosion hazard potential.

The Mond Index provides separate indices for fire, internal explosion and aerial explosion potential, in addition to an overall hazard rating index. The first step in the use of this index is the division of the plant into smaller units to identify areas that requires hazard analysis. The dominant material in the unit of interest is then selected to determine

the material factor; a material factor is calculated for each unit based on the heat of combustion. Factors affecting the hazard potential of the process are determined; these are the special material hazards, general process hazards, special process hazards, layout hazards, and the acute hazards. All but the last two items are similar in principle to the equivalent factor in the Dow Guide, although again, they are developed to give a more comprehensive treatment. The Layout factor was novel. It is intended to bring out more clearly the advantageous effects that spacing, access, structure heights, drainage, etc., can have on hazard potential. An index is then calculated as a combination of these factors.

To use either Dow or Mond indices at an early stage in process design could reveal hazard potential which is relatively easy to alleviate before the design is advanced. The effects of any design modifications should be evaluated by recalculation of the indices. These indices are more relevant to the chemical and petrochemical industries, but complements other hazard analysis studies.

One major issue with the above mentioned hazard indices is that they should incorporate some kind of judgment of the relative importance of the various types of hazards and potential injuries or damage into the evaluation of the index. The user of the index either defers to the judgment of the developer of the index, or must modify it to incorporate personal judgment. If each user modifies the index based on personal judgment, there cannot be a valid comparison among different users (Hendershot 1997). Gupta (1997) gave some changes for the Dow F&EI to make it give a more realistic value for the developing countries. Another disadvantage is that the above indices are not suitable for route selection because they require detailed plant specifications (Edwards and Lawrence 1993). Route selection means early stage chemical manufacturing planning from feedstock to final products. Hence, these indices cannot be used in optimization models for early stage planning especially in large industries with a large number of options because they require detailed plant operational data which are not available at the early planning stage.

Examples of other comprehensive hazard indices, that are relatively new and not widely used, are Hazard Identification and Ranking (HIRA) technique (Khan and Abbasi 1998a) and Safety Weighted Hazard Index (SWeHI) (Khan et al. 2001).

5.4.2 Simple Indices

Simple safety indices have been used in the earliest stage of planning and when the most detailed process information is still lacking. Developing a simple hazard index for systems is not an easy task; it requires knowledge of what is important for the viability of the system involved and how that contributes to safety. The number of representative indicators in the index should be as small as possible, but as large as essential. Such simple indices are, by their nature, applicable only for specific functions and should not be employed for more general safety comparison.

In the petrochemical industry, the first forms of simple safety indices for planning started in the 1980s after the development of optimization models for that industry. The indices at that time were very simple; they were the first introduction of safety into planning. Fathi-Afshar and Yang (1985) selected the chemical TLV as an indicator for a health objective function. Chemical 1 is considered more harmful than chemical 2 if TLV_1 is less than TLV_2 ; so the index is represented as the reciprocal of TLV.

Also, very simple hazard indices were used when planning involved hazard identification for a large number of plants. The National Fire Protection Association (NFPA) (1994) has developed a system for indicating the health, flammability and reactivity hazards of chemicals. The system is based on giving a number (from 0 to 4) to a chemical indicating its effect. Al-Sharrah et al. (2001) used these NFPA health ratings as an index for an environmental objective in planning. This model was composed of 83 plants with 65 chemicals.

Other groups of safety indices present a more detailed approach to quantifying safety in the early stage of planning (i.e. inherent safety indices). Though detailed, they

are relatively simple when compared to the Dow and Mond indices. The indices depend on the materials handled and the process operated with all values being determined, not estimated or based on judgment. The first example is the Edwards and Lawrence (1993) index. This inherent safety index is intended for analyzing the choice of process route; i.e. the raw materials used and the sequence of the reaction steps. The index has been calculated as a total score, which is the sum of a chemical score and a process score. The chemical score consists of inventory, flammability as flash point and boiling point, explosiveness as a difference between explosion limits, and toxicity as TLV. The process score includes temperature, pressure and yield. Yield is the product of conversion and selectivity; a high yield implies efficient usage of raw material, with the consequence that there is no need for recycles and therefore less inventory. Some of the scores are based on similar tables in Dow and Mond indices and others have been constructed by dividing the domain of the values of the parameters into ranges and assigning a score to each range.

Another example is the Heikkila et al. (1996) index which considers a wider range of factors affecting the inherent safety of a process and it is an extension to the Edwards and Lawrence (1993) index. The index is divided into the two main categories, usually used in studies of risk indices: *chemical* and *process inherent safety*. The *chemical inherent safety index* describes the effect of the choice of raw materials and other chemicals on the inherent safety of the process. It considers the following aspects: heat of the main reaction including the diluents in the reactor, heat of potential side reactions, flammability as a flash point, explosiveness as a difference between explosion limits, toxicity as TLV, corrosiveness and incompatibility of chemicals, which represents the potential reaction hazards from an accidental mixing of the chemicals. The *process inherent safety index* describes the effect of the type of process equipment and processing conditions on the inherent safety. The following parameters are considered: inventory of chemicals, process temperature and pressure, the type of processing equipment and the structure of the process. The total inherent safety index is the sum of chemical and process indices. The details and examples of the index are clearly shown in Heikkila (1999).

Cave and Edwards (1997) proposed the Environmental Hazard Index (EHI) that ranks routes (raw materials and reactions to produce the final product) in chemical plant development by the estimated environmental impact of a total release of chemical inventory. The index considers the hazard to the aquatic and the terrestrial ecosystems. Also, an index by Gunasekera and Edwards (2001, 2003), called the Atmospheric Hazard Index (AHI), can be used to assess the potential impact of airborne releases from a chemical production plant. A catastrophic failure of the plant is assumed and the impact on the atmospheric environment is estimated. The method is designed to assess possible alternative process routes to make a chemical, in order to determine the route that has the least adverse atmospheric environmental impact. Thus, the routes that are inherently environmentally hazardous can be identified and avoided when the selection is made in the early stage of production plant design. The atmospheric impact categories considered were the toxicity, photochemical smog, acid deposition, global warming and ozone depletion of a chemical when it is released catastrophically into the environment.

The simple hazard indices discussed are suitable for route selection but with the following limitations:

1. The NFPA ratings and TLV are too simple and can give inaccurate relative toxicity of some chemicals.
2. Edwards and Lawrence (1993) and Heikkilä (1996) indices require some operational data such as temperature, pressure and yield which some times are not available at early planning stages.
3. Cave and Edwards (1997) and Gunasekera and Edwards (2001, 2003) indices were developed mainly to assess the potential impact of a chemical release on the environment without a clear indication of the adverse effect on people.

The literature on hazard indices gives different names and classifications for the indices using the terms risk, safety or hazard. For example, Hendershot (1997) considered Dow fire and explosion index and Dow chemical exposure index as *risk indices*. Khan

and Abbasi (2001) broadly characterized safety and risk studies into three groups: quantitative techniques, qualitative techniques and probabilistic techniques and Gentile et al. (2003) named three *quantification methodologies*:

1. A collection of several well-known indices used to evaluate various safety aspects. The results cannot be aggregated under an overall index.
2. A single overall index that evaluates aspects relative to inherent safety and the results aggregated under an overall number.
3. A risk-based approach.

5.5 Chemical Accidents Databases

An accident in the process industries is an unplanned or unwanted occurrence, leading to any one or combination of:

- Death, injury, or hospitalization of personnel.
- Damage to company property (including fire).
- Spill of hydrocarbons or other chemical.

Chemical plants are complex, tightly-coupled operations. Tightly-coupled means one event or process affects another event or process directly and quickly, thus making human intervention difficult when something goes wrong. Complex means that events cannot be predicted reliably because many different things can go wrong in many different ways. This is why every chemical plant in the world is an accident waiting to happen (Rachel's 1994). A major accident in one sector of the industry gives no market advantage to a competitor, if it leads to a general loss of confidence in the industry by the public (Kirchsteiger 2003).

Accidents databases are collections of data on chemical accidents. Major accidents databases were the result of federal law while others were compiled for private institutes or companies. The law requires that certain facilities report their toxic release and inventories together with any accidents that harm workers, the public, and the environment annually. In the past 30 years, special attention has been given to designing

and developing a database of chemical accident histories. As a result, there exist a number of such databases, some of them covering specific countries and some covering wider geographical areas. Statistical analysis with data processing has led to several scientific publications and technical guidelines issued by research institutes and governmental agencies. For example, Kirchsteiger (1999b) analyzed data of major accidents in the European Union and Belke (2000) analyzed data for chemical accidents risks in U.S. industry, all using accidents databases. Balasubramanian and Louvar (2002) studied seven accidents databases and identified that, even with the existing problems in the databases, some important information can be extracted and the description of accidents is useful and educational. Data in the databases are very valuable and many useful conclusions and statistics were found from analyzing them.

5.5.1 Database Contents

Most databases contain the following information. The length and details presented depending on the number and type of processes and chemicals present at the facility reporting the incident and on the interests of the database itself:

1. Registration information (e.g. facility name, address, process chemicals, nature of business, etc.)
2. The event:
 - The date and time
 - Names of chemicals released, Chemical Abstracts Service (CAS) registry number and hazard class
 - Source of release
 - Quantity of chemicals released and where to (soil, air, etc.)
 - On-site and off-site impacts or incident consequences (death, injury, evacuation property damage)
 - Initiating event (mechanical, human or natural phenomenon), and factors contributing to the release.
3. Information on the date of completing the last process hazard analysis, the major hazards identified by that analysis, process controls used to address those

hazards, and information on maintenance, training, compliance audits, and incident investigation.

Actual causes of incidents are not recorded in a database. Rather, only the presumed initiating event is identified; i.e. what apparently happened and where the system appeared to have broken down.

Despite some limitations, i.e. not being sufficiently comprehensive, existing databases confirm that the problem of chemical safety is large, and the frequency of serious chemical incidents is significant enough to warrant national concern.

5.5.2 Major Accidents Databases

A large quantity of information regarding chemical accidents has been gathered and stored in databases. In an interactive way, users may access such databases in order to retrieve information regarding similar accident situations that have been raised in the past and extract useful conclusions regarding probable actions to be taken. This feature is important in rare event circumstances as in major chemical accidents. Kourniotis et al. (1999) conducted a survey on the well-established major chemical accidents databases; information was retrieved through the Internet in order to test the availability of such data to the public. The results are shown in Table 5.2.

Table 5.2: Chemical Accidents Databases and their Public Availability through the Internet (Kourniotis et al. 1999)

Database Name	Num. of accidents publicly available	Period covered	Area covered	Agency
MARS	365/365	1980 to present	EU	MAHB
FACTS	0/~20000		World wide	TNO
MHIDAS	0/~5000	1964 to present	World wide	HSE
ERNS	All/10,000s	1987 to present	USA	EPA
CHEMAX	0/~5000		World wide	JRC
APELL	~350/?	1970 to present	Worldwide	UNEP
ARIP	All/4905	1986-1995	USA	EPA
ADID	?/~1100	1968 to present	Japan	ADIC
IRAS	0/?		Mainly USA	CCPS

Abbreviations are:

- ADIC:** Advanced Digital Information Corporation
- APELL:** Awareness and Preparedness for Emergences at Local Levels.
- ARIP:** Accidental Release Information Program
- CCPS:** Centre of Chemical Process Safety of the American Institute of Chemical Engineering (AIChE)
- EPA:** Environmental Protection Agency.
- ERNS:** Emergency Response Notification System.
- FACTS:** Failure and Accidental Technical Information System
- HSE:** Health and Safety Executive.
- IRAS:** Incident Reporting and Analysis System.
- JRC:** Joint Research Centre
- MAHB:** Major Accident Hazard Bureau
- MARS:** Major Accidental Reporting System
- MHIDAS:** Major Hazard Incident Data Service

TNO: Netherlands Organization for Applied Scientific Research.
UNEP: United Nation Environmental Programming.

The second column in Table 5.2 shows two numbers in the form x/y and these indicate that x accidents available to the public from y accidents in the database. The “~” symbol means approximately.

Checking the data in Table 5.2 reveals that it is correct except for:

- ARIP database covers the period 1986 – 1999 with 4945 accidents.
- ADID database could not be identified or found on the Internet.
- MARS database could not be accessed due to security reasons.

Other small and institute-related chemical accidents databases were found to be available on the Internet. The first one was the Emission of Unwanted Compounds Linked to Industrial Disasters and Emergencies database (EUCLIDE) developed by the Department of Chemical Engineering of the University of Pisa (Italy) and the Major Hazard Bureau of the European Community. The second one was the Relational Information System for Chemical Accidents Database (RISCAD) developed by the National Institute of Advanced Industrial Science and Technology (Japan). However, the two databases were small when compared with other databases like the ARIP database that contains a higher number of accidents (10 times more) with detailed accident descriptions.

From the major accidents databases available on the internet, the ARIP database was the most useful due to its size and format, therefore it was used later in developing a risk index. Accidental Release Information Program (ARIP) is associated with U.S. industry where all U.S. facilities are required by law to report non-routine releases of certain substances when those releases exceed a reportable quantity. These reports are submitted in to the National Response Centre, the U.S. Coast Guard, and Environmental Protection Agency (EPA) regional offices. EPA compiles the reports into the Emergency

Response Notification System (ERNS) database. EPA then uses ERNS data to select releases for the ARIP questionnaire. The ARIP questionnaire consists of 23 questions about the facility, the circumstances and causes of the incident, and the accidental release prevention practices and technologies in place prior to, and added or changed as a result of, the event. The questionnaire focuses on several areas of accident prevention including hazard assessments, training, emergency response, public notification procedures, mitigation techniques, and prevention equipment and controls.

Another important, and widely recognized, chemical accidents database is the Risk Management Plans database (RMP*info). It is a result of a law by U.S. congress to certain chemical facilities to submit summary reports every five years. These reports contain significant information on each facility's accident history, accident prevention program, and the potential consequence of a hypothetical accidental chemical release. These data have been assembled into a searchable computerized database and was originally intended to be available to the general public via the Internet. However, the chemical industry and U.S. security agencies raised concerns that some of the data would allow terrorists to easily identify those facilities likely to cause the greatest harm to the public in the event of a release. These concerns promoted Congress to pass legislation in August 1999, that, along with subsequent federal regulations, currently restricts public access to portions of the RMP*info database.

5.5.3 Analysis of Accidents Databases

The ability to learn from previous incidents has long been regarded as an essential aspect of any program designed to reduce the frequency and severity of future incidents. Many major events, which capture media attention, continue to implicate "failure to learn from previous losses". If obvious similarities are apparent between an existing operation and one that experienced loss, follow-up action is more likely to be pursued and future loss may be avoided.

Belke (2000) wrote a very useful analysis from the RMP*info database; it was a preliminary characterization of the database. One useful analysis was the normalized accident rates; accident rates are commonly normalized by dividing the number of incidents by some measure of the number of opportunities for an accident. This allows large and small facilities to be compared fairly over a given period. However, since hazardous chemical facilities vary so greatly in size, number of processes, chemical quantities stored and produced, operating schedules, and other characteristics, it is difficult to say which single divisor best represents the number of accident opportunities. Belke (2000) used the number of processes in the facility using the chemical and the aggregate chemical quantity as normalization factors. Table 5.3 shows the results.

Normalized accident rates, or accident frequency represented by “Number of Accidents per Process per Year”, listed in Table 5.3 shows similarities in rates for some group of chemicals. Following inspection of column two in Table 5.3, five groups of chemical were identified and these are presented in Table 5.4.

Table 5.3: Normalized Accidents Rates from RMP*info Chemicals (Belke 2000)

Chemical name	Number of Accidents per Process per Year	Number of Accidents per Mlbs stored per Year
1. Ammonia	0.016	0.014
2. Chlorine	0.022	0.16
3. Hydrogen Fluoride	0.064	0.27
4. Flammable Mixture	0.0074	0.00075
5. Chlorine Dioxide	0.155	1.97
6. Propane	0.006	0.0012
7. Sulfur Dioxide	0.013	0.011
8. Ammonia (aqueous)	0.017	0.018
9. Hydrogen Chloride	0.060	0.25
10. Hydrogen	0.031	0.024
11. Methane	0.027	0.0064
12. Butane	0.011	0.00089
13. Ethylene Oxide	0.027	0.045
14. Hydrogen Sulfide	0.067	0.5
15. Formaldehyde	0.009	0.024
16. Isobutane	0.010	0.011
17. Pentane	0.013	0.0052
18. Titanium tetrachloride	0.056	0.090
19. Phosgene	0.044	2.49
20. Nitric Acid	0.038	0.047
21. Ethane	0.014	0.00071
22. Oleum	0.022	0.011
23. Ethylene	0.014	0.00089
24. Vinyl Chloride	0.042	0.0051
25. Trichlorosilane	0.034	0.10

Table 5.4: Normalized Accidents Rates from RMP*info Chemicals; a Group Form

Chemical group	Accidents Frequency: Number of Accidents per Process per Year	Mean Group Frequency
Group 1: Hydrogen sulfide Hydrogen fluoride Hydrogen chloride	0.067 0.064 0.060	0.064
Group 2: Phosgene Vinyl chloride	0.044 0.042	0.043
Group 3: Hydrogen Methane Chlorine	0.031 0.027 0.022	0.027
Group 4: Ammonia Ethane Pentane Ethylene Butane Iso-Butane	0.016 0.014 0.013 0.014 0.011 0.010	0.013
Group 5: Formaldehyde Flammable mixture	0.009 0.007	0.008

Although some chemicals in the groups share some physical and/or chemical properties, the group name or a general classification has not been identified or determined yet. However, chemicals in the above table, which correspond to high accident frequencies, e.g. hydrogen sulfide, are chemicals that cause corrosion problems. Fontana (1987) indicated that most of the corrosion difficulties for refinery operations are due to inorganics such as hydrogen sulfide.

When studying the corrosion resistance of some chemicals in Table 5.4 it was found that the accident frequency decreased with increasing corrosion resistance. This can be seen more clearly when numerical values are assigned to corrosion resistance. Most Industrial plants are made from either 304 stainless steel, 316 stainless steel or carbon steel, chemical compatibilities, from corrosion tables, can be classified as excellent, good, fair or severe effect. To identify numerical values for corrosion resistance, numerical values were first assigned to the classifications for example:

Excellent = 4

Good=3

Fair =2

Severe effect= 1

Hydrogen sulfide has a compatibility of fair, excellent, and severe effect with 304 stainless steel, 316 stainless steel and carbon steel respectively; this gives a total score for compatibility of 7. Similarly, the score for hydrogen fluoride is 7, methane 9, chlorine 10, ammonia 11, and butane 12. Table 5.4 shows that these chemicals have descending accidents frequencies.

Unfortunately, not all the chemicals, in Table 5.4, have complete compatibility data, but relating chemical corrosion to accidents is a first step towards identifying chemical accident causes. The Dow F&EI and Heikkila (1999) indices considered corrosion in evaluating the indices. Dow gave a penalty for corrosion and erosion in the

range 0.1 to 0.75, and Heikkila gave a score of 0, 1 and 2 for the construction material carbon steel, stainless steel and better material respectively. It can be stated now that there exists an inverse relation between accident frequency and a chemical's compatibility with the construction material.

Other useful information from accidents databases is the hazardous effect of a chemical material in terms of the number of people affected by the release of that chemical. It is well known that the health and safety effects of chemicals on people are an important issue. These effects can be estimated from toxicity data like LD_{50} , LC_{50} , or TLV. However, information on the actual effects is shown in accidents databases. The Accidental Release Information Program (ARIP) (1999) database lists information on chemical accidents including the amount of chemical released and the number of people affected.

People affected include fatalities, people injured and people hospitalized. However, some incidents involving the release of hazardous chemicals reported in the databases indicate that the number of people affected by the release was zero. This can be a result of nobody being near at the time of an incident. However, it is important to be able to estimate the number of people affected following a release. For this reason, a relationship was sought between the number of people affected and toxicity data. Equation 5.1 represents a relationship between the LD_{50} and the number of people affected per tonne of chemical released. Equation 5.1 was found from a regression of the data in Table 5.5 which lists some chemicals that have known values of LD_{50} and valid accidents data from ARIP. This relationship can be used to estimate the number of people affected by a chemical knowing the LD_{50} for that chemical.

Table 5.5: People Affected per Tonne of Chemical Released and the Lethal Dose

Chemical	LD ₅₀ rat mg/kg	Affected people/tonne From ARIP
Acetic acid	3,310	0.0229
Acrylic acid	340	0.0561
Ammonium hydroxide	350	0.2449
Benzene	930	0.1465
Carbon tetrachloride	2,350	0.1827
Chloroform	1,194	0.0179
Dichloromethane	1,600	0.2064
Ethylene oxide	72	1.0800
Formaldehyde	100	1.0151
Phenol	317	0.6386
Phosphoric acid	1530	0.0133
Potassium hydroxide	365	0.0270
Propylene oxide	380	0.2821
Sulfuric acid	2,140	0.0213
Toluene	636	0.0747
Vinyl acetate	2,920	0.1866
Vinyl chloride	500	0.0417
Xylene	4,300	0.2348

$$\text{People affected / tonne} = (5.4764) LD_{50}^{-0.5881} \quad (5.1)$$

The regression of Equation 5.1 is shown in Figure 5.1 with an R^2 value of 0.2482. Although, the accuracy of the equation is low, Figure 5.1 shows a clear relation in the form of a power function between the affected people and the LD_{50} . Also, the accuracy of the equation is not expected to be very high because the data for affected people and the amount released were taken from a single accidents database. In addition, some incidents in the database have reported the release of a chemical which was not 100% pure and for some chemicals the number of incidents counted was not very high. It is strongly believed that the accuracy of the equation can be drastically increased if a larger number of incidents were included. Note that the LD_{50} was taken from the Material Safety Data Sheet (MSDS) and the number of people affected per tonne of chemical released was taken from ARIP accidents database.

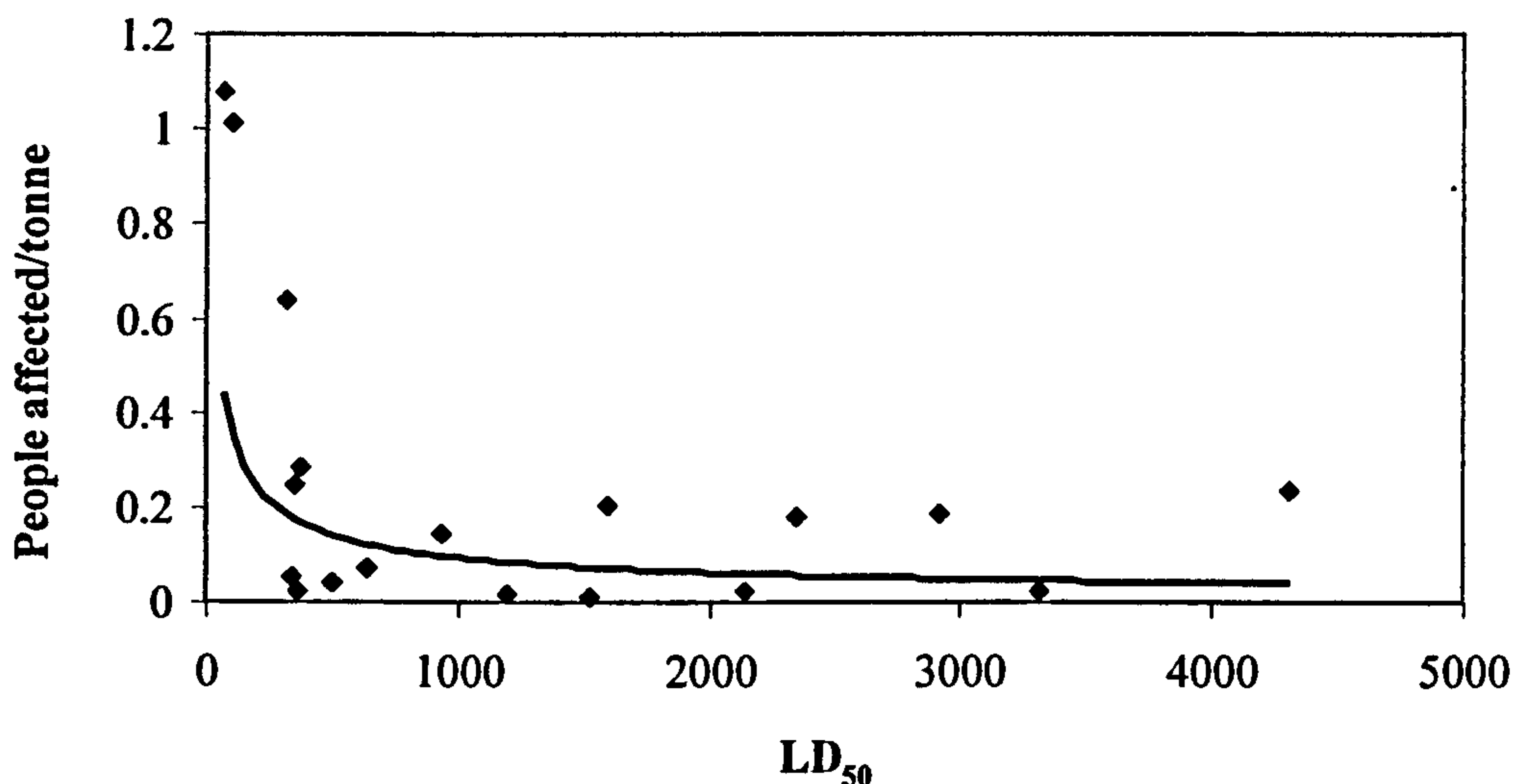


Figure 5.1: People Affected per Tonne of Chemical Released and the Lethal Dose

Accidents reported in the accidents database include toxic, fire and explosion incidents and the number of affected people in Table 5.5 is the sum of these three types of accidents. Attributing the number of people affected to a toxic effect only, as in Equation 5.1, assumes that the number of people affected by toxic release dominates over fire and

explosion effects. Belke (2000) indicated that the toxic effect of a chemical is far more severe than its fire effect. He stated the following:

- In general, toxic release scenarios result in a greater endpoint distance than flammable worst case scenarios. The distance to the endpoint is the distance from the release location to the point at which the toxic vapour cloud, heat from a fire, or blast wave from an explosion cease to have harmful effects.
- The median endpoint distance for toxic worst case scenarios is 1.6 miles, while the median endpoint distance for flammable worst case scenarios is 0.4 miles.
- Under the RMP rule, the population potentially affected by a release is defined as the residential population inside a circle with radius equal to the end point distance. The median population for flammable worst case scenarios is 15 people, while the median for toxic worst case scenarios is 1500 people- two full orders of magnitude greater, whereas the difference in the median value for the endpoint distance is only a factor of four.
- Flammable worst case scenarios are, on average, less severe than toxic alternative scenarios. Notably, most flammable alternative release scenarios would not even affect any members of the off-site public.

This was the result of an analysis done on the Risk Management Program (RMP*info) accidents database. This database was also analyzed by Al-Qurashi (2000) and it was found that 81% of the releases reported in the database are from toxic substances.

The above analysis from the RMP*info accidents database indicates that the toxic effect of chemicals is dominant over its fire and explosive effects. Consequently, a simplified relationship, such as Equation 5.1, to relate the number of people affected to LD₅₀ only can give acceptable results, although it was a regression of data representing the number of people affected from the toxic, explosion and fire effects of chemical releases.

Equation 5.2 can be looked at from another angle; it is an empirical formula that translates animal risk (LD_{50}) to human risk (people affected per tonne). This assumed relation is considered as a standard assumption in risk assessment. Regulatory agencies have developed a host of standards assumptions, which span most of the critical analytical areas in risk and include translating animal risk estimation to human risk prediction (American Chemical Society 1998). Assumptions invariably play a significant role in the quantitative stages of risk assessment as hard data may not be readily available, and they provide a way forward where scientific understanding may be incomplete or non-existent.

5.6 Proposing a New Risk Index

5.6.1 Why a New Index?

Our original focus was to plan Kuwait's petrochemical industry. This task usually starts at the Supreme Oil Council in Kuwait. For this council and at this early stage of planning and route selection, the safety part of planning has to be easily understood and must include some kind of experience. If an index is to be used in this situation, it has to be simple and need general plant information where planning may include tens of possible plants. Looking at the available indices (comprehensive and simple), their usage in route selection is limited for the reasons discussed in Section 5.4. In addition, the desire to incorporate past experience on chemical accidents led to the development of a new risk index. However, it is strongly stressed that the new index is not designed to replace the well known and established indices but to be useful in cases where planning of a very large number of plants is needed with limited amount of operational data.

5.6.2 Index Structure

Starting from the basic definition of risk, which was the product of the incident probability and the magnitude of the harmful effects, a simple risk index K is proposed. It is an index that can be applied to chemical plants using the properties of the major chemicals associated with production. It is an index to quantify risk to human life and

falls into the group of simple early stage planning and route selection hazard indices. The index is:

$$K = Freq \times Haz \times Inv \times Size \quad (5.2)$$

Where

Freq = Frequency of accidents, number of accidents per process per year

Haz = Hazardous effect of a chemical, number of people affected per tonne of chemical released

Inv = Inventory of chemical released, tonne per accident

Size = Size of plant, number of major processes in plant

This gives an overall unit of the index *K* as number of people affected per year, and it represents the potential maximum number of people affected if an accident caused the release of all the plant inventory of a chemical. Affected people include fatalities, people injured and hospitalized. The plant is assumed to have major processes in which a major chemical is being treated and an accident in any part of the plant may cause, in an extreme case, the release of the plant inventory.

The general definition of risk includes probability, whereas this work uses frequency because of the availability of frequency data and the difficulty of estimating a probability, as discussed previously. The frequency of accidents (*Freq*) can be taken from Belke (2000) as shown in Table 5.3. If the chemical is not found in Table 5.3, an estimate of the frequency is taken from a similar chemical or from Table 5.4, according to which group the chemical can be related; in this case, the mean group frequency is used. The hazard of a chemical (*Haz*) is calculated from the ARIP accidents database by looking at all the available accidents associated with the chemical and dividing the number of people affected by the amount released. If no accidents were reported for the chemical or if the reported number of people affected is zero, Equation 5.1 can be used to estimate this number. Although values for *Freq* and *Haz* has been taken, for this work,

from Belke (2000) and ARIP accident database, other accidents databases could provide values for these parameters.

The inventory (*Inv*) is taken as the maximum production inventory in a petrochemical plant; usually it is one month of production. The minimum economic production rate can be used for evaluating the inventory if the actual production rate has not been determined or planned. Minimum economic production rates are usually known for most plant from plant economics references such as Stanford Research Institute (SRI) reports. Finally, *Size* of a plant, in term of major processes, can vary from one plant to another but usually a chemical goes through production stage, purification stage and a final product storage stage. Therefore, a general number for *Size* is taken as three. Calculations of the index for some chemicals are shown in Table 5.6 and values plotted in Figure 5.2.

The values used for the index parameters are best estimates if other information is unavailable. Certainly, detailed information about a production plant and the chemical involved will result a more realistic evaluation of the risk index. The index can also be used in other cases as follows:

1. The index can be applied to a chemical plant including major and non-major chemicals. The index in this case is calculated as the summation of the individual chemicals indices.
2. The inventory of one month of production is used for calculating a theoretical maximum for the risk. Consequently, a high value for inventory is used. The index can give a more realistic (non maximum) value of the risk if it is applied to existing plants with accurate inventories.
3. The number used for the size is a representative number (an average). The actual number of major processes can be used.

4. The index can be applied for chemicals in the plant which are not stored. In this case, an estimate for their inventory in the process equipment can be used.
5. The index can be used to estimate risk from a single process in a plant; in this case the *Size* will be taken as one and *Inv* will be taken as the inventory of chemicals within the process equipment.

Table 5.6: Risk Index Results

Chemical	<i>Freq</i> Accidents/process yr	<i>Haz</i> People affected/tonne	<i>Inv</i> Tonne/accident	<i>Size</i> No. of process /plant	<i>K</i> People affected / plant . yr
Acetaldehyde	0.008	0.1202*	5625	3	11.2
Acetic acid	0.038	0.0229	5625	3	14.7
Acrolein	0.064	0.5763*	12.5	3	1.4
Acrylic acid	0.038	0.0561	7500	3	47.9
Acrylonitrile	0.042	0.4224*	7500	3	399.2
Ammonia	0.016	0.1357	8750	3	57
Benzene	0.008	0.1465	8333	3	293
Butadiene	0.013	0.1233*	2083	3	10.0
Carbon tetrachloride	0.056	0.1827	1875	3	57.6
Chlorine	0.022	0.8105	7500	3	401.2
Cumene	0.008	0.0742*	5000	3	8.9
Ethane	0.014	0.1526	4366	3	28
Ethyl benzene	0.008	0.0451*	15000	3	16.2
Formaldehyde	0.009	1.8414	1250	3	62.1
Hydrogen chloride	0.06	0.4273	1666	3	128.1
Hydrogen cyanide	0.064	5.9972	2500	3	2878.7
Hydrogen fluoride	0.064	0.0116	1458	3	3.2
Nitric acid	0.038	0.2298	1875	3	49.1
Pentane	0.013	0.1515*	417	3	2.5
Phenol	0.008	0.0002	3750	3	0.02
Phosphoric acid	0.038	0.0133	14400	3	21.8
Styrene	0.008	0.4484	18750	3	201.78
Sulfuric acid	0.038	0.0149	26666	3	45.3
Toluene	0.008	0.0747	5833	3	10.5
Vinyl acetate	0.042	0.1866	5625	3	132.3
Vinyl chloride	0.042	0.0337	10417	3	44.2
Xylene	0.008	0.2348	5000	3	28.2

* calculated from LD₅₀

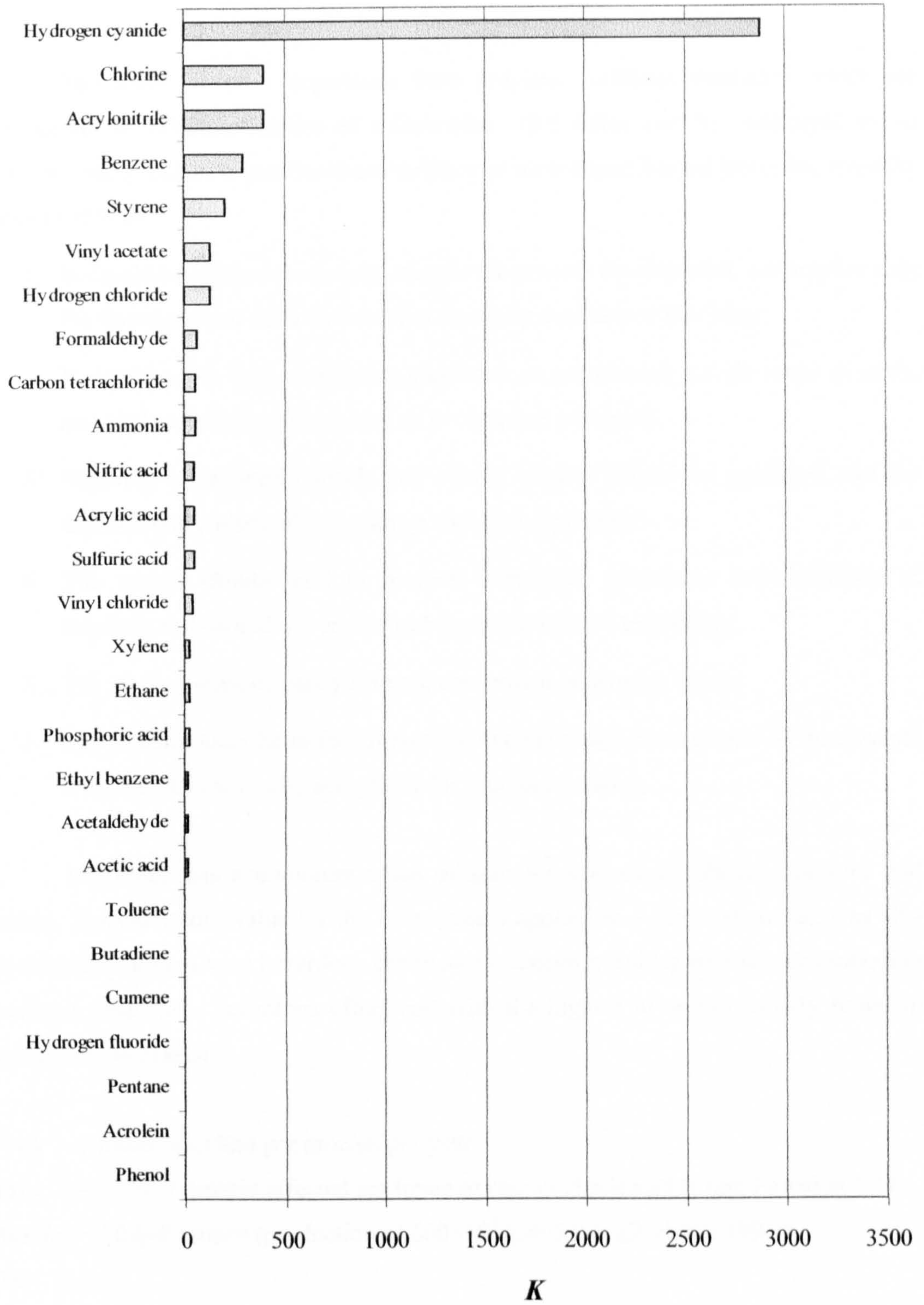


Figure 5.2: Risk index K for some Chemicals.

The index includes experience from previous accidents databases, which are considered as valuable sources of information. This index can be considered as an inherent safety index; it has the characteristics of an inherent hazard index indicated by Tyler (1985) as:

1. It should be applied at an early stage in the process development, and require only the flowsheet and other information normally available at that stage.
2. It should cover both continuous and batch processes over a wide range of scale, and apply to single units as well as to complete processes.
3. Ranking of separate hazards and overall hazards should be produced, and the fundamental causes of the rankings should be apparent.
4. The results should tend to promote simplified processes, safer methods of handling and should not unreasonably penalize novel technology.
5. The method must be easily learned, convenient, and quick to use.
6. The ranking must be in the correct relative order and there should be an absolute level which is normally acceptable for routine operation.

The index has a minimum value of zero for safe chemicals (e.g. plastics and resins). The maximum value for the index, when applied to a single chemical, was also calculated. Taking a very hazardous chemical (hydrogen cyanide) with its corresponding accidents frequency, hazardous effect and with the highest inventory usually found in petrochemical plants:

Freq = 0.064 accident per process per year

Haz = 5.9972 people affected per tonne of chemical released (using Equation 5.1)

Max Inv = 50,000 tonnes (production of 600×10^3 tonne / yr, (Rachel's 1994))

Size = 3

Max K = 57,573 people affected / yr

For each chemical, the index is directly proportional to inventory and thus it is related to the intensification concept of inherent safety. By decreasing the inventory by a factor of 10, the index will reduce by a factor of 10 also. This is different from other indices in terms of inventory dependence. Hendershot (2000) calculated the Dow F&EI for ethyl acrylate storage for different inventories; the index was reduced by a factor of 1.16 when the inventory was reduced from 2 million lb to 0.2 million lb (10 times reduction). For Heikkila (1999), the index decreased by 2 for the same inventories; knowing that Heikkila index has the order of 20s the reduction factor is roughly 1.1. Using the same inventories in Edwards and Lawrence (1993) index, the reduction in the index was only 1 and with an index order of 15, the reduction factor is roughly 1.1. Therefore, the new index is sensitive to inventory and reflects a direct relationship between the hazard and the amount of hazardous material whereas the other indices are relatively insensitive to this parameter.

The accuracy with which the index is determined depends on the accuracy of its four factors, namely accidents frequency (*Freq*), the hazardous effect of the chemical (*Haz*), the inventory (*Inv*) and the size of the plant (*Size*). In any stage of planning, even in the first stages, an estimate of the plant size and inventory can be found with good accuracy. This makes estimating the frequency of accidents and the hazardous effect of the chemical the main two factors that affect the accuracy of the index or estimating the effect of the plant accidents on people. Good values of *Haz* come from good accidents databases, the number of historical incidents has to be as high as possible and the number of affected people has to be accurately counted together with the amount of chemical released. If no data is available, an estimate can be found from Equation 5.1. Although the accuracy of this equation is not very high, it provides an estimate only for those cases where no data is available in accidents databases. The chemical accidents frequencies can also be estimated from accidents database if the number of processes using the chemical is listed in the database, otherwise Belke (2000) analysis and Table 5.4 are a good source of information.

The error in the two terms *Haz* and *Freq* should be as low as possible because the error in the index *K* will be approximately the sum of the error in its terms. If the *Inv* and *Size* were considered accurate and the error in *Haz* is *e1* and the error in *Freq* is *e2* then:

$$\begin{aligned} K_{\text{accurate}} &= \text{Haz} (1 \pm e1) \times \text{Freq} (1 \pm e2) \times \text{Inv} \times \text{Size} \\ &= \text{Haz} \times \text{Freq} \times \text{Inv} \times \text{Size} (1 \pm (e1 + e2) + e1 e2) \end{aligned}$$

for small errors $e1 e2 \ll (e1 + e2)$ then

$$K_{\text{accurate}} \approx K (1 \pm (e1 + e2))$$

Appendix C contains a paper that has been prepared on the work described in this chapter and has been submitted for publication to the “*Process Safety and Environmental Protection*” journal with the title, “A New Safety Risk Index for use in Petrochemical Planning”.

5.7 Conclusion

Identifying and addressing the factors contributing to industrial chemical accidents is a first step in reducing and hopefully eliminating such accidents. One way of doing that is to translate the large number of system components and features in the HSE fields to a representative number as an index. Before developing a risk index, accidents databases were studied and some useful relations were concluded; the most important of which is the power relation between the number of people affected from a chemical release and the chemical LD₅₀. Also, the causation between corrosion and high chemical accidents frequencies. These relations are worthy of attention and further studies.

The new risk index, developed in this chapter, was formulated to represent a potential maximum number of people affected if an accident caused the release of the whole of the plants chemical inventory. This index will be used later as a risk objective

for route selection in planning petrochemical networks. The merits of this index can be expressed as follows:

- Can be simply used for risk comparison.
- Can be applied in initial process assessment, even as early as the conceptual design stage of a plant.
- Incorporates past experience and data on chemical accidents into risk evaluation and comparison.
- Can be used for the planning of new plants.

Chapter 6

Model Formulation and Solution

The petrochemical industry is a large complex of processes and chemicals which are defined as a sector of the global chemical industry. Petrochemicals are chemicals that are made from feedstocks, which are derived from petroleum, coal, and natural gas. Examples of such feedstocks are ethane, propane, naphtha, and toluene. The end products of this industry are mainly plastics, resins fibres, and rubbers. Many of these end products are further processed by other sectors of the chemical industry and end up as daily consumable products. Besides the feedstocks and the end products, there are also intermediate products; these might also be end products in themselves, because there is a demand for them in other sectors of the chemical industry. Chemicals such as these are phenol, styrene, propylene and acrylonitrile. Modelling a petrochemical industry has to take into account the relationship between the chemicals and their sources and destinations. The petrochemical model in this work is an optimization model composed of constraints and objective function(s) under some assumptions. The main model assumptions are:

1. The petrochemical network is constructed from plants each containing a number of processes achieving a main chemical transformation between the feedstock and the product.
2. The plant inventory of chemicals is mainly in the storage section. Equipment inventory is assumed much smaller than storage inventory and hence can be neglected in the calculation of risk of chemical release.
3. A number of intermediate chemicals are produced and then totally consumed in the petrochemical network; their net production rate is zero.

6.1 Model Constraints

Let:

N be the number of chemicals involved in the operation of M plants,

X_j be the annual level of production of plant j ,

Q_i be the annual amount produced of chemical i ,

F_i be the annual amount of chemical i used as a feedstock, and

o_{ij} be the output coefficient of chemical i from plant j .

The main constraints that govern the operation of the petrochemical network are the material balance constraints:

$$F_i + \sum_{j=1}^M o_{ij} X_j = Q_i \quad i = 1, 2, \dots, N \quad (6.1)$$

These constraints ensure that the total quantity produced of each material i is equal to the sum of all the amounts produced by all the plants plus its quantity as a feedstock. For all the intermediate chemicals, Q_i will be set to zero because no output of these chemicals is required from the desired petrochemical network. This constraint applies only to the main chemicals in the plant, not secondary feedstocks or by-products.

The final products in the planned petrochemical industry will be governed by their demands in the petrochemical market, according to the country's share in that market. Constraints on Q_i for all final products are needed and they are formulated as:

$$Q_i \leq D_i U \quad i \in I_1 \quad (6.2)$$

Where D_i is the world demand for chemical i and it is multiplied by the upper limit of country's share in the petrochemical market, U . The above constraint is only applied for final products group I_1 .

Introducing the binary variables Y_j for each plant j will help in the selection requirement of the planning procedure. Y_j will be equal to 1 only if plant j is selected and zero if plant j is not selected. If plant j is selected, the production level must be at least equal to the minimum economic capacity B_j , therefore, for each plant j the following constraint is used:

$$B_j Y_j \leq X_j \leq H Y_j \quad j = 1, 2, \dots, M \quad (6.3)$$

Where H is a valid upper bound on production rates applicable to all plants.

The proposed improvement of Kuwait's petrochemical industry is directed towards building new plants to produce petrochemicals, so it is logical that only one plant should be selected to produce a single chemical. Then the following constraint is included for each chemical:

$$\sum Y_j \leq 1 \quad j \in J_1 \quad (6.4)$$

Where J_1 is the group of plants that produces a single chemical. This constraint ensures that a maximum of one plant is selected from each group.

For final products:

$$\sum Y_j = P \quad j \in J_2 \quad (6.5)$$

Where P is the number of final products selected from the proposed list of products, and J_2 is the group of all plants that produce a final product.

The supply of feedstock limitations will impose additional constraints on the selection and planning, i.e.:

$$F_i \leq S_i \quad i \in I_2 \quad (6.6)$$

Where S_i is the supply availability of feed chemical i . The feedstock F_i is a function of the optimization variable X_i while the supply S_i is a deterministic input parameter to the model. The above constraint only applies for some feedstock chemicals represented by the group I_2 . Not all the feedstock chemicals are included in I_2 because some are additives and some are needed in small quantities. Also, some petroleum-rich countries have few (if any) limitations on petroleum feedstocks.

An additional economic constraint is required for the limit on the investment budget. If cap_j is the capital investment cost for constructing plant j and Bg is the available budget, then the constraint is formulated as:

$$\sum_{j=1}^M cap_j \times Y_j \leq Bg \quad (6.7)$$

6.2 Model Objective Functions

Two objective functions are formulated in this study: an economic objective and a risk objective. For simplicity, the economic objective function is a maximum economical gain in the selected plants. The economical gain is represented by the overall added-value; it is the price of final products minus the cost of feedstocks for the petrochemical network. If C_i is the price (or cost) of chemical i , the added-value objective function will be represented by:

$$\max f_1 = \sum_j^M \sum_i^N o_{ij} C_i X_j \quad (6.8)$$

Note that the output coefficient o_{ij} of chemical i from plant j will be positive for chemicals produced and negative for chemicals consumed.

There is no one standard calculation form for the added-value, but the usual basis is the difference between sales income and cost of goods and bought in services. What should be and what should not be included in the calculation can be argued at length and largely depends on the purpose for which the data are to be used and by whom. Considering the nature and the size of the petrochemical network, the simplest measure possible for the added-value should be used, provided there is a clear indication, in that form, to the success of the industry.

The second objective function is formulated starting from the risk index K discussed previously in Chapter 5, the index was:

$$K = Freq \times Haz \times Inv \times Size$$

where

$Freq$ = Frequency of accidents, number of accidents per process per year

Haz = Hazardous effect of a chemical, number of people affected per tonne of chemical released

Inv = Inventory of chemical released, tonne per accident

$Size$ = Size of plant, number of major processes in plant

This gives an overall unit of the index K as number of people affected per year, and it represents the maximum number of people affected if an accident caused the release of all the plant inventory of a chemical. People affected include fatalities, people injured and hospitalized. The plant is assumed to have major processes in which a major chemical is being treated and an accident in any part of the plant may cause, in an extreme case, the release of the plant inventory.

Each plant in the petrochemical network was investigated to identify the chemicals associated with production. The three terms ($Freq$, Haz , and $Size$) of the index K , were calculated for each chemical in the plant, leaving the inventory (Inv) as a function of production (one month of production, or X_j divided by 12). This represents a

maximum inventory in a plant to calculate a representative maximum risk. The overall plant index was the summation of all plant chemicals indices, and the risk objective is formulated as:

$$\min f_2 = \sum_j^M \sum_i^N o_{ij} \left(Freq_i \times Haz_i \times Size_{ij} \times \frac{X_j}{12} \right) \quad (6.9)$$

The two objectives, minimize risk and maximize economic gain, are usually in conflict with one another; some valuable final products of resins and plastics need very hazardous chemicals for production. For example, Acrylonitrile Butadiene Styrene (ABS) resins needs acrylonitrile, which is very hazardous. Therefore, it is not possible, in many situations, to reduce the industrial risk without any decrease in economic gain. Therefore, one has to use multiple objectives techniques to reach a certain trade-off between them. Overall, the model described above is in the form of a Deterministic, Mixed Integer Linear Programming (MILP) model with Multiple Objectives (MO). This form of model will provide a strong planning and process selection tool. Deterministic means that all variables should be assigned a known value with no probability in their evaluation; Mixed Integer means that some variables are integer and some are continuous, Linear means that the model has linear constraints and linear objectives and finally, Multiple Objectives means having more than one objective function. The model will stay linear if the two objectives are combined in a linear form.

6.3 Model Data

Data collection is, as always, a major difficulty with large industrial projects. Much of it simply does not exist, or is not known. The time spent dealing with parameter data was a considerable part of this work's effort. In situations where data was scarce, best estimates were used indiscriminately. This proved to be an acceptable practice for two reasons. First, it is almost impossible to begin to structure the model without any data whatsoever, thus these numbers aided the early formulations of the model. Second, they could easily be changed after the model was up and running.

To construct the petrochemical network, first, the desired final products were defined and they are listed in Table 6.1 with the classification of Primary Final product (PF). These products are discussed in detail in Section 2.3 as the proposed final products for the development of Kuwait's petrochemical industry. The routes from the available basic feedstocks to the final product chemicals were determined by selecting a number of manufacturing plants and considering all the possible alternatives for producing these desired products. At the end, a network of 62 plants, linking the production and consumption of 51 chemicals, was formed.

A list of plants and chemicals considered within the model is presented in Appendix A. Some of the chemicals are catalysts, additives and inorganic reagents and some are considered as intermediate feedstocks and intermediate products in the petrochemical network. The chemicals that constitute the model are listed, numbered and classified according to their potential function in Table 6.1. The potential function of a chemical is determined assuming Primary Raw material (PR), Secondary Raw material (SR), Intermediate (products and feedstocks) (I), Primary Final product (PF), and Secondary Final product (SF). Primary raw materials are chemicals derived from petroleum and natural gas and form the basic feedstocks of the plant, whereas the secondary raw materials represent chemicals that are needed as additives or needed in small quantities. The intermediate chemicals are the chemicals that are produced and then consumed in the petrochemical network. Finally, the final products are also classified as primary and secondary. The primary products are the selected final products produced for the country's development and the secondary are by-products associated with the plants in the network. There are 51 chemicals included in the petrochemical model; of these, 13 are only secondary raw materials and secondary final products, which will not take part in the model constraints due to their small quantities. There are 18 intermediates, being both produced and consumed by the model, and 5 end products (primary final products). Primary raw materials constitute 15 chemicals, of which 3 have limited supplies from Kuwait's petroleum sources and they are ammonia, chlorine and naphtha.

Plants included in the model (listed in Appendix A) form a network shown in Figure 6.1 with each plant assigned an index j . Not all the chemicals needed in the development are assigned a production plant, only chemicals that are needed in a considerable amount and which represent major intermediates, not additives or catalysts. The chemicals that are needed in small quantities would be purchased to satisfy their demand in the network.

Some plants included in the model may be old or not used in the current industry, but they were included to give a general model of the industry. Aresa and Galatola (1999) studied two alternatives for environmental assessment of synthetic processes with one of these not being applied at the industrial level. Their justification was that, although the process is not implemented on an industrial scale, it is fascinating from the environmental point of view and can be extended to other feedstocks. Therefore, in the model proposed, all plant alternatives were taken into consideration.

Table 6.1: A list of Chemicals Included in the Model

PR= primary raw material, SR= secondary raw material, I= intermediate, PF= primary final product, SF= secondary final product.

Chemical	Function	Chemical	Function
1. Acetaldehyde	SF+I	27. Hydrogen chloride	SR+SF
2. Acetic acid	I	28. Hydrogen cyanide	I
3. Acetylene	I	29. Methane	PR+SF
4. Acrylonitrile	I	30. Methanol	I
5. Acrylonitrile butadiene styrene	PF	31. Naphtha	PR
6. Ammonia	PR	32. N-Butane	PR
7. Benzene	SF+I	33. N-Butylenes(1-and2-)	PR
8. Butadiene	I	34. Polybutadiene rubber	SR
9. Butenes –Mixed n-, iso, dienes, ...	SF	35. Polystyrene (crystal grade)	PF
10. C-4 fraction (mixed butanes, -enes, ...)	SF+PR	36. Polyvinyl alcohol	SR
11. Carbon dioxide	SR	37. Polyvinyl chloride	PF
12. Carbon monoxide	I	38. Propane	SF+PR
13. Chlorine	PR	39. Propylene (chemical grade)	SF+I
14. Coke	PR	40. Propylene (refinery grade)	PR
15. Cumene	PF	41. Propylene oxide	SF
16. Ethane	PR	42. Sodium hydroxide	SR
17. Ethanol	I	43. Styrene	I
18. Ethyl benzene	I	44. Sulfuric acid	I
19. Ethylene	SF+I	45. Sulfur	PR
20. Ethylene dichloride	I	46. Synthesis gas 3:1	I
21. Formic acid	SF	47. Synthesis gas 2:1	SF
22. Fuel gas	SF	48. Toluene	PR+SF
23. Fuel oil	SF+PR	49. Vinyl acetate monomer	PF
24. Gas oil	PR	50. Vinyl chloride	I
25. Gasoline	SF	51. Xylene (mixed)	SF
26. Hydrogen	SR+SF		

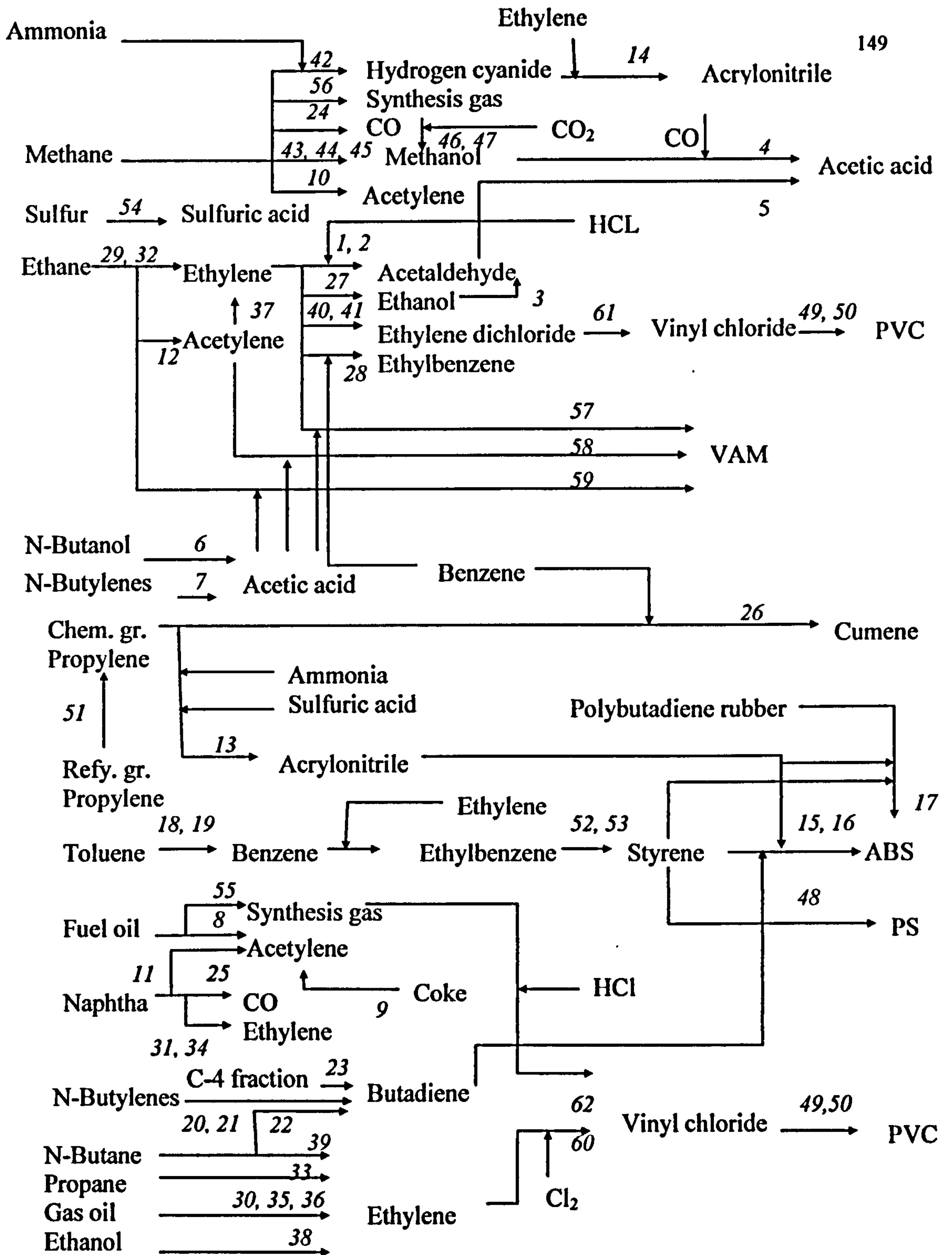


Figure 6.1: A Simplified Network of the Plants and Chemicals in the Model (numbers on the figure correspond to plants listed in Appendix A (SRI 1992))

The heart of the model is the material balance constraints. Hence, estimation of the output coefficients, σ_{ij} , is a key step in constructing the model. For this purpose, yield data for each chemical transformation is required. In many cases, plant yields are variable and depend on what product mix is desired or on what capital expenditure can be afforded. The model uses average yields reported at commercial installations and were taken from Stanford Research Institute (SRI) reports (1992).

The supply of feedstock and demand for final products are needed to complete the construction of the model constraint set. Supply and demand data were taken from different sources mainly from recent SRI reports and Kuwait's Petrochemical Industries Company (PIC) annual reports. Table 6.2 shows the values for the supply and demand.

Table 6.2: Supply and Demand Data.

Feedstock Chemical	Supply (10 ³ tonne/year)	Final Product Chemical	Demand (10 ³ tonne/year)
Ammonia	575	ABS	20,000
Chlorine	16	Cumene	7,217
Naphtha	2,500	Polystyrene (Crystal Grade)	4,000
		Polyvinyl Chloride	6,803
		Vinyl Acetate Monomer	4,000

The constraint on the final products demand, Equation 6.2, uses a value for Kuwait's share in the petrochemical market. An overview of Kuwait's exports of some chemicals like methanol and fertilizers have shown that Kuwait's share is roughly 1% of the total world petrochemical market. However, Al-Sharrah (2000) recommended that, after development, Kuwait must increase its share in the petrochemical market to at least 4%, to get a good economical utilization of the industry and its products. Therefore, U in

Equation 6.2 was assigned the value of 4%. The next constraint, Equation 6.3, needs minimum economic production rates B_j . These values were taken for all technologies in the models from SRI reports (1992). In the constraint, H is a valid upper limit for production rates X_j . The importance of assigning a reasonable value for H came from its effect on the model solution. A low value for H resulted in excluding some good high production rates from the model solution. A high value for H will result in increasing the solution space and hence, the model will display greater computational difficulties.

The P in Equation 6.5 is the number of final products needed to be selected from a set of proposed final products. For this study, we have a case for selecting four products and therefore, P was assigned the value of four. The fixed capital for Equation 6.7 was estimated from SRI reports (1992) and updated to the current year using a plant cost index. The available budget was taken from the PIC annual report (2003/2004).

Data needed for the economic objective function in the model are prices of final products and cost of main feedstocks. Final products prices were presented and then forecasted together with oil prices in Chapter 4. For the main feedstocks, historical cost lists show very low cost changes, and some researchers believe that these may follow larger cost cycles than petrochemicals; therefore current costs were used with the model.

For the risk objective, data sources were discussed in Chapter 5. The calculations were in the form of the number of people affected per year per tonne of chemical produced. When this number is multiplied by the annual production X_j , the full form of the risk index K is obtained.

Most of the model data are listed with each technology in Appendix A.

6.4 Model Solution

The final form of the model is a MILP model with 70 continuous variables, 62 binary variables, 185 constraints and two objectives forming a moderately sized model. While binary variables are very useful in the model formulation, it is at a cost; computing time becomes very long. The complexity of the problem grows exponentially as the number of binary decision variables increase linearly. This situation can produce an intractable or unsolvable problem, even in a moderately sized model formulation. This is where a specialized solver algorithm is employed that can iterate to a near optimal solution in much less time by using algorithms and techniques to check only a small portion of the total problem.

When dealing with a model formulation of this complexity, the only option for solving it is the use of a computer. With the computing power available on a desktop PC, it is now a reality that a problem of this type can be solved conveniently. The petrochemical MILP model was solved using the commercial optimization package GAMS (Brook et al. 1992); the acronym stands for General Algebraic Modelling System. A sample GAMS output is listed in Appendix B. The GAMS itself does not solve the model, but passes it to one of a number of separate solvers according to the selection of the modeller and the model type. The solver used mostly in this work was CPLEX; it is an optimization solver used for linear, network, integer programming, and mixed integer programming. It was originally developed by Robert E. Bixby and sold via CPLEX optimization Inc., which was bought by ILOG, Inc. in 1997.

CPLEX uses a branch-and-bound approach for problems containing integer variables. The optimization algorithm maintains a hierarchy of related linear programming sub-problems, known collectively as a *search tree*. At each node on the search tree, a sub-problem is created and evaluated using the branch-and-bound solving algorithm. This approach can create many combinations of sub-problems but the CPLEX algorithm employs a search mechanism that passes over (rejects) many of the sub-optimal solutions. It is extremely time consuming for the solver to check every possible sub-

problem solution, so it uses algorithms and techniques such as cuts, heuristics and a variety of branching and node selection strategies that gains a very near optimal solution to the overall problem.

When the objective functions were combined using the L_p norm method, the model was not linear for p greater than one. In this case another GAMS solver was used to handle the Mixed Integer Non-Linear Programming model. The solver was SBB which uses the branch-and-bound approach but with a non-linear solver at each node.

Both risk and economic objective functions were tested with the model separately. The model was solved using a single objective function to get the industry bounding structure. The economic objective was also solved with forecasted prices of chemicals. Several solutions were obtained with different final product prices taken for the planning horizon (forecasted prices for the years 2010, 2020, and 2030). The forecasted prices were taken from causal models discussed in Chapter 4; these prices are not indexed to a base year, therefore they represent actual dollars. Also, different multiple objectives optimization methods were tested with the model to generate solutions.

Overall, the model solution gave the selected final products (four out of five chemicals), the corresponding petrochemical network of plants from the basic feedstocks to final products and plants production rates. The tables below show results (rounded to three significant figures) for different solution methods and indicate three values from the solution: the rejected final product chemical; the value of the economic objective; and the value of the risk objective. Note that the number of final products for the development of the petrochemical industry is five, but it is only desired to select four, i.e. to reject one chemical.

6.4.1 Solution with a Single Objective

Economic objective

The model was solved with a single economic objective using current prices and forecasted prices. The forecast was done using two causal models with oil price as an input, (1) transfer function and (2) ARX forecast. The results are shown in Table 6.3.

Table 6.3: Solution with Economic Objective

Price for Economic Objective	Rejected Chemical	Economic Objective (10 ⁶ \$/yr)	Corresponding Risk (people affected/yr)
Current prices	Cumene	1,550	33,900
Transfer Function Forecast	2010	PS	2,000
	2020	VAM	2,660
	2030	VAM	2,450
ARX Forecast	2010	PS	1,070
	2020	VAM	1,390
	2030	PS	1,300

Risk objective

The model was solved with a single risk objective; the results are shown in Table 6.4 with the corresponding economic objective calculated using current prices.

Table 6.4: Solution with Risk Objective

Single Risk Objective	Rejected Chemical	Risk Objective (people affected/yr)	Corresponding Economics (10 ⁶ \$/yr)
	ABS	2,210	249

6.4.2 Solution with Multiple Objectives

The model was solved with different multiple objective methods that combine the two objectives in different ways.

Weighted Objective method

The model was solved with a weighted objective method; the objective function has the form:

$$\text{Min. } f = -w_1 (\text{Economic}/\text{Economic}^*) + w_2 (\text{Risk}/\text{Risk}^*) \quad \text{Where } w_1 + w_2 = 1$$

The two objectives are normalized using their values from single objective optimization, *Economic** and *Risk**, having values of 1,550 (10^6 \$/yr) and 2,210 (people affected/yr) respectively. Results are shown below in Table 6.5 with economics at current prices:

Table 6.5: Solution with Weighted Objective Method

w_1	Rejected Chemical	Economic Objective (10^6 \$/yr)	Risk Objective (people affected/yr)
1	Cumene	1,550	33,900
0.9	ABS	466	2,940
0.8	ABS	394	2,540
0.7	ABS	394	2,530
0.6	ABS	257	2,210
0.5	ABS	257	2,210
0.4	ABS	257	2,210
0.3	ABS	257	2,210
0.2	ABS	249	2,210
0.1	ABS	249	2,210
0	ABS	249	2,210

Trade-off Method (ϵ -constraint)

The model was solved using the multiple objectives ϵ -constraint method. The model used a single economic objective with an additional constraint that the risk objective is between its maximum and minimum values. The maximum risk objective was found from Table 6.3 taking current prices and the minimum from Table 6.4. The ratio between the maximum and minimum risk was 15.3. Therefore, the constraint on risk objective is:

$$Risk \leq MI \times Risk_{minimum} \quad \text{and} \quad 1 < MI < 15.3$$

The results are listed below in Table 6.6.

Table 6.6: Solution with ϵ -Constraint Method (Economic Objective)

<i>MI</i>	Rejected Chemical	Economic Objective (10 ⁶ \$/yr)	Corresponding Risk (people affected/yr)
2	ABS	506	4,420
4	ABS	588	5,380
6	ABS	588	6,090
8	PS	1,040	17,700
10	PS	1,250	22,100
12	Cumene	1,420	26,500
14	Cumene	1,510	29,700

The model was solved again using the multiple objectives ϵ -constraint method but with a single risk objective and an additional constraint that the economic objective is between its maximum and minimum values. The maximum economics objective was found from Table 6.3 taking current prices and the minimum from Table 6.4. The ratio between the maximum and minimum economics was 6.2. Therefore, the constraint on economic objective is:

$$Economic \geq M2 \times Economic_{minimum} \quad \text{and} \quad 1 < M2 < 6.2$$

The results are listed below in Table 6.7.

Table 6.7: Solution with ϵ -Constraint Method (Risk Objective)

$M2$	Rejected Chemical	Risk Objective (people affected/yr)	Corresponding Economics (10^6 \$/yr)
1	ABS	2,210	249
2	ABS	3,320	499
3	PVC	15,500	748
4	PS	16,800	998
5	Cumene	23,300	1,250
6	Cumene	28,300	1,500

Weighted L_p norm method

The model was solved with weighted L_p norm objective method; the objective function has the form:

$$Min. \quad f = \left[w1 \left(\frac{Economic - Economic^*}{Economic^*} \right)^p + w2 \left(\frac{Risk - Risk^*}{Risk^*} \right)^p \right]^{1/p}$$

Where $Economic^*$ and $Risk^*$ are, as before, objective value from single objective optimization. Different values for p were tested with the objective function, a value of $p=1$ gave similar results to the weighted method (Table 6.5), a value of $p=2$ gave the results shown in Table 6.8 and values of $p>2$ did not reach any optimal solution because the calculations reached very high numerical values when evaluating the objective.

Table 6.8: Solution with Weighted L_p Norm Objective Method ($p=2$)

w_1	Rejected Chemical	Economic Objective (10^6 \$/yr)	Risk Objective (people affected/yr)
1	Cumene	1,550	33,900
0.9	ABS	484	3,230
0.8	ABS	466	2,940
0.7	ABS	466	2,940
0.6	ABS	441	2,800
0.5	ABS	409	2,610
0.4	ABS	394	2,530
0.3	ABS	394	2,520
0.2	ABS	385	2,500
0.1	ABS	306	2,330
0	ABS	249	2,210

The solutions obtained so far are plotted to obtain the Pareto optimal curve. This curve helps to visualize the set of optimal solutions and to identify regions of the solution that should be investigated. The curve is a plot of one objective versus the other as shown in Figure 6.2. The Pareto curve has two frontiers, the bottom one is formed from all solutions (single and multiple objective) when using current prices of chemicals and the top frontier is formed when using forecasted prices. The forecasted prices are relatively higher than current prices, therefore a higher value of the economic objective is found. The curve with its two frontiers show good continuity with some gaps. To try to cover the gaps in the Pareto curve, many solution trials for the model with different combinations of objectives were done but no new solutions were generated. Possibly no solutions exist for some ranges of the objective functions. Similar discrete Pareto curves from MILP models were used efficiently by Bagajewicz and Cabrera (2003) and Bonfill et al. (2004) for decision-making.

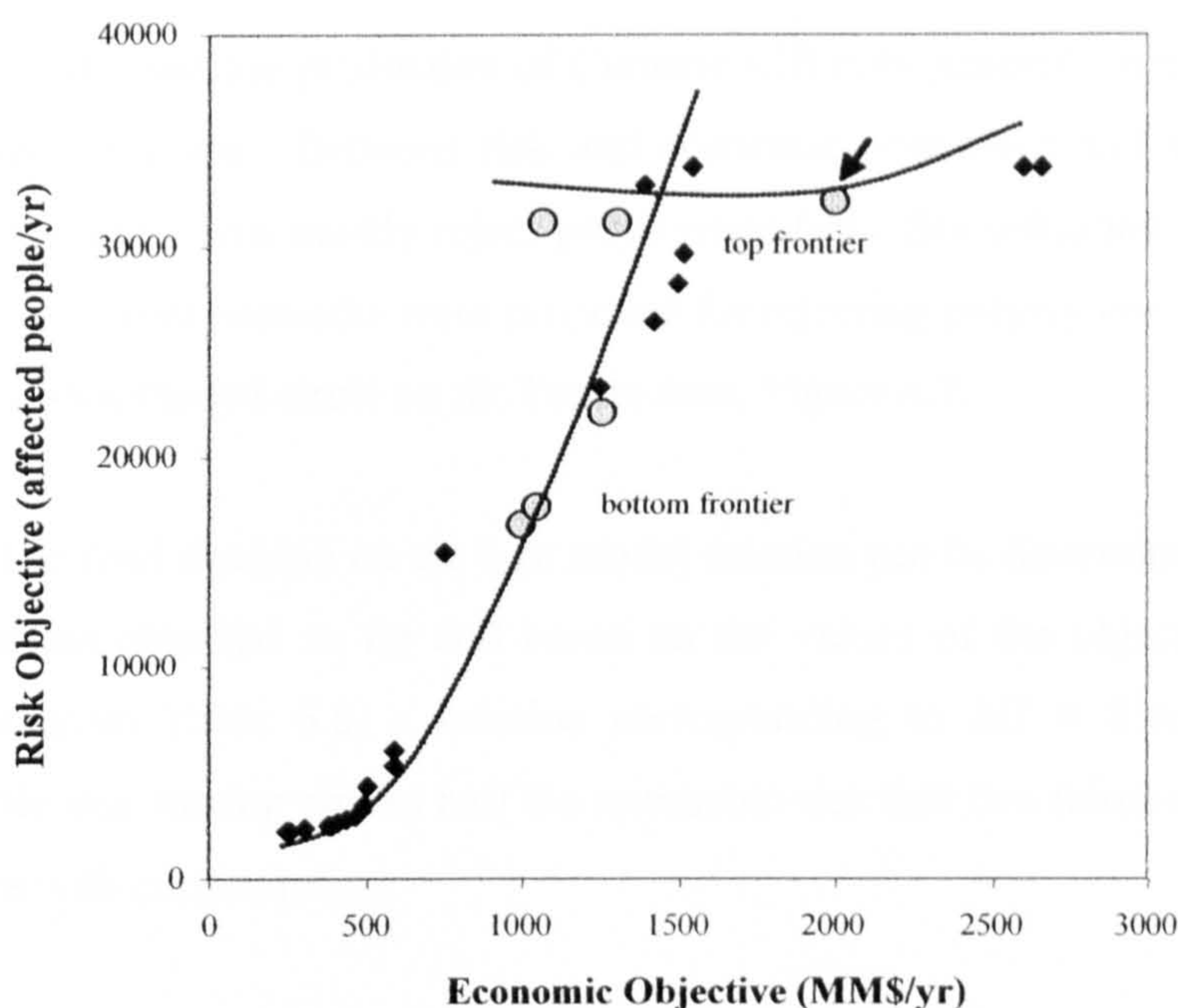


Figure 6.2: The Pareto Optimal Curve

6.5 Results Interpretation

It can be seen from the results that high values of economic gain correspond to high production risk for most petrochemical networks producing the desired final products and vice versa. The two multiple objective (MO) methods, the weighted method and the weighted L_p , give unsatisfactory results where an even spread of weights did not produce an even spread of points in objective values. Results from the weighted and the L_p MO methods were poor and were very similar to results from single objectives. Therefore weighted and L_p methods results were excluded from the final decision. Abido (2001) favoured the ε -constraint over the weighted objective after identifying a number of difficulties in its application.

Overall, the results showed that risk was minimized if ABS was rejected. The results also showed that economics was maximized with current prices if Cumene was rejected. The production of ABS needs the production of Acrylonitrile, with a very high

risk to people, and the production of Cumene will only generate minimal economic gain due to its low price. Between risk and economic objectives and also with forecasted prices, the model will mostly reject polystyrene (PS). Six solutions of the model giving only five different networks were proposed for rejecting polystyrene. These solutions are marked with a shaded circle on the Pareto curve, Figure 6.2.

The final decision on the best model solution can be determined at this stage from the solutions obtained so far and based on the values of the objective functions. ; for example, from Table 6.6, a solution corresponding to $MI = 8$ may be taken as an acceptable one, having almost half the maximum risk and two thirds maximum economic objective with current prices.

Another decision method that can be used is a manufacturing strategy tool. The tool is the GE/McKinsey matrix with "*Industry Attractiveness*" presented as the average growth rate of all chemicals in the solution network and "*Business Strength*" as the present value of the network with a 10% interest rate; this interest rate is used for most future plans in petrochemicals. The size of the circles in the matrix is the average production rate of the final product chemicals from the petrochemical network. For the "*Industry Attractiveness*", it is important to include the growth rates of all chemicals in the network and not only the final product. This will encourage the selection of an industry with attractive chemical (intermediate and final products) and it is useful if, under certain circumstances, decision-makers required to produce one of these intermediates. A useful source of chemicals growth rates are recent issues of the *Chemical Market Reporter*.

Solutions, rejecting PS, are located in the GE/McKinsey matrix and shown in Figure 6.3. Figure 6.3 indicates that some model solutions will give a petrochemical network that is strategically not very attractive and not sufficiently strong to keep its position in the world market. The best solution from the GE/McKinsey matrix shown in Figure 6.3 is found to be the highest left-most circle in the matrix and pointed at with an

arrow in Figures 6.3 and 6.2. This is considered as the best strategic solution and it is a network of 14 plants listed with their production rates in Table 6.9 and forming the network plotted in Figure 6.4. The network has the following features:

Network chemicals average growth rate = 2.91 %

Network Present value (10% interest rate) = 988 10^6 \$

Economic objective = 2,000 10^6 \$/yr

Risk objective = 31,900 people affected/yr

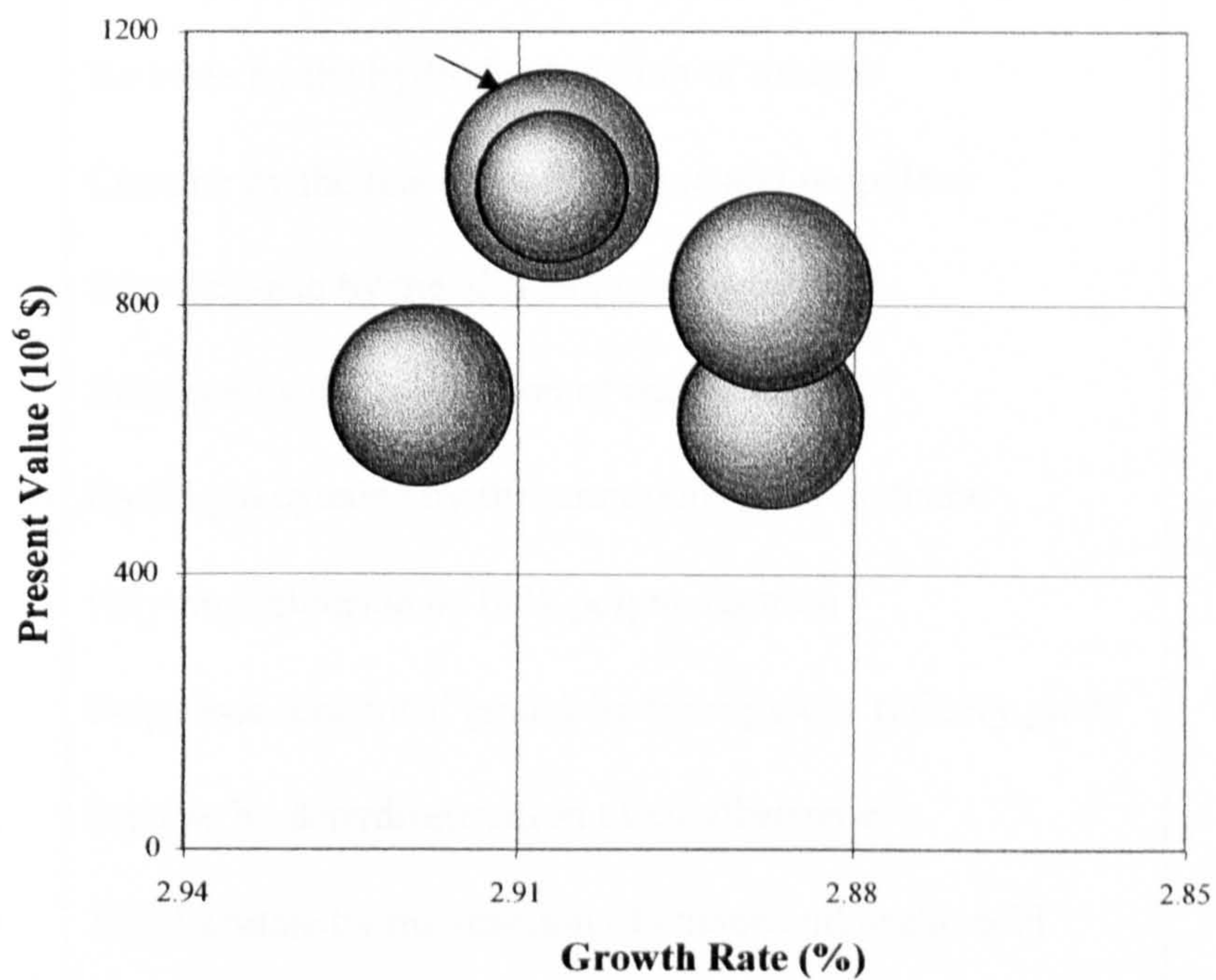


Figure 6.3: Model Solutions on the GE/McKinsey Matrix

Table 6.9: Plants Recommended by the Best Strategic Solution of the Petrochemical Model

Plant Index, <i>j</i>	Plant	Production Rate (10³ tonne/yr)
6	Acetic Acid by oxidation of N-butanol	122
12	Acetylene by the pyrolysis of ethane	447
14	Acrylonitrile by the cyanation/oxidation of ethylene	176
17	ABS by bulk/suspension polymerization	800
18	Benzene by the hydrodealkylation of toluene	633
26	Cumene by the reaction of benzene and propylene	289
28	Ethylbenzene by the alkylation of benzene	615
37	Ethylene by hydrogenation of acetylene	300
42	Hydrogen cyanide by the ammoxidation of methane	106
49	Polyvinyl chloride by bulk polymerization	272
51	Propylene (chemical grade) from propylene refinery grade	109
52	Styrene by dehydrogenation of ethylbenzene	536
59	Vinyl acetate by the reaction of ethane and acetic acid	160
62	Vinyl chloride by the hydrochlorination of acetylene	279

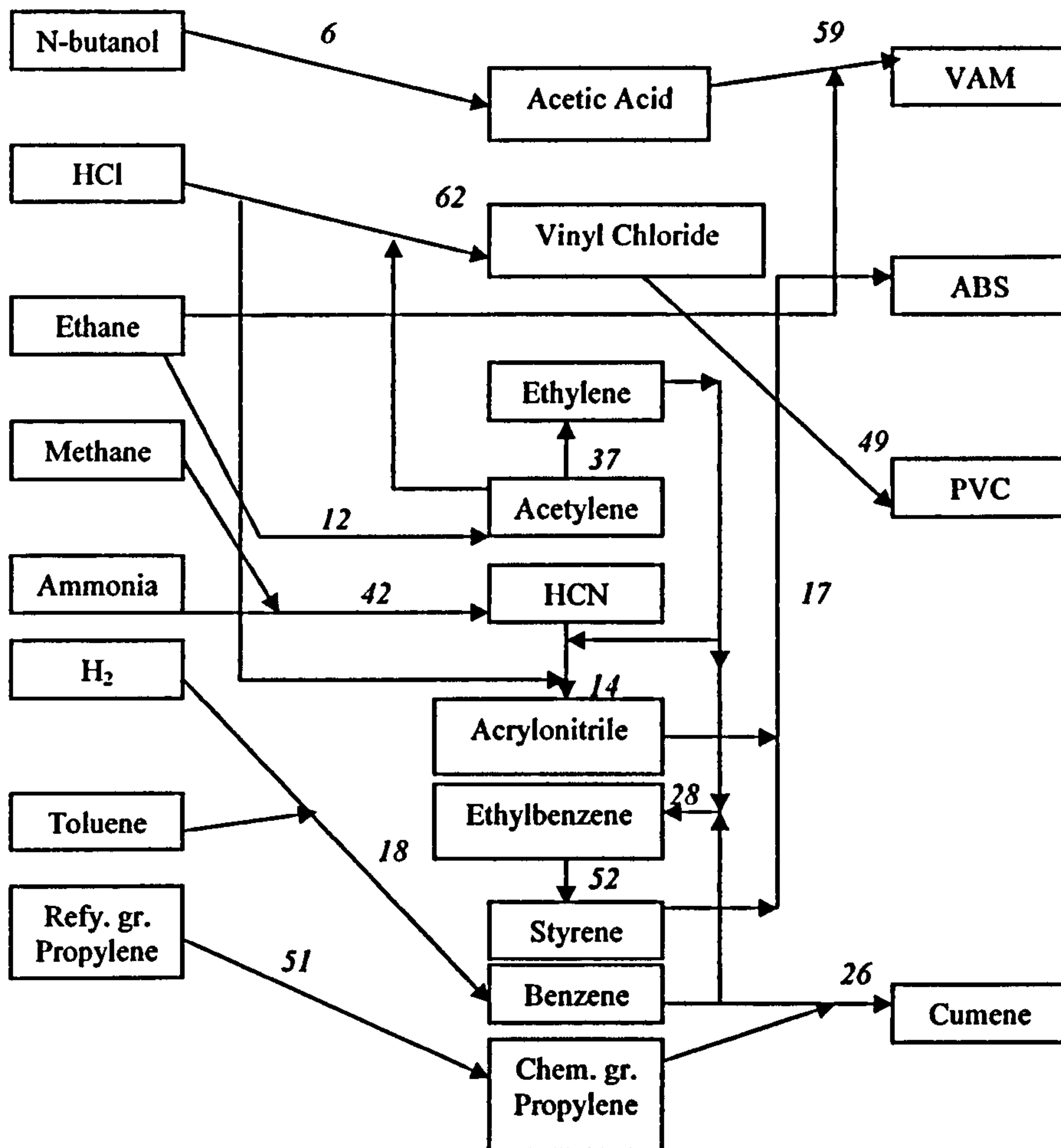


Figure 6.4: The Planned Petrochemical Network from Basic Feedstock to Final Product Chemicals (numbers indicate plant indices)




It is worth mentioning that other solutions that lie in the three cells at the top left of Figure 6.3 are also attractive depending on the decision-makers point of view. Other solutions may give lower risk, which is required in some situations. Also, the ranges used for the GE/McKinsey matrix axis are not fixed and are usually determined according to the industry low and high values of attractiveness and strength.

Single objective solutions and the final strategic solution are shown in Figure 6.5 in the form of selected plants; each plant is assigned a number (index j). Thirteen plants were selected by the economics objective and eleven by the risk objective. Seven plants are shared by both objectives; however, by examining the situation more closely, one can observe that 2 out of the 7 plants have been selected merely due to the lack of alternatives. After eliminating two such cases there remains only 5 plants which are favoured by both objectives. However, these observations suggest that, if a safer industry is desired, about 55% of the plants (with alternative routes) which have been proven to be cost efficient will have to be abandoned. Looking at Figure 6.4 again, more than 70% of the plants favoured by the two objectives were also selected by the strategic solution. This proves the validity of the proposed decision-making method to give a balanced solution between risk and economics.

Appendix C contains a paper that has been prepared from the work of Chapter 6. The paper has been accepted for publication in the journal "*Chemical Engineering Research and Design*" with the title "Decision-Making for Petrochemical Planning Using Multiobjective and Strategic Tools".

1	2	3	4	5	<u>6</u>
7	8	9	10	11	<u>12</u>
13	<u>14</u>	15	16	<u>17</u>	<u>18</u>
19	20	21	22	23	24
25	<u>26</u>	27	<u>28</u>	29	30
31	32	33	34	35	36
<u>37</u>	38	39	40	41	<u>42</u>
43	44	45	46	47	48
<u>49</u>	50	<u>51</u>	<u>52</u>	53	54
55	56	57	58	<u>59</u>	60
61	<u>62</u>				

Figure 6.5: Comparison between Single Objectives Solutions and the Final Strategic Solution.

-  Process selected by the Risk objective function
-  Process selected by the Economic objective function
-  Process selected by the Strategic tool

Risk Acceptability

Determining the acceptability of risk is often the most challenging aspect of risk assessment. Some regulators provide guidelines or criteria that can be used to interpret whether the facility under study is considered below the level of acceptable risk. The risk from the selected model solution, representing the planned petrochemical network, is 31,900 people affected per year and this includes people hospitalized, injured or dead. This risk is a theoretical maximum, or potential, risk for a chemical release accident and must be examined against the current standards and risk criteria in industrial risk assessment.

The most important question on risk acceptability that is related to this work is: If a petrochemical network is working with the current acceptable safety standards, what maximum risk is expected to result? There are many international and national standards about this aspect. One useful and clear example is in the state of Queensland, Australia. The “Guidelines for Major Hazard Facility” (Queensland Government 2002), prepared by the Chemical Hazard and Emergency Management (CHEM) unit in association with the Queensland Government presents numbers for acceptable risk criteria. In the guidelines, the target for individual fatality risk for residential and industrial sites were 1 and 50 in a million per year respectively. Squire (2001) also, gave a hierarchical statistical nature of injuries; he indicated that for each fatality, there are 30 lost-time injuries, 300 recordable injuries and 30,000 near misses injuries. These numbers add up to give an approximate theoretical maximum for affected people accompanying a fatality because evaluating a *theoretical maximum* risk needs data and analysis, not only about recorded chemical incidents but possibly about “Near Miss” incidents. A “Near Miss” is defined as an unplanned event, where a serious or minor incident would probably have occurred had circumstances been only slightly different or had the activity been continued.

Kammen (2005) gave an estimation of the number of plant workers that are expected to be in industrial areas, he estimated 20 engineers per plant and an employee to

engineer ratio of 20 to 10. The above mentioned numbers are useful for risk calculation from industrial sites.

The planned petrochemical network will be established in one of Kuwait's industrial areas, but there is one problem with Kuwait's demographic nature in that most of the inhabited areas are near the seaside and some are surrounding industrial areas. Also, many studies about the demographical and meteorological parameters and their relation to risk of plants emissions indicated that plant releases may cover all of Kuwait; see for example (Elkilani and Bouhamra 2002). From all of the above risk criteria and facts, if the industrial and residential population is taken as Kuwait's entire population, 2,335,648 in 2005, and the planned industry of 14 plants is operating within acceptable safety standards the following can be calculated:

- Estimated total number of employees for the plants = 5880 employee.
- Acceptable fatality rate on industrial sites = 0.294 per year
- Acceptable fatality rate in residential areas = 2.33 per year
- Total acceptable fatality rate = 2.62 per year
- Maximum affected people = 79,600 per year

The last number is the potential maximum risk on people according to Squire (2001) accident analysis and according to the current industry standards and criteria. Compared to the results of risk for the selected network which was calculated from the proposed risk index, 31,900 people affected per year, the planned petrochemical network is expected to operate, in Kuwait, within currently acceptable risk criteria.

6.6 Conclusion

The petrochemical industry has been structured for two design objectives of maximum economic gain and minimum operational risk. In this chapter, the new risk index was used as an objective for route selection in planning the petrochemical networks and the economic objective was used with current and forecasted prices. Considering the

two objectives independently, the bounding structure of the industry has been generated and, using the concept of multiple objectives programming, a set of attainable industrial structures which fall within the bounding structure were identified. Results indicate that high economic gain is usually accompanied by high risk on people, and a balanced industry should have economics and safety as importance decision tools. However, it can be shown that, in this case, where the multiple objectives (risk and economics) and single objective (forecasted economics) exist, the values of the objectives are not the only important issues. The variables selected, or rejected, in the optimal solution have the same importance.

Chapter 6 has also provided the tools for deciding on future strategy of an industry. Any development in the petrochemical industry should take the growth of the product and its size into its strategic plan. A good plan will insure not only short-term profit but also most importantly, the need for sustainability of success represented by a good business strategy. The method adopted in this work provides the design engineer and the industrial planner the necessary mathematical tools for planning the operation of a petrochemical network which is sound economically and at the same time responsive to safety and risk constraints.

Chapter 7

Conclusions and Recommendations for Future Work

In this work, a model was formulated to plan the development of Kuwait's petrochemical industry by taking into consideration two of the major forces that shape the industry in the world, namely economics and plant safety. There are number of conclusions that can be derived from this study.

First of all, petrochemicals are the most feasible industries for development in Kuwait. This country has the advantage of good oil resources and good international relations for marketing. If successful, the development of the Kuwait petrochemical industry would provide the best prospect for steady economic growth with decreasing emphasis on the export of oil. The expected economic added-value from producing petrochemicals would insure less income dependence on crude oil.

The changing economic environment gives importance to forecasting variables that affect the industry. Not only the short-range forecast but also the long-range forecast is essential, especially when past trends in the variables of interest are analysed. Well known cycles are now considered as strong drivers of the economy throughout the world and the petrochemical industry should select its plans according to these cycles. Also, there is a clear relationship between changes in oil price and prices in the petrochemical market, the lag effect in this relation would provide Kuwait with more stability from the income generated from petrochemicals, and therefore give a better opportunity of making necessary adjustments.

On the other hand, petrochemical plants are a major source of risk to the people and the environment. Safety is expected to have a serious impact on the industry if it is not well planned, and included in all stages of planning and plant selection. Future development of a petrochemical plant will not be possible if there is a possibility of

considerable harmful effects on people. Including the predicted harmful effect of chemical accidents in the planning procedure, incorporates the concept of inherent safety. To include safety in planning of the petrochemical industry, a new risk index was developed to estimate the possible effect of a chemical accident on people. This risk index was used effectively as an objective function within the planning model.

The two major forces of economics and safety that were used as a basis for planning lead to many possible acceptable ideas for development. The decision is not easy and it needs tools to assist in providing the confidence in the final decision. Using a strategic tool to select the final decision for planning the industry provides such confidence in the final results. It allows different plans to be analyzed in terms of dimensions of value to the industry. A general overview of this work is a decision based on four requirements; two objectives for the MILP model and two metrics for the strategic tool. Decomposing the overall problem into two levels with two requirements (objectives) in each level is undertaken to provide good visualization of the results and decision options. The Pareto curve and the GE/McKinsey matrix were the visualization tools used for the first and the second levels respectively. Combining the four requirements as objectives for the model, i.e. economic gain, risk, growth rate and present value, will make results visualisation more complex.

The proposed approach and the decision-making tool can be applied for more than two objectives in the MILP model. The steps will be similar with a difference only in generating the solutions in the MO optimization stage. When the number of objectives increase, the procedure for generating the Pareto optimal solutions will be more comprehensive.

Although it was applied to Kuwait, this thesis proposes a systematic decision-making procedure and a quantitative data analysis method for planning a development in any petrochemical industry. Reaching the final planning decision comprised the generation of possible plans from the model solution. Not all steps must be followed nor

all combinations of the objectives must be tested. With the decision-makers experience and requirements, a final plan can be achieved using only part of the model solution steps. This work used modelling, quantification, forecasting and other analytical techniques for planning. Although a great part of the planning process will always be intuitive, analytical techniques, modelling, and optimization can be of great value and can permit vast improvements in the planning process.

Finally, in order for the model to produce more useful results, the following key recommendations are identified:

- Further work is needed to try to improve the accuracy of the new risk index by incorporating data from other accidents databases in evaluating its terms. Using other accidents databases is required to refine the simplified relationship between the number of people affected and toxicity data (Equation 5.1). Additionally, results predicted by the index must be compared with other published methods (e.g., Dow indices) based on a number of different case studies. The aim is to test the ability of this proposed simple index to evaluate the relative risk of industrial process.
- It has been identified that chemical accidents are associated with process corrosion; this relation needs to be properly tested by data with extended range of accident frequency and corrosion resistance.
- The petrochemical model provided a decision-making tool for planning the industry. It is evident that further effort needs to be placed in model data input to account for the changes in the industry. This is where the model has the most room for improvement. One way to accomplish that is by sensitivity analysis on the major data sets in the model such as process risk and demand.
- The use of two objective functions with the model could be extended to account for other industry requirements such as environmental protection. In addition, the strategic tool, GE / McKinsey matrix, can be transferred into an objective

function and included in the model. Although, increasing the number of objectives will increase the computational difficulty of the model, however, it will provide confidence that the selected model solution will provide a plan that satisfies more needs.

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Appendix A

Plants Included in the Petrochemical Model

Table A.1, shown in the following pages, summarizes the plants, which are included in the petrochemical model. The coefficients given for the chemicals in each plant are the tonnes of chemical produced or consumed per tonne of main product (the coefficient is 1.0 for the main product by definition). It is used in the model as ϕ_{ij} the output coefficient of chemical i from plant j . Materials consumed are differentiated from materials produced by negative coefficient. Reagents are not included in this tabulation. Also the minimum economic production rate and the fixed capital, based on the year 1992, is listed for each plant. All the data in this appendix were taken from SRI reports (1992).

Table A.1: Plant Included in the Model

<i>j</i>	Plant	Output coefficient <i>t</i> <i>o_{ij}</i>	Fixed Capital (10 ⁶ \$)	Minimum Eco. Prod. Rate (10 ³ tonne/yr.)
1	Acetaldehyde # 1: One Step Oxidation from Ethylene Acetaldehyde Ethylene Hydrogen Chloride	1 -0.68 -0.0033	74	67.5
2	Acetaldehyde # 2: Two Step Oxidation from Ethylene Acetaldehyde Ethylene (Hydrogen Chloride)	1 -0.68 -0.023	74	67.5
3	Acetaldehyde # 3: Oxidation of Ethanol Acetaldehyde Ethanol	1 -1.2	74	67.5
4	Acetic Acid # 1: Low Pressure Carbonylation of Methanol Acetic Acid Carbon monoxide Methanol	1 -0.61 -0.57	185.5	180
5	Acetic Acid # 2: Air Oxidation of Acetaldehyde Acetic Acid Acetaldehyde	1 -0.78	74.1	67.5
6	Acetic Acid # 3: Oxidation of n-Butanol Acetic Acid n-Butanol	1 -0.83	74.1	67.5
7	Acetic Acid # 4 : Direct Oxidation of n-Butylenes Acetic Acid n-Butylenes (1- and 2-) Butenes -Mixed n-, iso-, dienes, ... Formic Acid	1 -1.01 0.09 0.06	74.1	67.5
8	Acetylene # 1 : Submerged Flame Process Acetylene Fuel Oil (High Sulfur) Synthesis Gas 2:1 Fuel Gas Ethylene	1 -8.34 5.47 1.3 1.15	32.2	22.5
9	Acetylene # 2 : Hydration of Calcium Carbide Acetylene Coke	1 -1.86	32.2	22.5
10	Acetylene # 3 : Pyrolysis of Methane (Partial Oxidation) Acetylene Methane Synthesis Gas 2:1	1 -4.23 4.01	32.2	22.5

11	Acetylene # 4 : Pyrolysis of Naphtha (One-Stage Partial Oxidation) Acetylene Naphtha Fuel Gas Coke	1 -4.31 0.84 -0.01	32.2	22.5
12	Acetylene # 5 : Pyrolysis of Ethane (Regenerative Process) Acetylene Ethane Fuel Gas Fuel Oil (Low Sulfur)	1 -3 0.57 0.18	32.2	22.5
13	Acrylonitrile # 1: Ammoxiation of Propylene Acrylonitrile Chemical Grade Propylene Ammonia Sulfuric Acid	1 -1.2 -0.428 -0.152	364.6	90
14	Acrylonitrile # 2 : Cyanation/Oxidation of Ethylene Acrylonitrile Ethylene Hydrogen Cyanide Hydrogen Chloride	1 -0.76 -0.6 -0.17	364.6	90
15	Acrylonitrile-Butadiene-Styrene # 1:By Emulsion/Emulsion Polymerization Acrylonitrile-Butadiene-Styrene Styrene Butadiene Acrylonitrile Sodium Hydroxide	1 -0.5409 -0.2451 -0.1937 -0.0042	83.6	25
16	Acrylonitrile-Butadiene-Styrene # 2: By Suspension/Emulsion Polymerization Acrylonitrile-Butadiene-Styrene Styrene Butadiene Acrylonitrile	1 -0.54 -0.25 -0.19	70.8	25
17	Acrylonitrile-Butadiene-Styrene # 3: Bulk/Suspension Polymerization Acrylonitrile-Butadiene-Styrene Styrene Acrylonitrile Polybutadiene Rubber	1 -0.67 -0.22 -0.07	70.8	25
18	Benzene # 1: Hydrodealkylation of Toluene Benzene Toluene Methane Hydrogen	1 -1.2 0.24 -0.07	44.5	125

19	Benzene # 2 : Disproportion of Toluene Benzene Toluene Xylenes (Mixed) Fuel Gas	1 -2.69 1.16 0.01	44.5	100
20	Butadiene # 1 : Dehydrogenation of n-Butylenes Butadiene n-Butylenes (1- and 2-) Ammonia Sulfuric Acid	1 -1.46 -0.01 -0.01	61.1	25
21	Butadiene # 2 : Oxidative Dehydrogenation of n-Butylenes Butadiene n-Butylenes (1- and 2-)	1 -1.316	61.1	25
22	Butadiene # 3 : Dehydrogenation of n-Butane Butadiene n-Butane	1 -1.793	61.1	25
23	Butadiene # 4 : By Extractive Distillation Butadiene C-4 fraction - Mixed butanes , -enes, ... Butenes- Mixed n-, iso-, dienes, ...	1 -2.374 1.3	61.1	25
24	Carbon monoxide # 1 : Steam Reforming of Natural Gas Carbon monoxide Methane Hydrogen	1 -0.635 0.23	160	27.3
25	Carbon monoxide # 2 : From Naphtha Carbon monoxide Naphtha Hydrogen	1 -0.8 0.25	160	27.3
26	Cumene # 1 : Reaction of Benzene and Propylene Cumene Benzene Chemical Grade Propylene	1 -0.6733 -0.3783	33.7	60
27	Ethanol # 1 : Hydration of Ethylene Ethanol Ethylene Fuel Gas Hydrogen Sodium Hydroxide	1 -0.7477 0.06 -0.0031 -0.0026	191.3	125
28	Ethylbenzene # 1: Alkylation of Benzene Ethylbenzene Benzene Ethylene Fuel Oil (Low Sulfur)	1 -0.74 -0.27 0.01	69.6	250

29	Ethylene # 1 : Steam Cracking of Ethane-Propane (50-50wt%)		501	250
	Ethylene	1		
	Ethane	-0.815		
	Propane	-0.815		
	Fuel Gas	0.36		
	Chemical Grade Propylene	0.1697		
	C-4 fraction - Mixed butanes , -enes, ...	0.0601		
30	Ethylene # 2 : Steam Cracking of Gas Oil (High Severity)		839.2	250
	Ethylene	1		
	Gas Oil	-3.9042		
	Gasoline	0.6426		
	Chemical Grade Propylene	0.6032		
	Fuel Oil (Low Sulfur)	0.5361		
	C-4 fraction - Mixed butanes , -enes, ...	0.3461		
	Sodium Hydroxide	-0.0022		
31	Ethylene # 3 : Steam Cracking of Naphtha (High Severity)		762	250
	Ethylene	1		
	Naphtha	-3.17		
	Gasoline	0.7061		
	Fuel Gas	0.5		
	Chemical Grade Propylene	0.4539		
	C-4 fraction - Mixed butanes , -enes, ...	0.307		
	Fuel Oil (Low Sulfur)	0.1008		
	Sodium Hydroxide	-0.00035		
32	Ethylene # 4 : Pyrolysis of Ethane		519.4	250
	Ethylene	1		
	Ethane	-1.22		
	Fuel Gas	0.14		
	C-4 fraction - Mixed butanes , -enes, ...	0.04		
	Chemical Grade Propylene	0.02		
	Gasoline	0.02		
	Sodium Hydroxide	-0.01		
33	Ethylene # 5 : Pyrolysis of Propane		636.2	250
	Ethylene	1		
	Propane	-2.12		
	Fuel Gas	0.6		
	Chemical Grade Propylene	0.28		
	C-4 fraction - Mixed butanes , -enes, ...	0.11		
	Gasoline	0.1		
	Fuel Oil (Low Sulfur)	0.03		

34	Ethylene # 6 : Pyrolysis of Naphtha (Low Severity)		108	250
	Ethylene	1		
	Naphtha	-3.9		
	Gasoline	1.3		
	Fuel Gas	0.58		
	Chemical Grade Propylene	0.42		
	Fuel Oil (Low Sulfur)	0.3		
	C-4 fraction - Mixed butanes , -enes, ...	0.3		
35	Ethylene # 7 : Pyrolysis of Gas Oil (Low Severity)		108	250
	Ethylene	1		
	Gas Oil	-6.02		
	Fuel Oil (Low Sulfur)	2.16		
	Gasoline	1.1		
	Chemical Grade Propylene	0.85		
	C-4 fraction - Mixed butanes , -enes, ...	0.53		
	Fuel Gas	0.39		
36	Ethylene # 8 : Steam Cracking of Gas Oil (Medium Severity)		108	250
	Ethylene	1		
	Gas Oil	-4.8		
	Fuel Oil (Low Sulfur)	1.45		
	Gasoline	0.73		
	Chemical Grade Propylene	0.63		
	C-4 fraction - Mixed butanes , -enes, ...	0.55		
	Fuel Gas	0.43		
37	Ethylene # 9 : Hydrogenation of Acetylene		108	250
	Ethylene	1		
	Fuel Gas	1.24		
	Acetylene	-1.09		
	Hydrogen	-0.31		
38	Ethylene # 10 : Dehydration of Ethanol		108	250
	Ethylene	1		
	Ethanol	1.75		
39	Ethylene # 11 : Pyrolysis of Butane		108	250
	Ethylene	1		
	n-Butane	-2.5		
	Fuel Gas	0.58		
	Chemical Grade Propylene	0.43		
	C-4 fraction - Mixed butanes , -enes, ...	0.26		
	Gasoline	0.2		
	Fuel Oil (Low Sulfur)	0.04		
40	Ethylene Dichloride # 1 : Chlorination of Ethylene		22.7	180
	Ethylene Dichloride	1		
	Chlorine	-0.7		
	Ethylene	-0.36		

41	Ethylene Dichloride # 2 : Oxychlorination of Ethylene Ethylene Dichloride Hydrochloric Acid Ethylene	73.4 1 -0.94 -0.34	73.4	180
42	Hydrogen Cyanide # 1: Ammoxidation of Methane Hydrogen Cyanide Methane Ammonia	1 -1.02 -0.75	101.6	30
43	Methanol # 1 : From Methane (Low Pressure) Methanol Methane	1 -0.49	345.4	410
44	Methanol # 2 : From Methane (Medium Pressure) Methanol Methane	1 -0.49	345.4	410
45	Methanol # 3 : From Methane (High Pressure) Methanol Methane	1 -0.5	345.4	410
46	Methanol # 4 : From Syn. Gas (High Pressure) Methanol Synthesis Gas 3:1 Carbon Dioxide	1 -0.923 -0.32	345.4	410
47	Methanol # 5 : From Syn. Gas (Low Pressure) Methanol Synthesis Gas 3:1 Carbon Dioxide Sulfuric Acid	1 -0.89 -0.36 -0.02	345.4	410
48	Polystyrene (Crystal Grade) # 1 : By Bulk Polymerization Polystyrene (Crystal Grade) Styrene	1 -1.02	18.4	15
49	Polyvinyl Chloride # 1 : Bulk Polymerization Polyvinyl Chloride Vinyl Chloride Sodium Hydroxide	1 -1.025 -0.0005	91	50
50	Polyvinyl Chloride # 2 : Suspension Polymerization Polyvinyl Chloride Vinyl Chloride Sodium Hydroxide Hydrogen Chloride Toluene Polyvinyl Alcohol	1 -1.025 -0.0041 -0.0033 -0.0023 -0.0015	164.3	90
51	Chemical Grade Propylene # 1 : Chemical Grade Propylene from Refinery Grade Chemical Grade Propylene Refinery Grade Propylene Propane	1 -1.33 0.33	49.1	90

52	Styrene # 1 : Dehydrogenation of Ethylbenzene		216	225
	Styrene	1		
	Ethylbenzene	-1.148		
	Toluene	0.052		
	Benzene	0.032		
53	Styrene # 2 : From Ethylbenzene by Hydroperoxide Process		216	225
	Styrene	1		
	Ethylbenzene	-1.139		
	Propylene Oxide	0.408		
	Chemical Grade Propylene	-0.3248		
	Sodium Hydroxide	-0.013		
54	Sulfuric Acid # 1 : Double Absorption Process		80.8	320
	Sulfuric Acid	1		
	Sulfur	-0.328		
55	Synthesis gas 3:1 # 1 : Partial Oxidation of Residual Oil		167.1	937
	Synthesis gas 3:1	1		
	Fuel Oil (High Sulfur)	-0.91		
56	Synthesis gas 3:1 # 2 : Methane Reforming		167.1	937
	Synthesis gas 3:1	1		
	Methane	-0.49		
57	Vinyl Acetate # 1 : Reaction of Ethylene and Acetic Acid		126.2	67.5
	vinyl Acetate	1		
	Acetic Acid	-0.704		
	Ethylene	-0.393		
58	Vinyl Acetate # 2 : Reaction of Acetylene and Acetic Acid		91.8	67.5
	Vinyl Acetate	1		
	Acetic Acid	-0.72		
	Acetylene	-0.32		
	Acetaldehyde	0.01		
59	Vinyl Acetate # 3 : Reaction of Ethane and Acetic Acid		91.8	67.5
	Vinyl Acetate	1		
	Acetic Acid	-0.76		
	Ethane	-0.44		
60	Vinyl Chloride # 1 : Chlorination and Oxychlorination of		218.7	250
	Ethylene			
	Vinyl Chloride	1		
	Chlorine	-0.606		
	Ethylene	-0.475		
	Sodium Hydroxide	-0.007		
61	Vinyl Chloride # 2 : Dehydrochlorination of Ethylene		95.9	125
	Dichloride			
	Vinyl Chloride	1		
	Ethylene Dichloride	-1.66		
	Hydrogen Chloride	0.61		

62	Vinyl Chloride # 3 : Hydrochlorination of Acetylene		95.9	200
	Vinyl Chloride	1		
	Hydrogen Chloride	-0.6		
	Acetylene	-0.43		
	Sodium Hydroxide	-0.01		

Appendix B

Sample Model Program Output File

This appendix contains one output list file from the model's program. The output file is the solution obtained from GAMS commercial optimization package.

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Thesis

6 SETS

7 I constraints /1*26/

8 J process /1*70/

9

10

11 TABLE A(I,J) constraints coefficients

12	1	2	3	4	5	6	7	8	9	10	11	
			12	13	14	15	16	17	18	19	20	
13	1	1	1	0	-0.78	0	0	0	0	0	0	
			0	0	0	0	0	0	0	0	0	
14	2	0	0	1	1	1	1	0	0	0	0	
			0	0	0	0	0	0	0	0	0	
15	3	0	0	0	0	0	0	1	1	1	1	
			1	0	0	0	0	0	0	0	0	
16	4	0	0	0	0	0	0	0	0	0	0	
			0	1	1	-1.937	-.19	-.22	0	0	0	0
17	5	0	0	0	0	0	0	0	0	0	0	
			0	0	0	1	1	1	0	0	0	
18	6	0	0	0	0	0	0	0	0	0	0	
			0	0	0	0	0	0	1	1	0	
19	7	0	0	0	0	0	0	0	0	0	0	
			0	0	0	-2.451	-.25	0	0	0	0	1
20	8	0	0	-0.61	0	0	0	0	0	0	0	
			0	0	0	0	0	0	0	0	0	
21	10	0	0	-1.3	0	0	0	0	0	0	0	
			0	0	0	0	0	0	0	0	0	
22	12	-0.6	-0.68	0	0	0	0	0	1.15	0	0	0
			0	0	-0.76	0	0	0	0	0	0	
23	14	0	0	0	0	0	0	0	0	0	0	
			0	0	-0.6	0	0	0	0	0	0	
24	15	0	0	0	-0.57	0	0	0	0	0	0	
			0	0	0	0	0	0	0	0	0	
25	18	0	0	0	0	0	0	0	0	0	0	
			0	-1.2	0	0	0	0	0	0	0	
26	19	0	0	0	0	0	0	0	0	0	0	
			0	0	0	-0.5409	-.54	-.67	0	0	0	0
27	20	0	0	0	0	0	0	0	0	0	0	
			0	-0.152	0	0	0	0	0	0	-0.01	
28	24	0	0	0	0	0	0	0	0	0	0	
			0	0.428	0	0	0	0	0	0	0.01	
29	26	0	0	0	0	0	0	0	0	0	4.31	
			0	0	0	0	0	0	0	0	0	
30	+	21	22	23	24	25	26	27	28	29	30	31
			32	33	34	35	36	37	38	39	40	
31	3	0	0	0	0	0	0	0	0	0	0	
			0	0	0	0	0	-1.09	0	0	0	
32	6	0	0	0	0	-0.6733	0	-0.74	0	0	0	
			0	0	0	0	0	0	0	0	0	
33	7	1	1	1	0	0	0	0	0	0	0	
			0	0	0	0	0	0	0	0	0	
34	8	0	0	0	1	1	0	0	0	0	0	
			0	0	0	0	0	0	0	0	0	
35	9	0	0	0	0	0	1	0	0	0	0	

Thesis

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98  PARAMETER CAP(J) Fixed capital /1 74,2 74,3 74,4 185.5,5 74.1,6 74.1,7
    74.1,8 32.2,9 32.2,10 32.2,11 32.2,12 32.2,
99    13 364.6,14 364.6,15 83.6,16 70.8,17
    70.8,18 44.5,19 44.5,20 61.1,21 61.1,22 61.1,23 61.1,
100   24 160,25 160,26 33.7,27 191.3,28 69.6,
    29 561,30 839.2,31 762,32 519.4,33 636.2,
101   34 108,35 108,36 108,37 108,38 108,39 108,40 22.7,41 73.4,42 101.6,43 345.4,
102   44 345.4,45 345.4,46 345.4,47 345.4,48
    18.4,49 91,50 164.3,51 49.1,52 216,53 216,54 80.8,55 167.1,56 167.1,
103   57 126.2,58 91.8,59 91.8,60 218.7,61 95.9,62 95.9,63 0,64 0,65 0,66 0,67 0/;
104
105
106
107  VARIABLES X(J),Y(J),Z;
108  POSITIVE VARIABLES X(J);
109  BINARY VARIABLES Y(J);
110
111
112
113  EQUATIONS ASSI(I),LIM1(J),LIM2(J),LIM3,S1,S2,S3,S4,S6,S7,S8,S9,S10,
114    S11,S12,S13,S14,S15,S16,S17,S19,S20,
115    S21,S22,S23,S27,S29,S30,OBJ;
116  ASSI(I).. SUM(J,A(I,J)*X(J))=E=0;
117  LIM1(J).. X(J)-B(J)*Y(J)=G=0;
118  LIM2(J).. X(J)-1000*Y(J)=L=0;
119  LIM3.. SUM(J,Y(J)*CAP(J))=L=10000;
120
121
122
123
124  S1.. Y("1")+Y("2")+Y("3")=L=1;
125  S2.. Y("7")+Y("4")+Y("5")+Y("6")=L=1;
126  S3.. Y("8")+Y("9")+Y("10")+Y("11")+Y("12")=L=1;
127  S4.. Y("14")+Y("13")=L=1;
128  S6.. Y("16")+Y("17")+Y("15")=L=1;
129  S7.. Y("18")+Y("19")=L=1;
130  S8.. Y("20")+Y("21")+Y("22")+Y("23")=L=1;
131  S9.. Y("25")+Y("24")=L=1;
132  S10.. Y("26")=L=1;
133  S11.. Y("27")=L=1;
134  S12.. Y("28")=L=1;
135  S13.. Y("29")+Y("30")+Y("31")+Y("32")+Y("33")+Y("34")+Y("35")+Y("36")
    +Y("37")+Y("38")+Y("39")=L=1;
136  S14.. Y("40")+Y("41")=L=1;
137  S15.. Y("42")=L=1;
138  S16.. Y("43")+Y("44")+Y("45")+Y("46")+Y("47")=L=1;
139  S17.. Y("48")=L=1;
140  S19.. Y("49")+Y("50")=L=1;
141  S20.. Y("51")=L=1;
142  S21.. Y("52")+Y("53")=L=1;
143  S22.. Y("54")=L=1;
144  S23.. Y("55")+Y("56")=L=1;
145  S27.. Y("57")+Y("58")+Y("59")=L=1;

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146 S29.. Y("60")+Y("61")+Y("62")=L=1;
147 S30.. Y("63")+Y("64")+Y("65")+Y("66")+Y("67")=E=4;
148 w1=0;
149 w2=1;
150
151 OBJ.. Z=E=SUM(J,w2*RI(J)*X(J)/2208-w1*ADD(J)*X(J)/154558);
152
153
154 F=4;
155 X.UP("63")=200*F;
156 X.UP("64")=40*F;
157 X.UP("65")=68.039*F;
158 X.UP("66")=72.165*F;
159 X.UP("67")=40*F;
160 X.UP("68")=575.765;
161 X.UP("69")=16.371;
162 X.UP("70")=2500;
163
164
165 MODEL THESIS /ALL/;
166
167 OPTION LIMROW=0;
168 OPTION LIMCOL=0;
169 OPTION MIP=CPLEX;
170 OPTION ITERLIM=60000;
171 SOLVE THESIS USING MIP MINIMIZING Z;
172
173     PARAMETER    risk
174                  economy;
175 risk = SUM(J, RI(J)*X.L(J));
176 economy = SUM(J, ADD(J)*X.L(J));
177
178 DISPLAY risk, economy;

```

COMPILATION TIME = 0.010 SECONDS 0.8 Mb WIN205-130

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Thesis
Model Statistics SOLVE THESIS USING MIP FROM LINE 171

MODEL STATISTICS

BLOCKS OF EQUATIONS	29	SINGLE EQUATIONS	192
BLOCKS OF VARIABLES	3	SINGLE VARIABLES	141
NON ZERO ELEMENTS	605	DISCRETE VARIABLES	70

GENERATION TIME = 0.050 SECONDS 1.6 Mb WIN205-130

EXECUTION TIME = 0.050 SECONDS 1.6 Mb WIN205-130

SOLVE SUMMARY

MODEL THESIS OBJECTIVE Z
TYPE MIP DIRECTION MINIMIZE
SOLVER CPLEX FROM LINE 171

**** SOLVER STATUS 1 NORMAL COMPLETION
**** MODEL STATUS 1 OPTIMAL
**** OBJECTIVE VALUE 1.0001

RESOURCE USAGE, LIMIT 0.140 1000.000
ITERATION COUNT, LIMIT 193 60000

GAMS/Cplex Jan 31, 2002 WIN.CP.CP 20.5 021.022.039.VIS For Cplex 7.5
Cplex 7.5.0, GAMS Link 21
Licensed for 1 use of lp, mip and barrier.
Proven optimal solution.

MIP Solution: 1.000148 (193 iterations, 2 nodes)
Final LP: 1.000148 (0 iterations)
Best integer solution possible: 1.000148
Absolute gap: 0.000000
Relative gap: 0.000000

--- EQU ASSI

	LOWER	LEVEL	UPPER	MARGINAL
1
2	.	.	.	-0.001
3
4
5
6	.	.	.	2.8727E-4
7
8
9	.	.	.	EPS
10
11	.	.	.	0.002
12	.	.	.	6.0740E-4
13	.	.	.	7.6211E-4
14
15
16	.	.	.	EPS
17	.	.	.	EPS
18	.	.	.	-0.001
19	.	.	.	-4.061E-4
20
21
22	.	.	.	EPS
23	.	.	.	-1.889E-4

Thesis

EQU ASSI

	LOWER	LEVEL	UPPER	MARGINAL
24
25
26

--- EQU LIM1

	LOWER	LEVEL	UPPER	MARGINAL
1	.	.	+INF	.
2	.	.	+INF	.
3	.	.	+INF	.
4	.	.	+INF	.
5	.	.	+INF	.
6	.	.	+INF	0.002
7	.	.	+INF	.
8	.	.	+INF	.
9	.	.	+INF	.
10	.	.	+INF	.
11	.	.	+INF	.
12	.	.	+INF	.
13	.	.	+INF	.
14	.	.	+INF	.
15	.	.	+INF	.
16	.	.	+INF	.
17	.	.	+INF	.
18	. 28.781	.	+INF	.
19	.	.	+INF	.
20	.	.	+INF	.
21	.	.	+INF	.
22	.	.	+INF	.
23	.	.	+INF	.
24	.	.	+INF	.
25	.	.	+INF	.
26	. 4.428	.	+INF	.
27	.	.	+INF	.
28	. 11.840	.	+INF	.
29	.	.	+INF	.
30	.	.	+INF	.
31	.	.	+INF	.
32	.	.	+INF	.
33	. 7.047	.	+INF	.
34	.	.	+INF	.
35	.	.	+INF	.
36	.	.	+INF	.
37	.	.	+INF	.
38	.	.	+INF	.
39	.	.	+INF	.
40	.	.	+INF	.
41	. 27.500	.	+INF	.
42	.	.	+INF	.

Thesis

EQU LIM1				
	LOWER	LEVEL	UPPER	MARGINAL
43	.	.	+INF	.
44	.	.	+INF	.
45	.	.	+INF	.
46	.	.	+INF	.
47	.	.	+INF	.
48	.	63.431	+INF	.
49	.	71.951	+INF	.
50	.	.	+INF	.
51	.	.	+INF	.
52	.	.	+INF	0.005
53	.	.	+INF	.
54	.	.	+INF	.
55	.	.	+INF	.
56	.	.	+INF	.
57	.	.	+INF	.
58	.	.	+INF	.
59	.	21.316	+INF	.
60	.	.	+INF	.
61	.	.	+INF	0.004
62	.	.	+INF	.
63	.	.	+INF	.
64	.	21.316	+INF	.
65	.	71.951	+INF	.
66	.	4.428	+INF	.
67	.	63.431	+INF	.
68	.	.	+INF	.
69	.	.	+INF	.
70	.	.	+INF	.

--- EQU LIM2				
	LOWER	LEVEL	UPPER	MARGINAL
1	-INF	.	.	.
2	-INF	.	.	.
3	-INF	.	.	.
4	-INF	.	.	.
5	-INF	.	.	.
6	-INF	-932.500	.	.
7	-INF	.	.	.
8	-INF	.	-4.237E-4	.
9	-INF	.	.	.
10	-INF	.	.	.
11	-INF	.	.	.
12	-INF	.	.	.
13	-INF	.	.	.
14	-INF	.	.	.
15	-INF	.	.	.
16	-INF	.	.	.
17	-INF	.	.	.

Thesis

EQU LIM2

	LOWER	LEVEL	UPPER	MARGINAL
18	-INF	-891.219	.	.
19	-INF	.	.	.
20	-INF	.	.	.
21	-INF	.	.	.
22	-INF	.	.	.
23	-INF	.	.	.
24	-INF	.	.	.
25	-INF	.	.	.
26	-INF	-935.572	.	.
27	-INF	.	.	.
28	-INF	-908.160	.	.
29	-INF	.	.	.
30	-INF	.	.	.
31	-INF	.	.	.
32	-INF	.	-2.339E-4	.
33	-INF	-912.953	.	.
34	-INF	.	.	.
35	-INF	.	.	.
36	-INF	.	.	.
37	-INF	.	-4.028E-4	.
38	-INF	.	-3.959E-4	.
39	-INF	.	.	.
40	-INF	.	.	.
41	-INF	-792.500	.	.
42	-INF	.	.	.
43	-INF	.	.	.
44	-INF	.	.	.
45	-INF	.	.	.
46	-INF	.	.	.
47	-INF	.	.	.
48	-INF	-921.569	.	.
49	-INF	-878.049	.	.
50	-INF	.	.	.
51	-INF	.	.	.
52	-INF	-920.000	.	.
53	-INF	.	.	.
54	-INF	.	.	.
55	-INF	.	.	.
56	-INF	.	.	.
57	-INF	.	.	.
58	-INF	.	.	.
59	-INF	-911.184	.	.
60	-INF	.	.	.
61	-INF	-875.000	.	.
62	-INF	.	.	.
63	-INF	.	.	.
64	-INF	-911.184	.	.
65	-INF	-878.049	.	.
66	-INF	-935.572	.	.
67	-INF	-921.569	.	.
68	-INF	-1000.000	.	.

Thesis

EQU LIM2

LOWER LEVEL UPPER MARGINAL

69 -INF -1000.000 . .
 70 -INF -1000.000 . .

LOWER LEVEL UPPER MARGINAL

--- EQU LIM3 -INF 1444.600 10000.000 .
 --- EQU S1 -INF . 1.000 .
 --- EQU S2 -INF 1.000 1.000 .
 --- EQU S3 -INF . 1.000 .
 --- EQU S4 -INF . 1.000 .
 --- EQU S6 -INF . 1.000 .
 --- EQU S7 -INF 1.000 1.000 .
 --- EQU S8 -INF . 1.000 .
 --- EQU S9 -INF . 1.000 .
 --- EQU S10 -INF 1.000 1.000 .
 --- EQU S11 -INF . 1.000 .
 --- EQU S12 -INF 1.000 1.000 .
 --- EQU S13 -INF 1.000 1.000 .
 --- EQU S14 -INF 1.000 1.000 .
 --- EQU S15 -INF . 1.000 .
 --- EQU S16 -INF . 1.000 .
 --- EQU S17 -INF 1.000 1.000 .
 --- EQU S19 -INF 1.000 1.000 .
 --- EQU S20 -INF . 1.000 .
 --- EQU S21 -INF 1.000 1.000 .
 --- EQU S22 -INF . 1.000 .
 --- EQU S23 -INF . 1.000 .
 --- EQU S27 -INF 1.000 1.000 .
 --- EQU S29 -INF 1.000 1.000 .
 --- EQU S30 4.000 4.000 4.000 .
 --- EQU OBJ . . . 1.000

--- VAR X

LOWER LEVEL UPPER MARGINAL

1 . . +INF 5.1888E-4
 2 . . +INF 6.2463E-4
 3 . . +INF 2.1753E-4
 4 . . +INF 0.002
 5 . . +INF 0.002
 6 . 67.500 +INF .
 7 . . +INF 0.002
 8 . . +INF .
 9 . . +INF 4.8913E-5
 10 . . +INF 0.001
 11 . . +INF 0.007
 12 . . +INF 5.6966E-4
 13 . . +INF 0.001
 14 . . +INF 0.029

Thesis

VAR X

	LOWER	LEVEL	UPPER	MARGINAL
15	.	.	+INF	4.3362E-4
16	.	.	+INF	4.8761E-4
17	.	.	+INF	4.4192E-4
18	.108.781	.	+INF	.
19	.	.	+INF	3.7065E-4
20	.	.	+INF	2.6223E-4
21	.	.	+INF	2.5898E-4
22	.	.	+INF	4.0494E-4
23	.	.	+INF	5.4617E-4
24	.	.	+INF	2.3940E-4
25	.	.	+INF	0.001
26	.64.428	.	+INF	.
27	.	.	+INF	6.0474E-4
28	.91.840	.	+INF	.
29	.	.	+INF	2.2766E-5
30	.	.	+INF	5.8409E-4
31	.	.	+INF	0.005
32	.	.	+INF	.
33	.87.047	.	+INF	.
34	.	.	+INF	0.006
35	.	.	+INF	0.001
36	.	.	+INF	7.5100E-4
37	.	.	+INF	.
38	.	.	+INF	.
39	.	.	+INF	4.0878E-4
40	.	.	+INF	0.001
41	.207.500	.	+INF	.
42	.	.	+INF	0.044
43	.	.	+INF	2.4040E-4
44	.	.	+INF	2.4040E-4
45	.	.	+INF	2.4040E-4
46	.	.	+INF	1.0104E-4
47	.	.	+INF	1.0226E-4
48	.78.431	.	+INF	.
49	.121.951	.	+INF	.
50	.	.	+INF	9.7373E-6
51	.	.	+INF	0.001
52	.80.000	.	+INF	.
53	.	.	+INF	0.005
54	.	.	+INF	8.0285E-5
55	.	.	+INF	1.1322E-5
56	.	.	+INF	1.6114E-4
57	.	.	+INF	2.1602E-5
58	.	.	+INF	2.3605E-4
59	.88.816	.	+INF	.
60	.	.	+INF	0.002
61	.125.000	.	+INF	.
62	.	.	+INF	0.002
63	.	.800.000	EPS	.
64	.88.816	160.000	.	.
65	.121.951	272.156	.	.

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VAR X

	LOWER	LEVEL	UPPER	MARGINAL
66	.	64.428	288.660	.
67	.	78.431	160.000	.
68	.	.	575.765	EPS
69	.	.	16.371	EPS
70	.	.	2500.000	EPS

--- VAR Y

	LOWER	LEVEL	UPPER	MARGINAL
1	.	.	1.000	EPS
2	.	.	1.000	EPS
3	.	.	1.000	EPS
4	.	.	1.000	EPS
5	.	.	1.000	EPS
6	.	1.000	1.000	0.105
7	.	.	1.000	EPS
8	.	.	1.000	-0.424
9	.	.	1.000	EPS
10	.	.	1.000	EPS
11	.	.	1.000	EPS
12	.	.	1.000	EPS
13	.	.	1.000	EPS
14	.	.	1.000	EPS
15	.	.	1.000	EPS
16	.	.	1.000	EPS
17	.	.	1.000	EPS
18	.	1.000	1.000	EPS
19	.	.	1.000	EPS
20	.	.	1.000	EPS
21	.	.	1.000	EPS
22	.	.	1.000	EPS
23	.	.	1.000	EPS
24	.	.	1.000	EPS
25	.	.	1.000	EPS
26	.	1.000	1.000	EPS
27	.	.	1.000	EPS
28	.	1.000	1.000	EPS
29	.	.	1.000	EPS
30	.	.	1.000	EPS
31	.	.	1.000	EPS
32	.	.	1.000	-0.234
33	.	1.000	1.000	EPS
34	.	.	1.000	EPS
35	.	.	1.000	EPS
36	.	.	1.000	EPS
37	.	.	1.000	-0.403
38	.	.	1.000	-0.396
39	.	.	1.000	EPS
40	.	.	1.000	EPS

VAR Y

	LOWER	LEVEL	UPPER	MARGINAL
41	.	1.000	1.000	EPS
42	.	.	1.000	EPS
43	.	.	1.000	EPS
44	.	.	1.000	EPS
45	.	.	1.000	EPS
46	.	.	1.000	EPS
47	.	.	1.000	EPS
48	.	1.000	1.000	EPS
49	.	1.000	1.000	EPS
50	.	.	1.000	EPS
51	.	.	1.000	EPS
52	.	1.000	1.000	0.435
53	.	.	1.000	EPS
54	.	.	1.000	EPS
55	.	.	1.000	EPS
56	.	.	1.000	EPS
57	.	.	1.000	EPS
58	.	.	1.000	EPS
59	.	1.000	1.000	EPS
60	.	.	1.000	EPS
61	.	1.000	1.000	0.460
62	.	.	1.000	EPS
63	.	.	1.000	EPS
64	.	1.000	1.000	EPS
65	.	1.000	1.000	EPS
66	.	1.000	1.000	EPS
67	.	1.000	1.000	EPS
68	.	1.000	1.000	EPS
69	.	1.000	1.000	EPS
70	.	1.000	1.000	EPS

	LOWER	LEVEL	UPPER	MARGINAL
--	-------	-------	-------	----------

--- VAR Z		-INF	1.000	+INF	.
-----------	--	------	-------	------	---

**** REPORT SUMMARY : 0 NONOPT
0 INFEASIBLE
0 UNBOUNDED

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Thesis
Execution

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---- 178 PARAMETER risk = 2208.328
PARAMETER economy = 24937.940

EXECUTION TIME = 0.000 SECONDS 1.6 Mb WIN205-130

**** FILE SUMMARY

INPUT C:\WINDOWS\GAMSDIR\GAMSDIR\GH11.GMS
OUTPUT C:\WINDOWS\GAMSDIR\GH11.LST

Appendix C

Papers from this Work

Appendix C contains three papers published or to be published from the work and results of this thesis:

Paper I

Modeling and Identification of Economic Disturbances in the Planning of Petrochemical Industry

Ghanima K. Al-Sharrah, Imad Alatiqi and Ali Elkamel

Industrial & Engineering Chemistry Research, Vol. 42, No. 20, pp 4678-4688, 2003

Paper II

A New Safety Risk Index for use in Petrochemical Planning

Al-Sharrah, G.K., Edwards, D., Hankinson, G.

Process Safety and Environmental Protection, to be published

Paper III

Decision-Making for Petrochemical Planning Using Multiobjective and Strategic Tools

G.K. Al-Sharrah , G. Hankinson , A. Elkamel

Chemical Engineering Research and Design, Vol. 80, No. A10, pp 1-12, 2006

Paper I

Modeling and Identification of Economic Disturbances in the Planning of Petrochemical Industry

Ghanima K. Al-Sharrah, Imad Alatqi and Ali Elkamel

Industrial & Engineering Chemistry Research, Vol. 42 No. 20, pp. 4678-
4688, 2003

Modeling and Identification of Economic Disturbances in the Planning of Petrochemical Industry

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Abstract

The petrochemical industry is a dynamic industry and can be seen as a network of chemicals from basic feedstock to final chemicals. The aim of this work is to identify and model long and short range disturbances that affect planning of the petrochemical industry. An application to the Kuwait Petrochemical Industry was performed. The major disturbance is the oil prices that affect chemical prices and consequently profit. Future chemical prices needed for planning are predicted using three forecasting models, simple time-series fitting and two causal models with oil prices, the second order plus dead time transfer function and ARX models. Oil prices for the causal models are first forecasted under the concept of market long cycles (K-waves) and short cycles (business or Kitchin cycles) and then used to forecast chemical prices. The forecasted chemical prices affect the planning of the petrochemical industry where different routs in the network are selected for different final products prices. It is found that including the market cycles and using the causal models for forecasting petrochemical products prices will provide possible scenarios for chemical price forecast and then a risk adjusted present value can be calculated.

Key Words: Planning; K-wave; forecasting; Petrochemical; Disturbances; Risk

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E-mail: imad@kuc01.kuniv.edu.kw

1. Introduction

The petrochemical industry is, as the name implies, based upon the production of chemicals from petroleum. There is more to the industry than just petroleum products; however, the petrochemical industry also deals with chemicals manufactured from by-products of petroleum refining, such as natural gas, gas oil, and tar.

The petrochemical industry is dynamic and is affected by different types of disturbances. The economic environment in which a chemical plant operates is a dynamic rather than a static one, and it undergoes continuous change. During the life of the plant the demand and prices for its product will change, as will all the factors that determine its profitability, e.g., labor, raw material, and utilities cost. Many of these factors can be included in a complete economic evaluation of a proposed plant.

Reasons for the dynamics of the chemical industries are not difficult to find. One of the most important reasons is the continual replacement of conventional materials, often of agricultural origin, by materials of synthesis origin, such as synthetic fibers, plastics, and synthetic rubbers. Another strong factor is the high demand for fertilizers and pesticides, required to raise and maintain high agricultural productivity. Rising standards of health care have resulted in increased demand for pharmaceuticals. These factors are also fed by a spirit of innovation, characteristic of this industry that has resulted in a constant stream of new or improved products.

The aim of this paper is to identify and model the long and short range cycles and to introduce them as disturbances to the petrochemical industry planning process. This should be viewed as a preliminary effort in incorporating dynamic disturbances in the planning exercise. The disturbance models are to be applied to planning model for petrochemical industry in the state of Kuwait. The implication of such disturbances on the economic viability of the planned industries will be discussed.

2. Disturbances on the Petrochemical Industry

Disturbances mean dynamic inputs to a system; for the petrochemical industry this include many factors such as prices and demand. The dynamic behavior in this industry is characterized by cycles with long-range duration (decades) and/or short-range duration (years).

2.1 Long-Range Disturbances:

Since the onset of the 20th century, students of the world economy have been drawing attention to certain long-term regularities in the behavior of the leading economies. The first to make this argument in a sustained manner was Nikolai Kondratieff, a Russian economist writing in the 1920s. Statistical work on the behavior of prices, and some output series, for the United States and Britain since the 1790s, led him to conclude that the existence of long waves was very probable, thereafter this has been named after him (Kondratieff wave or simply K-wave). Looking at the cause of this long-

wave, different approaches can be found in the literature, ranging from pure exogenous causality, for example, solar activity and/or astronomical configurations, to pure endogenous process of biological or social nature¹.

Kondratieff saw the capitalist world economy as evolving and self-correcting and, by implication; he denied the notion of an approaching collapse of capitalism that was common among Marxist economists. Kondratieff expressed the belief that the dynamics of free market economics are not linear and continually progressing upward in a cyclical manner. He acknowledged that each cycle advanced and developed the economy further and brought it to new height. The cyclical economic growth or K-wave is related to the innovation in products therefore each wave is associated with new technological environment; new products replace old ones. Kondratieff taught and believed in the intermediate 7-11 years cycle that many economics believe in today. However, Kondratieff taught that reducing the system to this small cycle only was simplistic and that a broader long-wave scope should be superimposed onto the development of the system. He also recognized the necessity of flexibility in the system and believed that the long cycles fluctuate between 45 and 60 years. Table 1 shows an outline for K-waves recognized by economists and the corresponding dominant forces during each wave².

Table 1: K-waves dates and forces

K-Wave	1 st Wave 1785-1843	2 nd Wave 1843-1894	3 rd Wave 1894-1941	4 th Wave 1941-199X
Industry	Textile	Railroads	Automobiles	Electrification
Material	Cotton	Iron	Steel	Plastic
Energy	Water	Wood	Coal	Oil
Communication	Overland	Telegraph	Telephone	Electronic
National Economy	France and Britain	Britain	Germany	United States

The foundation of Kondratieff's theory, and the element considered to be one of the most important aspects of his research, are the cycles impact on the rise and fall of prices. The movement of prices is key to understanding the K-wave and the effect that K-wave has on investment and planning. Raw material and commodity prices in the recent decades have closely followed the outline Kondratieff laid out for the rise and fall of the cycle³. Market dynamics of natural gas suggests also future cycles; as is indicated by U.S. Department of Energy⁴.

Kontratieff was not the only person to notice long-term cycles within the economy. In 1939, the great economist Joseph Schumpeter – the anther of the concept “Creative Destruction” - hypothesized that technology runs in fifty-year waves.

Schumpeter notices that bursts of technical transformation coincides with upturns in economic activity⁵. He assumed that they were the causes of that activity, new technology drive faster the economic growth and then the more the innovation in technology, the greater is the chance of damage to economy especially through loss of jobs. Konratieff found cycles in industrial production, Schumpeter found them in technical application. Then in the 1970s Jay Forrester and his team of computer modelers at the Sloan School of Management at Massachusetts Institute of Technology (MIT) came up with a persuasive long wave theory. It was an application of System dynamics created during the mid-1950s by Forrester. Forrester⁶ disapproved with the approach taken by operations research in the 1950s, where methods are applied to isolate company problems. He suggested that the success of industrial companies depends on the interaction between many flows of information, some are global⁷. In his paper⁸ he showed that economic models for capital goods – the metals, machines, chemicals, concrete, etc. - can generate long wave cycles about 50 years in length. Forrester work has inspired a group of researchers at the MIT to follow him, most notable is John Sterman. In his work he showed how interaction between multiple time scales in a non-linear model can lead to long waves cycles about 50 years in length, on top of shorter waves cycles^{9,10,11}. Another similar approach to explain the K-wave is the “learning dynamics of succeeding generations”¹. This approach, shown in Figure 1, explains the conceptual framework that generations follow and it is mainly successive processes of technological substitution or “Succeeding Technosphere”.

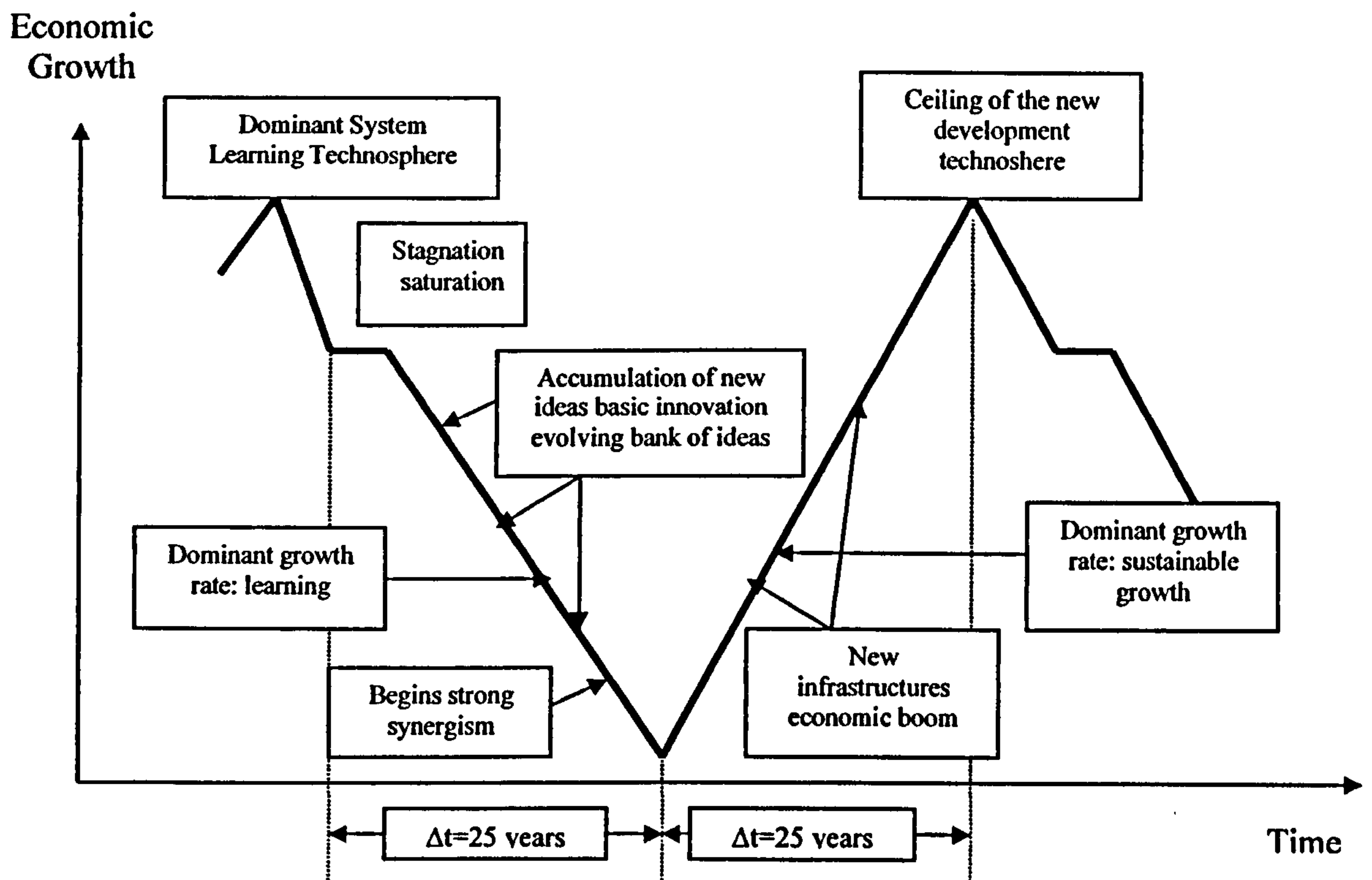


Figure 1: Learning dynamics of succeeding generations

Significance of the long wave:

We have discussed some history of the long wave since its discovery by Kondratieff. This long history, however, did not transfer the long wave to the main stream of investment community. Many economists and financial planners pass over its implications and it is not likely that the debate over its validity will end soon. For example, the current long wave implies declining stock market prices from 1998 to 2010. That means indexes like Dow Jones Industrial will be at best near their current level by 2010. Prominent writers pass over this prediction and forecast at least 100% appreciation for the same period¹². On the petrochemical industry side, there is little evidence that major consulting houses paid the slightest attention to the long wave. When the long wave top was realized in Asian markets in 1998, planners revised down their demand expectations and Asia was treated as an anomaly¹³. Recovery of demand was predicted for base chemicals and oil prices were predicted to remain weak¹⁴. Other prominent forecasters predicted declining prices for Oil from 2000 till 2003 in different scenarios around and below 20 \$/ bbl¹⁵. In fact and as already known, oil prices remained strong from 1999 till early 2003. Students of the long wave had different call at about the same time^{16,17}. Finally, a caution is in place. The cyclic phenomena is neither new nor its discussion is novel. However, the long wave and its incorporation in petrochemicals business planning seem to be quite rare. It is the risk of ignoring and/or abandoning a viable economic opportunity which the understanding of the long wave should help avert. K-waves are not exactly about history repeating itself; instead they are about the danger and reward of going forward¹⁸. Market analysts know that the cycles of human progress are based on a psychology which takes a long time to manifest and will not accrue in a strict periodic rhythm¹⁹. Although long wave understanding is essential, studying their effect was neglected especially in the petrochemical industry. Applications and uses of long cycles can be found for interest rates, commodities prices, stocks and bond forecasting^{20,21,22}.

Long-term cycles are key factors in analyzing or modeling the economic activity of large international industries such as the petrochemical industry and understanding them is essential for sound investment decision². Yimoyines²³ explained this by recognizing that the petrochemical industry is characterized by large plants that takes several of years to be build finally they come to stream together creating oversupply and thus the bottom of the cycle.

2.2 Short-Range Disturbances:

Energy prices, mainly oil price affect all industries and they are determined by the capacity use of OPEC members and other producers. The capacity use, however, is influenced by the simultaneous actions and interactions of numerous variables that affect supply, demand and producers actions. Figure 2 shows a representative diagram of variables affecting oil prices and consequently causing short-term disturbances to the petrochemical industry²⁴.

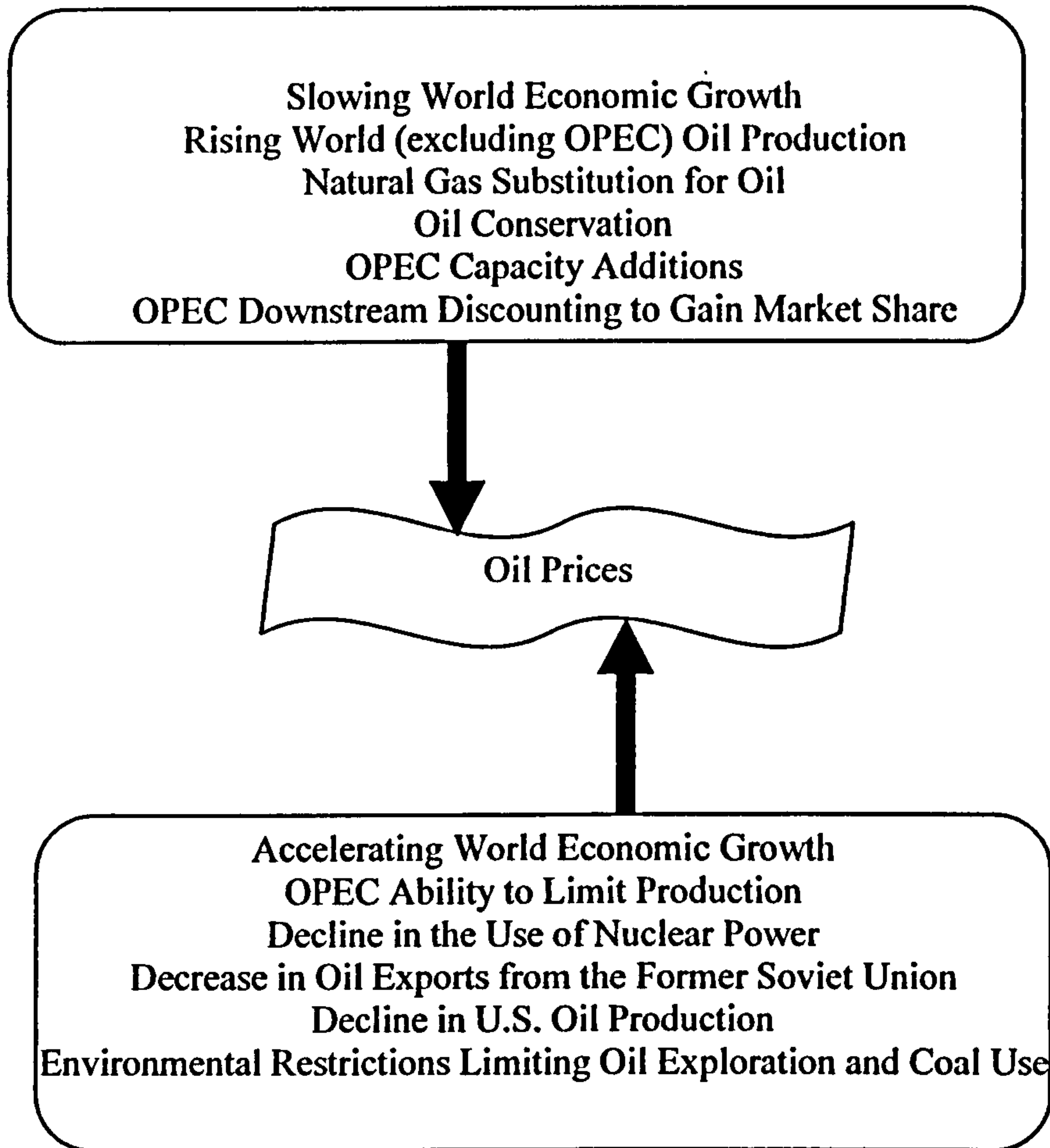


Figure 2: Variables Determining Oil prices in short-range

Short-term disturbances occur also in the form of cycles. A famous short cycle is the "Kitchin" $3\frac{1}{2}$ to 4 year cycle. It is also closely related to the business cycle that affect business activities, interest rates and wholesale and retail prices. A wide variety of linear and nonlinear time-series techniques have been employed to model short cycles features. Simpson et al.²⁵ forecasted the UK quarterly index of production using a model of business cycle. He adopted both linear and non-linear approaches. Kontolemis²⁶ also analyzed the US business cycle and identified the cycle turning points using four time-series indicators. By turning point we mean the cycle upward or downward peaks; these are key points in economic analysis because they separate a rising economy from a falling one.

3. Modeling the Petrochemical Industry

Mathematical models of the petrochemical industry have the objective of defining the inherent technical structure with which the world wide chemical industry must function. The structure is formed by the large but linked number of chemicals that are available on a commercial scale and by the rigid feedstock, by-products, and energy requirements of these chemicals. The products of one segment of the industry become the

feedstock for another segment; thereby defining a network of material and energy flows that constrains business activities.

Linear Programming as well as Mixed Integer Programming were used in modeling the petrochemical industry under deterministic and uncertainty approaches.

3.1 Deterministic Models

Deterministic models for the industry assume that all parameters included in the model, for example prices and demand, are known with certainty. The model is required to select the optimal technology paths for production of a given amount of chemicals under environmental or economic objective. For this it is assumed that a set of feedstocks is locally available in a limited quantity. Also, several alternative processes technologically are accessible for transforming feedstock into final products. These technologies are characterized by technical coefficients of consumption of raw materials, chemicals, utilities, labor, by-products production, investment cost for different plant sizes and operation and maintenance costs. These technologies introduce intermediate chemicals, which are produced and consumed in the system.

Many deterministic mathematical programming models have appeared over the years to plan the petrochemical industry. Rudd²⁷ defined the intermediate chemicals as a network and formulated the behavior of the petrochemical industry as a system of linear equations. He used the minimization of total production cost as an objective.

Different other researchers presented variants to the Linear Programming model of Stadtherr and Rudd with different objective functions. Al-Fadli et al.²⁸, and Fathi-Afshar et al.²⁹ selected the minimization of the total production cost, other studies, Stokic and Stevancevic³⁰, and Stadtherr and Rudd^{31,32}, selected minimizing feed stock consumption.

Multiobjective analysis in the modeling of the petrochemical industry was also considered. Fathi-Afshar and Yang³³ considered a dual objective of minimizing cost and gross toxicity. Sophos et al.³⁴ considered the minimization of entropy creation (lost work) and feedstock consumption.

Linear Programming Models showed their ability to identify the technological structure of the petrochemical industry that meets the needs of the economy, natural resources or environment as well as to test different development scenarios. However, these models must be taken with care since their results may recommend the production of a single chemical using more than one technology or a process with very low production rates. Using different technologies for one chemical is not recommended for small countries and building a plant with small production is not economically feasible. In order to overcome this problem, many researchers considered Mixed Integer Linear Programming (MILP) models. A MILP model was proposed by Jimenez et al.³⁵ and Jimenez and Rudd³⁶ to study the Mexican Petrochemical industry with a fixed charge operating cost as an objective function. The model selects a process to be installed if the

production cost of its product reaches a favorable level with respect to the cost of importing the chemical.

The development of the petrochemical industry in the Kingdom of Saudi Arabia was also studied with a MILP model. Al-Amer et al.³⁷ proposed a MILP model similar to Jimenez model with small modification in process capacity constraints. The objective function was the maximization of the total annual profit. Deterministic MILP was used by Al-Sharrah et al.^{38,39} and Jackson and Grossmann⁴⁰ for different economical and environmental objectives.

3.2 Models with Uncertainty

Many models were proposed for the chemical or the petrochemical industry that included uncertainty in formulating the model and not as a final stage of the solution in sensitivity analysis. Systems modeled were batch plants, small operations or process networks.

For optimization under uncertainty in batch chemical plants, Shah and Pantelides⁴¹ and, Petkov and Maranas⁴² considered uncertainty in product demand only, Ierapetritou and Pistikopoulos⁴³ considered uncertainty in processing time, size and product demand, Bhatia and Biegler⁴⁴ considered uncertainty in process reaction parameters and Lee and Malone⁴⁵ considered uncertainty in product demand and due dates.

Similar uncertain parameters were considered in the models of continuous processes. System parameters which may include operating temperature, reaction constants and yields were studied by Friedman and Reklaitis⁴⁶, Grossmann and Sargent⁴⁷, Halemane and Grossmann⁴⁸, Straub and Grossmann⁴⁹, Novak and Kravanja⁵⁰, Pintaric and Kravanja⁵¹ and Rooney and Biegler⁵². Uncertain demand only was included in the models of Acevedo and Pistikopoulos^{53,54} and Ahmed and Sahinidis⁵⁵. With the uncertain demand, Ierapetritou et al.⁵⁶ included supply and process yield, Liu and Sahinidis⁵⁷ and Acevedo and Pistikopoulos⁵⁸ included supply, and Bernardo et al.⁵⁹ included supply and prices.

Uncertainty in future chemicals prices will be considered in this study and is treated with forecasting tools.

4. Forecasting

Forecasting of future prices of petrochemicals are a major input to all aspects of production and market planning in the petrochemical industry. The two classes of forecasting techniques are qualitative, which use either experts, salespeople, or customers to make forecasts, and quantitative, most of which use historic data to make the forecasts. There are two basic types of models in the quantitative category: time series models and causal models.

4.1 Time-series models

These use past time-ordered sequences of observations of the forecasted variable. In this type of analysis only the time series history of the variable being forecasted is used in order to develop a model for predicting future values. Then, forecasts are made by extrapolating the fitted model. The extrapolation is based on the assumption that the future will continue on the same basis as the past.

There are four types of patterns usually seen in data series: horizontal, seasonal, cyclical, and trend. A horizontal pattern exists when there is no trend in the data. When such a pattern exists, the series generally is referred to as stationary, that is, it does not tend to increase or decrease over time in any systematic way. Thus it is just likely that the next value of the series will be above the mean value as it is that it will be below it. The kind of situations that generally exhibit a horizontal pattern would include products with stable sales and the demand of a chemical over fairly short time periods. The element of time is generally an important one in considering horizontal patterns, since in the short run even patterns that may exhibit a defined trend over several years might be assumed to be horizontal patterns for the purpose of short-term forecasting.

A seasonal pattern exists when a series fluctuates according to some seasonal factor. The season may be the month or the four seasons of the year, but they could also be the hours of the day, the days of the week, or the days in a month. Seasonal patterns exist for a number of different reasons, varying from the way in which an industry has chosen to handle certain operations (internally caused seasons) to external factors such as the weather.

A cyclical pattern is similar to a seasonal pattern, but the length of a single cycle is generally longer than one year. Many series in the industry follow this pattern as discussed earlier. The cyclical pattern is a difficult one to predict, because it does not repeat itself at constant intervals of time, and its duration is not uniform.

A trend pattern exists when there is a general increase or decrease in the value of the variable over time. The demand of many products that are related to the population, for example construction material and fuel, follow a trend pattern.

Although a number of other patterns can be found in specific series of data, the four we have discussed are the most important ones. They often can be found together or individually. In fact, some series actually combine a trend, a seasonal pattern, and a cyclical pattern in addition to the horizontal level, which is a part of all series.

One of the useful tools in analyzing time-series data of cyclical nature is the Fourier analysis; it is based on the concept that series can be approximated by a sum of sinusoids, each at a different frequency. It has been used in its basic form to study oil short cycles for example the cyclic behavior of the quarterly average of non-OPEC supply in the studies of Jazayeri and Yahyai⁶⁰, and it is identified; in a form called

“Dynamic Harmonic Regression”; as useful to investigate periodic phenomena for forecasting⁶¹. Ierapetritou et al.⁶² used a time-series model to generate necessary scenarios for future power prices.

4.2 Causal models

These models, relate statistically the time series of interest (dependent variable) to one or more other time series (independent variables) over the same time period. If these other variables are correlated with the variable of interest and there appears to be a logical cause for this correlation, then a statistical model describing this relationship can be constructed. Knowing the value of the correlated variable (independent variable), the model is used to forecast the dependent variable. The most applied causal model is the regression model. This approach attempts to quantitatively relate a chemical demand (dependent variable), for instance, to the causal forces (independent variables), which determine the chemical demand. Thus regression is a mathematical procedure that takes into account the relationship of the dependent variable and the independent variable(s). Therefore, regression is more powerful than subjective qualitative estimate because it enables the forecaster to measure explicitly the apparent association between variables over time, thus eliminating most of the guesswork.

While regression involves a single equation, econometric models can include any number of simultaneous multiple regression equations. The term econometric model is used to denote systems of linear multiple regression equations, each including several interdependent variables. Perhaps the best starting point for understanding the basics of econometric forecasting is regression. Regression analysis assumes that all of the independent variables included in the regression equation are determined by outside factors, that is, they are exogenous to the system. In econometric models, however, such an assumption is often unrealistic. To illustrate this point, one can assume that the demand of a chemical is a function of GDP, chemical price and oil price. In regression, all three independent variables are assumed to be exogenously determined; they are not influenced by the level of demand itself or by each other. This is a fair assumption as far as GDP is concerned, which is not influenced directly by the demand of a single chemical. However, for the chemical price there is unlikely to be a similar absence of influence. If the per-unit cost (and thus price) decreases sales volume increase (and vice versa), different levels of sales will result in different per-unit costs (and thus prices). Price forecasting in petrochemical planning may include tens of interdependencies and variables. An example is the price forecast elements considered by Chem Systems⁶³. These elements include production elements (crude oil price forecast, feedstock cost trend and alternative feedstock economics and production costs and technology trends) and profitability elements (current price, general macroeconomic forecast, specific petrochemical business area trends and opinion of petrochemical purchasers and sellers)

The main idea behind econometric modeling is that everything in the real world depends on everything else. The world is becoming more aware of this interdependence, but the concept is very difficult to deal with at an operational level. The practical question

is, of course, where to stop considering these interdependences. In an econometric model one is faced with many tasks similar to those in regression models. These tasks include⁶⁴:

1. Determining which variables to include in each equation (specification).
2. Determining the functional form (that is, linear, exponential, logarithmic, etc.) of each equation.
3. Estimating in a simultaneous manner the parameters of the equations.
4. Testing the statistical significance of the results.
5. Checking the validity of the assumption involved.

An obvious limitation to the use of causal models in general and econometric analysis in particular is the requirement of an extensive investigation of many explanatory variables. This process is usually time-consuming and costly. The other limitation is that only explanatory variables whose values are known can be used to forecast the dependent variable. Therefore simple regression with one dependent and one independent variable is more commonly used.

The form of the model that can be used as causal model is transfer functions or polynomials. Second order plus dead time model (SOPDT) is used extensively in system identification and it can be used as a forecasting model. Another useful model, used extensively in forecasting, is a polynomial form of a transfer function. It is explicitly defined as a polynomial between the input u (independent variable) and the output y (dependent variable). The current output $y(t)$ (dependent variable) is a function of previous na outputs and previous nb inputs delayed by nk together with some noise e . The model is named Auto-Regression with exogenous variable (ARX) model⁶⁵ and is presented as:

$$y(t) + a_1y(t-1) + \dots + a_{na}y(t-na) = b_1u(t-nk) + b_2u(t-nk-1) + \dots + b_{nb}u(t-nk-nb) + e(t) \quad (1)$$

Nogales et al.⁶⁶ used ARX and a transfer function causal model to forecast the next-day electricity prices. They used the electricity demand as the independent variable.

The petrochemical model proposed in this study is used with uncertain future prices of the final products. The uncertain price is found by quantitative forecasting.

5. Model Formulation

The model used in this study is a deterministic MILP model proposed by the authors³⁸ with some modifications and it is re-introduced below. Let N be the number of chemicals involved in the operation of M processes, X_j be the annual level of production of process j , Q_i the total amount produced of chemical i , F_i the amount of chemical i as a feedstock, and a_{ij} be the output coefficient of material i in process j . The main constraints that govern the operation of the petrochemical network are the material balance constraints:

$$F_i + \sum_{j=1}^M a_{ij} X_j = Q_i \quad i = 1, 2, \dots, N \quad (2)$$

These constraints ensure that the total quantity produced of each material i is equal to the sum of all amounts produced by all processes plus its quantity as a feedstock. For all the intermediate chemicals, Q_i will be set to zero because no output of these chemicals is required from the desired petrochemical network.

The final products in the planned petrochemical industry will be governed by their demands in the petrochemical market, according to the country's share in that market. Constraints on Q_i for all final products are needed and they are formulated as:

$$Q_i \leq D_i U \quad i \in I_1 \quad (3)$$

Where D_i is the world demand for chemical i and it is multiplied by the country's share in the petrochemical market, U represent valid and upper limits of the country's share. The above constraint is only applied for final products group I_1 .

Introducing the binary variables Y_j for each process j will help in the selection requirement of the planning procedure. Y_j will be equal to 1 only if process X_j is selected, and zero if process X_j is not selected.

The proposed improvement of petrochemical industry is directed towards building new plants to produce petrochemical. It is logical therefore, that only one process should be selected to produce a single chemical. Following constraints should be included for all chemicals:

$$\sum Y_j \leq 1 \quad j \in J_1 \quad (4)$$

Where J_1 is the group of processes that produces a single chemical. For final products:

$$\sum Y_j = K \quad j \in J_2 \quad (5)$$

Where K is the number of final products selected from the proposed list of products, and J_2 is the group of all process that produce a final product.

The supply of feedstocks limitations will impose additional constraints on the selection and planning, i.e.:

$$F_i \leq S_i \quad i \in I_2 \quad (6)$$

Where S_i is the supply availability of feed chemical i . The above constraint only applies for some feedstock chemicals represented by the group I_2 . Not all the feedstock chemicals are included in I_2 because some are additives and some are needed in small quantities. Also, some petroleum-rich countries have small limitations on petroleum feedstocks.

An additional economic constraint is required for the limit on the investment budget. If cap_j is the capital investment cost for constructing plant j and Bg is the available budget, then the constraint is formulated as:

$$\sum_{j=1}^M cap_j \times Y_j \leq Bg \quad (7)$$

For simplicity the objective function used is a maximum economical gain in the selected processes. The economical profit is represented by the overall added value; it is the price of final products minus the cost of feedstock for the petrochemical network. If C_i is the price of chemical i , the added-value objective function will be represented by:

The added value objective is applied on the network so only prices of final products and major feedstocks are considered.

$$\max . \quad Z_2 = \sum_j^M \sum_i^N a_{ij} C_i X_j \quad (8)$$

As chemical prices are considered to be changing during the planning horizon, they are treated using forecasting. Three forecasting models will be used, first time-series models where historic data on a chemical price is collected and it is correlated with time. When a reliable correlating function is found, a forecast of future price can be performed. The second and third forecasting models were causal models. In these models, the chemical prices are related to oil prices using a transfer function and ARX model, where oil price is the input and chemical price is the output. Historic data of oil prices and the chemical prices were used to find the best causal models. Oil price is a cyclical variable, so its forecast is based on cycle analysis aimed at finding a function to best describe its behavior. Oil prices forecast and chemical/oil causal models can then be used to forecast the chemical prices.

6. Illustrative Case Study:

Kuwaiti officials have expressed interest in accelerating development of the country's relatively small petrochemical industry. This would accomplish several goals; boosting the value of Kuwait's crude oil reserves; helping to protect Kuwait's revenues during periods of low crude prices; and boosting Kuwait revenues while adhering to OPEC crude oil quota limitation.

The desired final products were defined under the criteria of their importance to the global petrochemical and its relevance to Kuwait. The proposed final products are:

- Acrylonitrile Butadiene Styrene (ABS)
- Cumene
- Polystyrene, crystal grade (PS)
- Polyvinyl chloride (PVC)
- Vinyl acetate monomer (VAM)

It is desired to select four products out of the proposed ones and also to identify the best network of petrochemicals starting from the basic feedstocks that can produce these final products.

The routes from the final products to the basic feedstock chemicals were determined by selecting a number of manufacturing processes forming at the end a network. The selection of the chemicals came as an output of taking all possible alternatives of producing the desired products. A simplified network of the process is illustrated in Figure 3.

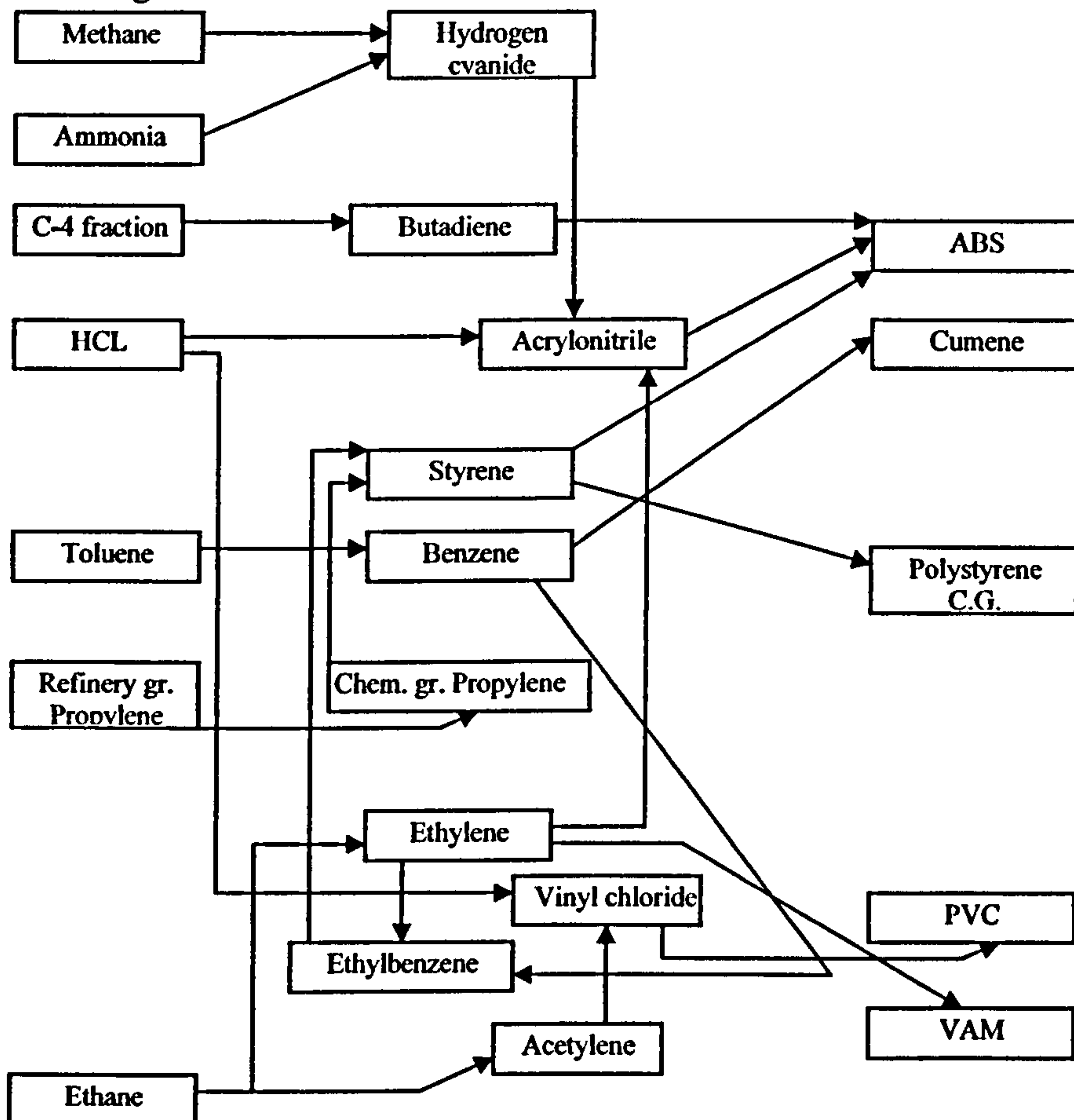


Figure 3: A simplified petrochemical network for the proposed products

The heart of the model is the material balance constraints. Hence, estimation of the output coefficient a_{ij} is a key step in constructing the model. For this purpose, yield data for each chemical transformation is required. In many cases, process yields are variable and depend on what product mix is desired or on what capital expenditure can be afforded. The model uses average yields reported at commercial installations.

Needed to complete the construction of the model constraint set are the supply of feedstock and demand of final products. Since the industry must compete for its feedstock and markets, supply and demand data were taken from different sources (mainly from recent SRI reports and Kuwait's Petrochemical Industries Company (PIC) annual reports). However, the supply and demand data are estimated using observed values of production and observed usage patterns

The data needed for the objective function in the model are prices of final products and main feedstocks; and these were taken mainly from "SRI reports" and "Chemical Market Reporter" journal. Oil prices needed for the causal model were taken mainly from Jenkins⁶⁷ and the internet. Prices of 1871-1899 were Pennsylvania crude, 1900-1944 were U.S average crude and 1945 and after were Arabian light. Figure 4 shows oil prices since 1871. It is clear that long and short range cycles characterize the prices. Inspection of Figure 4 and the price data of oil suggests a pattern of a pattern of 55 years long waves for oil. Peaks (tops) of these cycles occur in 1871, 1921 and 1980. A theoretical next bottom should register near 2007 this can be seen later through identification in time series.

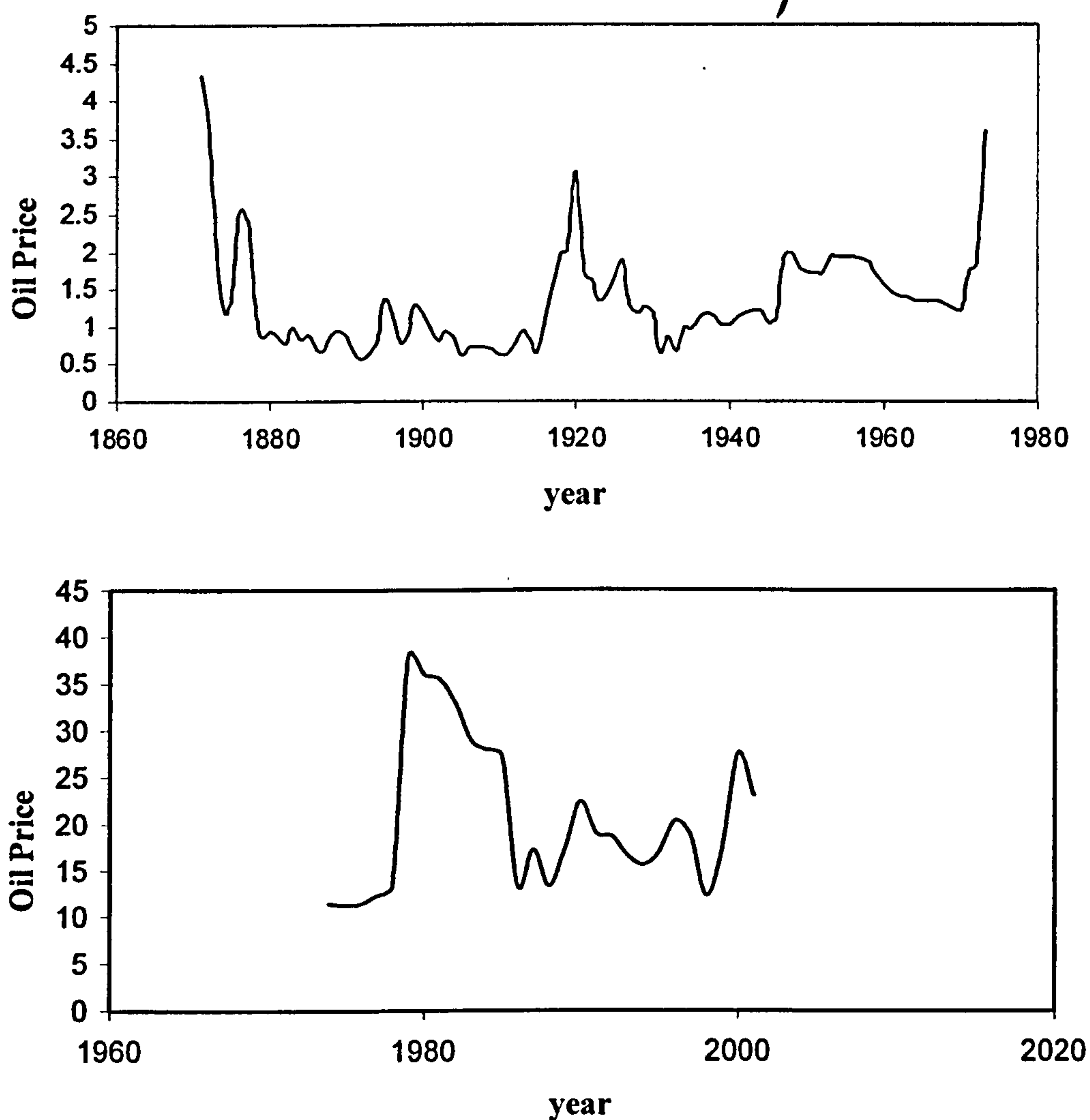


Figure 4: Historical data of oil prices (\$/bbl)

Price Forecast

Preparing a price forecast is done before solving the petrochemical model. The simple time-series forecast is applied. This model is basically finding a function with time that best fit the chemical prices data. First a simple third order polynomial of price with time was used. However its results were very poor since it indicated some negative prices or very high prices when used in the forecast. Secondly; because the price data are cyclical, Fourier analysis is applied with only one frequency together with a trend term. Results are presented below:

$$ABS (\$/kg) = -0.034 t + 32.984 \cos(5.857 t) + 15.047 \sin(5.857 t) + 257.839 \quad (9-a)$$

$$Cumene (\$/kg) = 0.005 t + 4.324 \cos(5.500 t) + 4.872 \sin(5.500 t) + 37.672 \quad (9-b)$$

$$PS (\$/kg) = 0.002 t + 7.561 \cos(5.782 t) + 13.854 \sin(5.782 t) + 97.882 \quad (9-c)$$

$$PVC (\$/kg) = 0.027 t - 12.061 \cos(5.533 t) - 0.273 \sin(5.533 t) + 17.865 \quad (9-d)$$

$$VAM (\$/kg) = 0.038 t - 13.465 \cos(6.011 t) - 12.387 \sin(6.011 t) + 13.944 \quad (9-e)$$

The above equations can be directly used to forecast chemical prices for the planning horizon.

For the causal model, identifying cycles in oil prices is done also by time-series Fourier analysis but with two frequencies in order to capture short and long cycles. The analysis result is:

$$\begin{aligned} oil\ price (\$/bbl) = & 0.0136 t + 9.4163 \cos(6.2 t) - 2.1974 \sin(6.2 t) \\ & + 1.921 \cos(8.5372 t) - 0.7131 \sin(8.5372 t) \end{aligned} \quad (10)$$

Where t is the time in years. A plot of actual and theoretical oil prices is given in Figure 5. The figure clearly shows the cyclicity in the data. Figure 5 also shows the prediction of oil prices till 2030; for the petrochemical industry, the long range horizon is considered as the time for building then running the plant through its expected life; this time is around three decades. Therefore all forecasts were done to year 2030. Oil price prediction suggests the next bottom in oil price to be in year 2006 at a price of 16.88 \$/bbl. This is consistent with the predictions for Kuwait Export Crude⁶⁸ and Dubai crude¹⁵, the bottom was at 2006 and at 17 \$/bbl and Dubai crude. But this bottom is slightly earlier than some analysts predictions for the K-wave next bottom. Notley⁶⁹ and Barker³ modeled interest rates and have predicted the next bottom at 2010 and 2009 respectively. This indicated that interest rates are affected by oil prices and follow the same trends. It also indicates that oil prices lead interest rate in the long wave sense by 3 to 4 years, which is logical with the role of oil as a driver of inflation.

The second stage in forecasting stage is finding the causal model between oil prices and products prices. The first causal model is represented by a transfer function relating oil prices as an input and products prices as an output. The transfer function is found in the form of a SOPDT. The transfer functions parameters given in Table 2 were found for the proposed final products. The significant parameter in the transfer function was the delay; its value was much higher than the time constant; except for VAM; this means that delays range from 4 to 13 years (1 to 3 business cycles) for the chemical prices to respond to oil price change but as soon as they respond, they respond relatively fast. This result is consistent with the fact that downstream industry take several years to be operational. The damping factor for all chemical prices was very small indicating high oscillatory underdamped response. The third stage in forecasting is using the forecasted oil price and the transfer functions to forecast products prices.

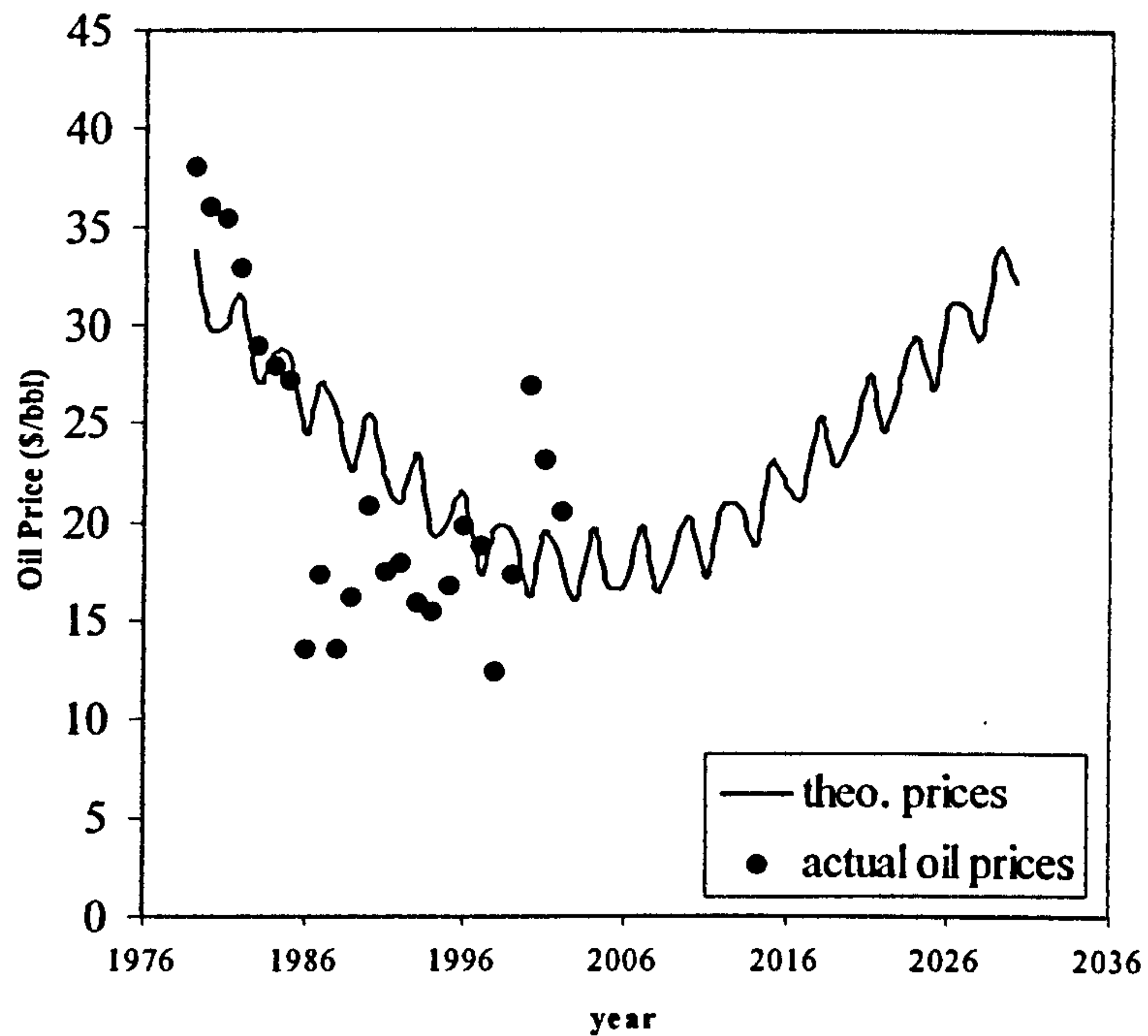


Figure 5:Oil prices (\$/bbl)

Table 2: SOPDT transfer function parameters relating chemical prices and oil prices.

	Gain K (c/kg)/(\$/bbl)	Time constant τ (year)	Damping factor ζ	Delay θ (year)
ABS	6.9801	0.1760	0.0316	5.8408
Cumene	2.4313	0.0831	0.0193	4.0313
PS (C.G.)	3.5699	0.0830	0.0177	6.7276
PVC	1.6729	0.1498	0.0450	13.3748
VAM	4.6014	0.1559	0.0064	0.0894

Note: transfer function is a relation between the change in prices of products to change in oil prices.

An alternative to the transfer function model is the ARX model represented by equation 1. ARX models for the chemical prices were found to be best in the order of 6 for na and nb and 2 for the delay nk ; this was concluded after many trials of model order. All forecasting results are presented in Figure 6 for ABS.

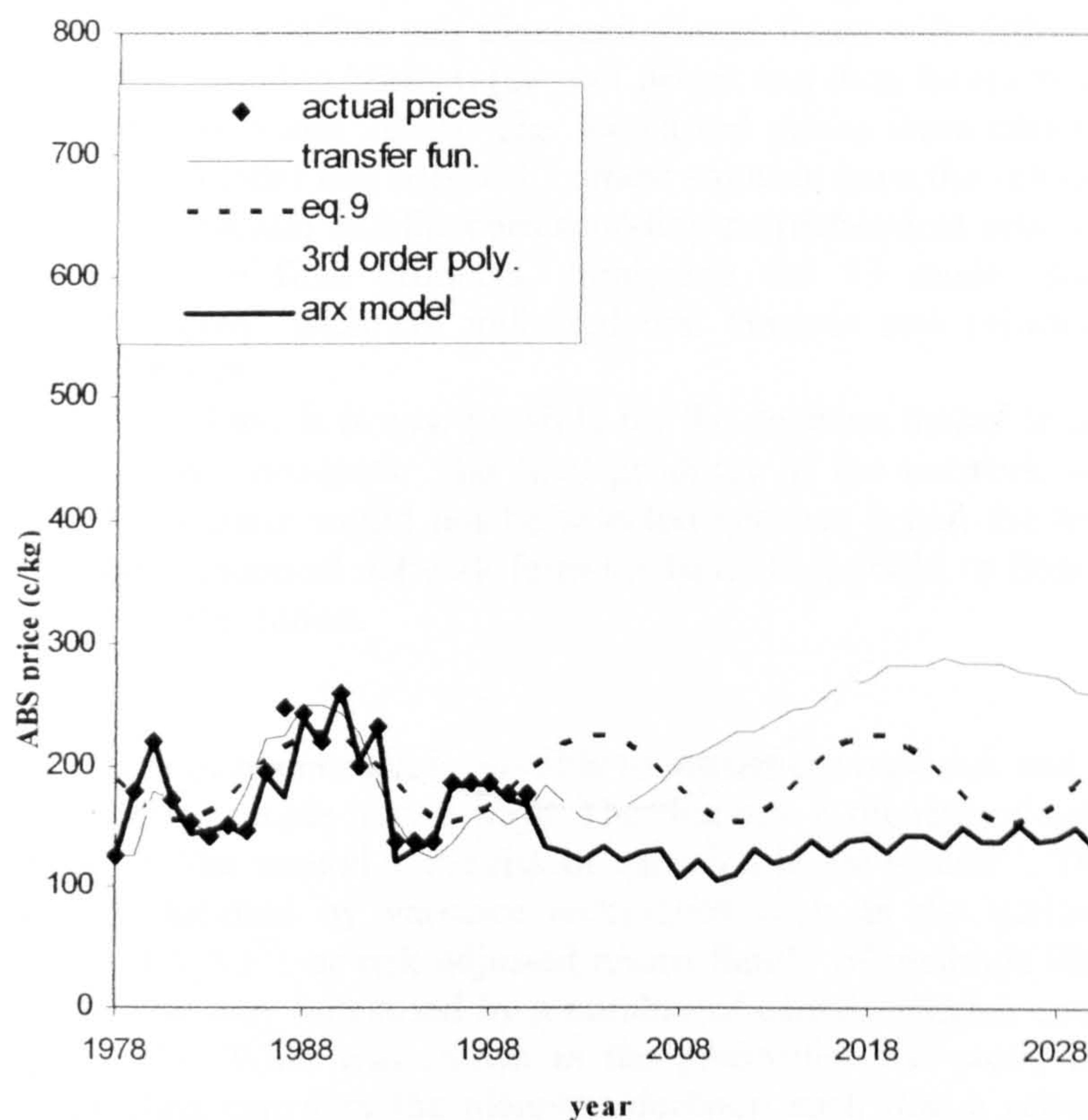


Figure 6: ABS actual and forecasted prices (c/kg)

Equations 9 and 10 and data in Table 2 were obtained using Nelder-Mead simplex direct search optimization in the MATLAB. A file was written for MATLAB defining the required form of the function and requesting for its parameters that best fit the data. The ARX models were found using the “System Identification toolbox” in MATLAB. Data used were prices from 1978 to 2000, prices for 2001 and 2002 were used to test the accuracy of the models. Actual chemical prices were compared with forecasted prices calculated from the causal models and the time series model (equations 9-a to 9-e). Results show an average absolute error of 14.8% with transfer function model, 1.82% with ARX model and 24.5% for the time-series model (equation 9). From the previous errors and Figure 6, it is clear that the causal models provide the more reasonable forecast of the chemical prices. The time series model gives pure cyclic behavior with no trends and the simple polynomial fit gives unrealistic forecast. Inspection of Figure 6 reveals an interesting trend for the ABS price pattern, with long term topping action between the years 2022-2024. The transfer function model and the ARX model both exhibit this

phenomenon, which implies the possibility that the long wave may apply to petrochemicals in additions to commodities.

Model Solution

The petrochemical MILP model was solved using the commercial optimization package GAMS⁷⁰. The solution was obtained several times with different final products prices taken for the planning horizon (current prices and then forecasted prices for 2005, 2010, 2015, 2020, 2025 and 2030). The forecasted prices were taken from the causal models. Overall, the model was solved 13 times; solution gave the selected final products (four out of five chemicals) and the corresponding petrochemical network of plants from the basic feedstock to final products. Analyzing the 13 model solutions with the corresponding “rejected” chemical indicated that cumene was rejected 7 times, PS 4 times and VAM 2 times.

From the model solutions, it is now possible for the decision maker to select the planned petrochemical network products. The final products of the network will be ABS, PS, PVC, and VAM. Cumene would not be selected because it had the highest number of rejections. The petrochemical network form the basic feedstocks to final products will be found from the model solution.

Risk Assessment:

At this stage of planning it is possible to introduce some risk and concepts. Risk is perceived by business people in two ways. The first one is the risk of not achieving target financial objective. The second is the risk of variation in the results⁷¹. The second type of risk can be well handled by variance techniques such as the variance of Expected Monetary Value (EMV)⁷², or risk adjusted return family of methods like Sharpe ratio⁷³. The first type of risk may be caused by a number of causes whether economic, political, technical or the like. What was shown in the preceding case study is how economic disturbance modeling can alter the planning decision such that a suboptimal choice of product selection can be avoided. The difference in aggregate revenue can be calculated and related to the net present value.

Consider the transfer function and the ARX models as two possible scenarios of forecasted chemical prices. A third scenario of prices of chemicals is added from the transfer function model with oil prices (peak amplitudes) reduced by 70%. The third scenario is considered to take account for some factors affecting the oil prices some of which started in recent years; these include environmental factors, reduced cost of production and alternative energies replacement. The present value PV of the products sales is calculated using the three proposed scenarios sc and an interest rate of 10%, the results were \$5.6 b, \$3.4 b, and \$5.5 b for the transfer function, ARX and oil price model respectively. An expected monetary value EMV can be calculated from the present values as the following:

$$EMV = \sum_{sc=1}^3 p_{sc} \times PV_{sc} \quad (11)$$

The present value of each scenario is multiplied by its probability of accordance p . the

variance can be calculated from:

$$\sigma^2 = \frac{\sum_{sc=1}^3 [PV_{sc} - EVM]^2}{2} \quad (12)$$

The large variance indicates the risk of making a decision on petrochemical process selection without paying attention to the economic disturbances.

Taking the probability simply as 0.333, the expected monetary value will be \$4.8 b. This number represents a risk adjusted present value with a variance value of 1.54.

We would like to address the risk problem from another angle, using historical account. The lack of appreciation for the long wave may result in a lot of disruption in the administration of project plans and strategic plans. Even the better understood and accepted cyclic phenomena typically cause disruptions in fund allocation and planning. It was noted by several observers that the chemical business cycles result in unfavorable investor response. During weak market periods, profits are low and investors refrain allocating money in new capacity. This inaction results in demand increasing and supply stable. After few years, shortage appears and prices rise and overshoot. Investors jump and put money above the required demand. By the time the added capacity goes on-stream, prices go down again due to the competition. Thus the boom-bust and cyclic phenomena^{74,23}.

Looking back to Figure 6 illustrates the potential risk of reacting to weak market conditions. The ARX model had the least numerical error and taken alone, investors may decide to abandon a plane of investing in ABS. Considering the transfer function model in analysis would provide additional insight to the probable scenarios. In fact, recent trends suggests that prices would be stronger than what would the ARX itself would have forecasted.

Implications for Oil Producing Countries:

Through incorporation of cyclic analysis, various difficulties that were encountered in the Kuwaiti petrochemical industry were explained. Most notable example is the Equate Chemicals Company. A Joint venture of Petrochemicals Industry co. (PIC) with Dow Chemicals, commenced production in 1997 for ethylene, polyethylene, and ethylene glycol. With four months delay in startup, prices were at the bottom of the business cycle. In 1998 the Asian crisis hit markets and products prices were substantially below forecast. To add insult to injury, technical problems were encountered at the same time and interruptions of operations took place. In the mean time, PIC and Equate sponsored a conference on Investment opportunities in Petrochemicals in Kuwait in October 1998. In this conference a critical analysis of the Asian crises from the perspective of the long wave was presented. It was suggested² that the crises was not isolated but part of an unfolding of a bigger picture. Further, it was suggested to incorporate cyclic disturbances in feasibility studies and forecasting. Weak prices continued for the first half of 1999 and operating income continued below target. As a result, the parent company of Equate required injection of additional capital. A cyclic study was performed by an international consultant who forecasted prices into

2010. The realization of cyclical nature of the chemicals business lead the Supreme Oil Council to support the additional capital and the continuation of support for the project. Operations soon recovered to target potential and beyond and by August 2001, phase 2 of the Olefin complex (2000 million USD capital) was approved. In addition, a much delayed and debated aromatics complex of 1400 million USD capital was also approved⁷⁵. The understanding of the short, intermediate and long wave phenomena contributed much to the continued support for petrochemical projects in Kuwait despite the tough challenges. In March 2003 Dow Chemicals signed strategic partnership with Petrochemicals Industry Company (the Parent of Equate) for the realization of the expansion. The proposed processes in this paper relies heavily on the raw materials provided by the olefin and aromatics complexes and with further understanding of the cyclic economic disturbances, confidence in the proposed products should increase and investors should stay committed.

7. Conclusion

A procedure for modeling disturbances in the petrochemical industry was proposed to best forecast chemical prices and consequently good planning in the long range. The advantages of this procedure are evident when it was able to identify a tool for product selection. Modeling of disturbances was based on oil prices that clearly followed the well known long and short range cycles. The modeled disturbance was used successfully with a chemical price/oil price causal models to forecast prices for the long range petrochemical planning horizon. The disturbances were applied to a petrochemical planning model for Kuwait, with purpose to study their effect on added value and economics.

It was found that the oil prices follow the traditional K-wave theory with an average period of 55 years. It was also found that oil prices lead interest rate in the long wave by 3 to 4 years.

From the tested forecasting models, the causal models in the form of second order pulse dead time (SOPDT) and ARX models were able to model the past prices and well forecast future prices. A risk adjusted present value was found from the present value of all possible price forecast scenarios. The large variance of the expected monetary value emphasizes the need for disturbance analysis in the decision making.

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Paper II

A New Safety Risk Index for use in Petrochemical Planning

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A New Safety Risk Index for use in Petrochemical Planning

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Abstract

Risk analysis is being used to evaluate and manage the potential of unwanted events in the chemical processing industry. The risk in this study is the risk posed by chemical plant accidents and it is presented in a simple quantitative form. A safety risk index is formulated that represents the maximum number of people that might be affected if an accident occurred that caused the release of all the plant inventory of a chemical. The index has four terms: frequency of accidents; hazardous effect of the chemical; inventory of the chemical released; size of the plant. The overall unit of the index is expressed as the number of people affected per year from the plant operation and is in a form suitable for the comparison of safety risk within a planning model for the development of the petrochemical industry.

Key words: Risk, Risk Index, Plant Accident, Hazardous Chemical

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INTRODUCTION

A decisive influence on the performance of the chemical industry is the toxicity of the chemicals and production safety in general. The raw material, the intermediate, and the finished products present the primary independent hazard element (Ward, 2002). They are a hazard even if only in storage, with no processing. Overlooking this increasingly important factor would be to ignore one of the major forces that shape the development of the industry. The issue of safely producing hazardous chemicals is as important as the economics of producing and selling them.

The hazardous effect of chemicals is manifested in three ways: flammability, explosivity and toxicity. The first step towards greater plant safety is being aware of the potentially dangerous properties of the substances, mixtures and reactions, i.e. whether they are inflammable, explosive or toxic.

In a process, not only the substances but also the equipment plays an important role. Equipment represents an inherent hazard, secondary to material because the equipment acts on the materials, and cannot be the cause of problems without the materials. Accident consequences due to equipment failure alone are mainly economic loss and an in-plant problem, while the equipment failure accompanied by a chemical release is usually an off-plant problem, mainly for human health and environmental damage. This means that chemical release is the major problem and that the existence of a hazardous chemical within the equipment increases the consequences of accidents.

An important and widely established term in the process industry is risk. The risk due to an industrial process or a technical installation is defined in the process industries as the combination of the incident probability and the magnitude of the harmful effects. Thus, this term strongly refers to probabilistic assessment. Another definition is expressed as – the time related, or location related likelihood of hazard actually resulting in an undesired event which can impose acute or chronic effect. Incident frequency can also be used instead of probability, and then the assessment is statistical.

Risk is a concept that is used in the chemical industry by practicing chemical engineers. The term risk is multifaceted and is used in many disciplines such as: finance, raw material supply, plant design and process change, and site selection. This work will focus on the basic concept of risk to human health and risk assessment as applied to the manufacturing, processing or use of chemicals and the impact of exposure to these chemicals on human beings.

The objective, in this work, was to develop a simple risk index that can be used in the early stage planning of chemical plants. The index need to be easily applied, include industrial experience and require only general plant information for its evaluation. In

many cases, early stage planning procedure requires risk evaluation and ranking for tens of plants with only limited availability of plant information. The index was structured in a form that is suitable for incorporation into optimization models for planning the development of the petrochemical industry from safety perspective. It can be used as an objective function or as a constraint together with other planning perspectives (see Al-Sharrah *et al*, 2006). The existing, internationally known and proven risk indices discussed later in this paper are not suitable for this purpose. The risk evaluated using the index provides an estimate of the potential risk on people resulting from a chemical plant accident.

RISK TOOLS AND CONCEPTS

The chemical process industries use a wide range of process analysis tools to identify, quantify and control risk in plant operations. Risk can be described and quantified using probability (or frequency) of damage, magnitude of potential harm and by index for the hazardous level of operation. Also, the history of chemical accidents in the process industries is a useful means of identifying sources of risk.

Probability and Frequency for Risk Assessment

Probability theory is one tool to reconstruct reality when incomplete knowledge on the initial conditions of a sequence of events in time is available (Kirchsteiger, 1999a). It helps to answer a basic risk question of how likely the event will happen?. Estimating a probability number for an event is based on an extensive study and data collection for that event including the failure of all its components and consequences. Probability, as an essential part of risk assessment, is used in the fields of occupational risk as the probability of accidents or any undesired event. The studies in this field began when insurance companies started to use science, psychology and statistics for their evaluations

The German author Marbe, in 1926, worked on the psychology of accidents, and, on the basis of the data of a large insurance company, he was able to show that the probability that a given person will have an accident varies directly with the number of accidents he has already had within a given time. This raised the possibility that those people who frequently suffer accidents are the same ones who repeatedly cause them. This finding became known as "Marbe's Law": a given individual's probability of having an accident is calculated on the basis of the number of accidents he has already had. This was one of the first times in the study of accidents when a conclusion employed the term "probability" and, furthermore, related probability to an observed frequency.

Although "Marbe's Law" was developed for human performance, it can be applied to other events and fields, including plant accidents and chemical releases. This concept of relating probability to frequency was used extensively due to the fact that

probability was not directly available for many events, especially if these events were complicated, multi-staged or new. Cuny and Lejeune (2003) supported this and indicated that estimating the probability is more problematic; the frequency approach is the most tangible; they estimated probability using its relative frequency.

Hazard Indices

The selection of appropriate measures of environmental or safety performance for a process will depend upon the nature of the environmental concerns, the type and quantity of information available and the degree of accuracy required in the representation. Several hazard analysis indices have been developed, some of them are internationally known and proven and some have been used and developed inside companies. The data required for each index is different and also, the results produced may vary. The different hazard indices are suitable for different stages of process development, design and operation. Some can be applied at a very early stage of planning and require an overall knowledge of the system under consideration, and some must be applied to existing units with full knowledge of all aspects of the unit. Some hazard indices are presented below with two different forms, comprehensive or detailed, and simple.

Detailed hazard indices

Detailed Indices, that consider many aspects of the unit under consideration, have been proposed from time to time for hazard identification. Noteworthy among them are the Dow fire and explosion index, Dow chemical exposure index and the Mond fire, explosion and toxicity index.

The Dow Fire and Explosion Hazard Index (Dow F&EI) index aims primarily at identifying fire, explosion and chemical reactivity hazards during a plant design and identifying equipment that would be likely to contribute to the creation of an incident. A number of aspects are explored in deriving their Dow F&EI. These are combined into three factors – material, general process and special process factors. Of these, the material factor is dominant.

Dow (1994) specified certain requirements that must be met before the F&EI can be applied to the process. An accurate plot plan of the manufacturing unit and the process flow sheet must be available. Moreover, the minimum inventory of the base material must not be less than 2,268 kg. If these requirements are not met, the hazard involved in a chemical process can be over-estimated by the index.

The Dow Chemical Exposure Index (Dow CEI) was developed to complement the Dow F&EI in the assessment of hazards associated with the release of toxic materials. This index is a measure of the relative acute toxicity risks to people within chemical plants and neighbouring communities. It may be used for initial process hazard analysis and in emergency response planning.

The information needed for the calculation of the Dow CEI includes physical and chemical properties of the material, a simplified process flow sheet, showing vessels and major pipe work with inventories, and an accurate plan of the plant and its surrounding.

Another detailed hazard index is the Mond Index. Members of the Explosion Hazard Section of ICI Mond Division (ICI Mond Division, 1993) developed the Mond Index from the Dow F&EI Hazard Classification Guide, principally for the chemical industry of ICI, following the Flixborough disaster. The main purpose of the Mond Index is to extend the applicability of the Dow F&EI to include a wider range of processes. It includes a consideration of toxicity hazards that was not accounted for in the Dow F&EI at that time. It expands the Dow F&EI to include a wider consideration of continuous and batch processes in the storage and loading/unloading areas and materials such as oxidative and other explosive materials, which are not considered fully in the Dow F&EI Hazard Classification Guide. Similar to the Dow F&EI, the application of the Mond Index highlights features of a plant having a significant fire and explosion hazard potential.

To use either the Dow F&EI or Mond Index procedures at an early stage in process design could reveal hazard potential which is relatively easy to alleviate before the design is advanced. The effects of any design modifications should be evaluated by recalculation of the indices. These indices are more relevant to the chemical and petrochemical industries and complement other hazard analysis studies.

Examples of other comprehensive hazard indices, that are relatively new and not widely used, are the Hazard Identification and Ranking (HIRA) technique (Khan and Abbasi, 1998) and Safety Weighted Hazard Index (SWeHI) (Khan *et al.*, 2001).

One major issue with the above mentioned hazard indices is that they incorporate judgment of the relative importance of the various types of hazards and potential injuries or damage into the evaluation of the index. The user of the index either defers to the judgment of the developer of the index, or must modify it to incorporate personal judgment. If each user modifies the index based on personal judgment, there cannot be a valid comparison among different users (Hendershot, 1997). For example, Gupta (1997) gave some changes for the Dow F&EI to make it give a more realistic value for developing countries. Another disadvantage is that the above indices are not suitable for

route selection because they require detailed plant specifications (Edwards and Lawrence, 1993). Route selection means early stage chemical manufacturing planning from feedstock to final products. Hence, these indices cannot be used in optimization models for early stage planning especially in large industries with large number of options. The Dow and Mond indices require detailed plant operational data which are not available at early planning stages.

Simple hazard indices

Simple hazard indices are used in the earliest stages of planning and when the most detailed process information is still lacking. Developing a simple hazard index for systems is not an easy task; it requires knowledge of what is important for the viability of the system involved and how that contributes to safety. The number of representative indicators in the index should be as small as possible, but as large as essential. Such simple hazard indices are, by their nature, applicable only for specific functions and should not be employed for more general safety comparisons.

In the petrochemical industry field, the first forms of simple safety indices for planning started in the 1980s after the development of optimization models for that industry. The indices at that time were very simple; they were the first introduction of safety into planning. Fathi-Afshar and Yang (1985) selected the chemical Threshold Limit Value (TLV) as an indicator for a health objective function. Chemical 1 is considered to be more harmful than chemical 2 if TLV_1 is less than TLV_2 ; so the index is represented as the reciprocal of TVL.

Very simple hazard indices were also used when planning involve hazard identification for a large number of plants. The National Fire Protection Association (NFPA) (1994) developed a system for indicating the health, flammability and reactivity hazards of chemicals. The system is based on giving a number (from 0 to 4) to a chemical indicating its effect. Al-Sharrah *et al.* (2001) used these NFPA health ratings as an index for an environmental objective in planning. This model was composed of 83 plants with 65 chemicals.

Other groups of safety indices present a more detailed approach to quantifying safety. Although more detailed, they are still relatively simple when compared to the Dow and Mond indices. The indices depend on the materials handled and the process operated with all values being determined, not estimated or based on judgment. The first example is Edwards and Lawrence (1993) index. This index is intended for analyzing the choice of process route; i.e. the raw materials used and the sequence of the reaction steps. This method is very reaction oriented. The index has been calculated as a total score, which is the sum of a chemical score and a process score. The chemical score consists of inventory, flammability as flash point and boiling point, explosiveness as a difference between explosion limits, and toxicity as TLV. The process score includes temperature, pressure and yield. Yield is the product of conversion and selectivity; a high yield implies

efficient usage of raw material, therefore, no need for recycles and therefore less inventory. Some of the scores are based on similar tables in Dow and Mond indices. Others have been constructed by dividing the domain of the values of the parameters into ranges and assigning a score to each range.

Another example is Heikkila *et al.* (1996) index which considers a wider range of factors affecting safety of a process and is an extension to Edwards and Lawrence (1993) index. The index is divided into the two main categories usually used in studies of risk indices: chemical and process safety. The index describes the effect of the choice of raw materials and other chemicals on the inherent safety of the process. It considers the following aspects: heat of the main reaction including the diluents in the reactor; heat of potential side reaction; flammability as a flash point; explosiveness as a difference between explosion limits; toxicity as TLV; corrosiveness; incompatibility of chemicals which represents the potential reaction hazards from an accidental mixing of the chemicals. The index describes the effect of the type of process equipment and processing conditions on safety. The following parameters are considered: inventory of chemicals, process temperature and pressure, the type of processing equipment and the structure of the process. The total index is the sum of chemical and process indices. The details and examples of the index are clearly shown in Heikkila (1999).

Cave and Edwards (1997) proposed the Environmental Hazard Index (EHI) that ranks routes (raw materials and reactions to produce the final product) in chemical plant development by the estimated environmental impact of a total release of chemical inventory. The index considers the hazard to the aquatic and the terrestrial ecosystems. An index by Gunasekera and Edwards (2001, 2003), called the Atmospheric Hazard Index (AHI), can be used to assess the potential impact of airborne releases from a chemical production plant. A catastrophic failure of the plant is assumed and the impact on the atmospheric environment is estimated. The method is designed to assess possible alternative process routes to make a chemical, in order to determine the route that has the least adverse atmospheric environmental impact. Thus the routes that are inherently environmentally hazardous can be identified and avoided when the selection is made in the early stage of production plant design. The atmospheric impact categories considered were the toxicity, photochemical smog, acid deposition, global warming and ozone depletion of a chemical when it is released catastrophically into the environment.

The simple hazard indices discussed are suitable for route selection but with the following limitations:

1. The NFPA ratings and TLV are two simple and can give inaccurate relative toxicity of some chemicals, for example the TLV for acrylonitrile is 2 ppm while for hydrogen peroxide is 1ppm; so according to their TLV, hydrogen peroxide is relatively more toxic than acrylonitrile which is not correct.

2. Edwards and Lawrence (1993) and Heikkilä (1996) indices require some operational data such as temperature, pressure and yield which are not available at early planning stages.
3. Cave and Edwards (1997) and Gunasekera and Edwards (2001,2003) indices were developed mainly to assess the potential impact of a chemical release on the environment without a clear indication of the adverse effect on humane beings.

In additions to the above points, the importance of learning from previous chemical incidence collected in databases led to developing a new index that incorporates this knowledge. However, it is strongly stressed that the new index is not designed to replace the well known and established indices but to be useful in cases where planning of a very large number of plants is needed with limited number of operational data.

The literature on hazard indices gives different names and classifications for the indices using the terms risk, safety or hazard. For example Hendershot (1997) considered the Dow F&EI and the Dow CEI as *risk indices*. Khan and Abbasi (2001) broadly characterized safety and risk studies into three groups: quantitative techniques, qualitative techniques and probabilistic techniques and Gentile *et al.* (2003) named three *quantification methodologies*:

1. A collection of several well-known indices used to evaluate various safety aspects. The results cannot be aggregated under an overall index.
2. A single overall index that evaluates aspects relative to inherent safety and the results aggregated under an overall number.
3. A risk-based approach.

Chemical Accidents Database

Chemical plants are complex, tightly – coupled operations. Tightly – coupled means one event or process affects another event or process directly and quickly, thus making human intervention difficult when something goes wrong. Complex means that events cannot be predicted reliably because many different things can go wrong in many different ways. This is why every chemical plant in the world is an accident waiting to happen (Rachel's, 1994). A major accident in one sector of the industry gives no market advantage to a competitor, if it leads to a general loss of confidence in the industry by the public (Kirchsteiger, 2003).

Accidents databases are collections of data on chemical accidents. Major accidents databases were the result of federal law while others were for private institutes or companies. The law requires that certain facilities report annually their toxic release and inventories together with any accidents that harm workers, the public, and the environment. In the past 30 years special attention has been given in designing and developing a database of chemical accident histories. As a result, there exist a number of

such databases, some of them covering specific countries and some covering wider geographical areas. Statistical analysis with data processing has led to several scientific publications and technical guidelines issued by research institutes and governmental agencies. For example, Kirchsteiger (1999b) analyzed data of major accidents in the European Union and Belke (2000) analyzed data for chemical accidents risks in U.S. industry, all using accidents databases. Balasubramanian and Louvar (2002) studied seven accidents databases and identified that, even with some existing problems in the databases, important information can be extracted and the description of accidents are useful and educational. Data in the databases are very valuable and many useful conclusions and statistics were found from analyzing them.

One major accidents database available on the internet is the Accidental Release Information Program (ARIP) (1999) database. It is one of the most useful databases due to its size, format and public availability. (ARIP) is associated with U.S. industry where all U.S. facilities are required by law to report non-routine releases of certain substances when those releases exceed a reportable quantity. These reports are submitted to the National Response Centre, the U.S. Coast Guard, and Environmental Protection Agency (EPA) regional offices. EPA compiles the reports into the Emergency Response Notification System (ERNS) database. EPA then uses ERNS data to select releases for the ARIP questionnaire. The ARIP questionnaire consists of 23 questions about the facility, the circumstances and causes of the incident, and the accidental release prevention practices and technologies in place prior to, and added or changed as a result of, the event. The questionnaire focuses on several areas of accident prevention including hazard assessments, training, emergency response, public notification procedures, mitigation techniques, and prevention equipment and controls.

Another important, and widely recognized, chemical accidents database is the Risk Management Plans database (RMP*info). It is a result of a law enacted by the U.S. congress to require certain chemical facilities to submit summary reports every five years. These reports contain significant information on each facility's accident history, accident prevention program, and the potential consequence of a hypothetical accidental chemical release. These data have been assembled into a searchable computerized database and was originally intended to be available to the general public via the Internet. However, the chemical industry and U.S. security agencies raised concerns that some of the data would allow terrorists to easily identify those facilities likely to cause the greatest harm to the public in the event of a release. These concerns promoted Congress to pass legislation in August 1999, that, along with subsequent federal regulations, currently restricts public access to portions of the RMP*info database.

Belke (2000) wrote a very useful analysis from the RMP*info database; it was a preliminary characterization of the database. One useful analysis was the normalized accident rates; accident rates are commonly normalized by dividing the number of incidents by some measure of the number of opportunities for an accident. This allows large and small facilities to be compared fairly over a given period. However, since

hazardous chemical facilities vary so greatly in size, number of processes, chemical quantities stored and produced, operating schedules, and other characteristics, it is difficult to say which single divisor best represents the number of accident opportunities. Belke (2000) used the number of processes in the facility using the chemical and the aggregate chemical quantity as normalization factors. Table 1 shows the results.

Table 1: Normalized accident rates from RMP*info chemicals (Belke, 2000)

Chemical name	Number of Accidents per Process per Year	Number of Accidents per Mlbs stored per Year
1. Ammonia	0.016	0.014
2. Chlorine	0.022	0.16
3. Hydrogen Fluoride	0.064	0.27
4. Flammable Mixture	0.0074	0.00075
5. Chlorine Dioxide	0.155	1.97
6. Propane	0.006	0.0012
7. Sulfur Dioxide	0.013	0.011
8. Ammonia (aqueous)	0.017	0.018
9. Hydrogen Chloride	0.060	0.25
10. Hydrogen	0.031	0.024
11. Methane	0.027	0.0064
12. Butane	0.011	0.00089
13. Ethylene Oxide	0.027	0.045
14. Hydrogen Sulfide	0.067	0.5
15. Formaldehyde	0.009	0.024
16. Isobutane	0.010	0.011
17. Pentane	0.013	0.0052
18. Titanium tetrachloride	0.056	0.090
19. Phosgene	0.044	2.49
20. Nitric Acid	0.038	0.047
21. Ethane	0.014	0.00071
22. Oleum	0.022	0.011
23. Ethylene	0.014	0.00089
24. Vinyl Chloride	0.042	0.0051
25. Trichlorosilane	0.034	0.10

APPROACH

Analysis of Accidents database

The ability to learn from previous incidents has long been regarded as an essential aspect of any program designed to reduce the frequency and severity of future incidents. Many major events which capture media attention continue to implicate "failure to learn from previous losses". If obvious similarities are apparent between an existing operation

and one that experienced loss, follow-up action is more likely to be pursued and future loss may be avoided.

Normalized accident rates, or accident frequencies represented by "Number of Accidents per Process per Year", listed in Table 1 show similarities in rates for some groups of chemicals. Following inspection of column two in Table 1, five groups of chemical were identified and these are presented in Table 2.

Table 2: Normalized accidents rates from RMP*info chemicals; a group form.

Chemical group	Accidents Frequency: Number of Accidents per Process per Year	Mean Group Frequency
Group 1: Hydrogen sulfide Hydrogen fluoride Hydrogen chloride	0.067 0.064 0.060	0.064
Group 2: Phosgene Vinyl chloride	0.044 0.042	0.043
Group 3: Hydrogen Methane Chlorine	0.031 0.027 0.022	0.027
Group 4: Ammonia Ethane Pentane Ethylene Butane Iso-Butane	0.016 0.014 0.013 0.014 0.011 0.010	0.013
Group 5: Formaldehyde Flammable mixture	0.009 0.007	0.008

Although some chemicals in the groups share some physical and/or chemical properties, the group name or a general classification has not been identified or determined yet. However, the chemicals in Table 2 that have high accident frequencies, e.g. hydrogen sulfide, are chemicals that cause corrosion problems. Fontana (1987) indicated that most of the corrosion difficulties for refinery operations are due to inorganics such as hydrogen sulfide. When studying the corrosion resistance of materials of construction to some chemicals in Table 2 it was found that the accident frequency

decreased with increasing corrosion resistance to the chemical. This can be seen more clearly when numerical values to corrosion resistance are assigned. Most Industrial plants are made from either carbon steel, 304 stainless steel or 316 stainless steel; chemical compatibilities, from corrosion tables, can be classified as being excellent, good, fair or having a severe effect. To identify numerical values for corrosion resistance, numerical values were first assigned to the classifications for example:

Excellent = 4

Good=3

Fair =2

Severe effect= 1

Hydrogen sulfide has a compatibility of fair, excellent, and severe effect with 304 stainless steel, 316 stainless steel and carbon steel respectively; this gives a total score for compatibility of 7. Similarly, the score for hydrogen fluoride is 7, methane 9, chlorine 10, ammonia 11, and butane 12. Table 2 shows that these chemicals have descending accident frequencies.

Unfortunately, not all the chemicals, in Table 2, have complete compatibility data, but relating chemical corrosion to accidents is a first step towards identifying chemical accidents causes. The Dow F&EI and Heikkila (1999) indices considered corrosion in evaluating their indices. Dow gave a penalty for corrosion and erosion in the range 0.1 to 0.75, and Heikkila gave a score of 0, 1 and 2 for the construction materials carbon steel, stainless steel and "better material" respectively. It can be stated now that there exists an inverse relation between accident frequency and a chemical's compatibility with the construction material.

Other useful information from accident databases is the hazardous effect of a chemical material in terms of the number of people affected by the release of that chemical. It is well known that the health and safety effect of chemicals on people is an important issue. These effects can be estimated from toxicity data like Lethal Dose LD₅₀, Lethal Concentration LC₅₀, or TLV. However, information on the actual effects is shown in accidents databases. The ARIP database lists information on chemical accidents including the amount of chemical released and the number of people affected. Affected people include fatalities, people injured and people hospitalized. However, some incidents involving the release of hazardous chemicals reported in the databases indicate that the number of people affected by the release was zero. This can be a result of nobody being in the vicinity of the accident at the time of the incident.

It is important to be able to estimate the number of affected people following a release. For this reason, a relationship was sought between the number of people affected and toxicity data. Equation 1 represents a relationship between the LD₅₀ and the number of people affected per tonne of chemical released. Equation 1 was found from a

regression of the data in Table 3 which lists some chemicals that have known values of LD_{50} and valid accidents data from ARIP. This relationship can be used to estimate the number of people affected by a chemical knowing the value of LD_{50} for a chemical. It is worth mentioning that the ARIP database was the only major accidents database accessible through the internet.

Table 3: Affected people per tonne of chemical released and the lethal dose

Chemical	LD_{50} rat mg/kg	Affected people/tonne From ARIP
Acetic acid	3310	0.0229
Acrylic acid	340	0.0561
Ammonium hydroxide	350	0.2449
Benzene	930	0.1465
Carbon tetrachloride	2350	0.1827
Chloroform	1194	0.0179
Dichloromethane	1600	0.2064
Ethylene oxide	72	1.0800
Formaldehyde	100	1.0151
Phenol	317	0.6386
Phosphoric acid	1530	0.0133
Potassium hydroxide	365	0.0270
Propylene oxide	380	0.2821
Sulfuric acid	2140	0.0213
Toluene	636	0.0747
Vinyl acetate	2920	0.1866
Vinyl chloride	500	0.0417
Xylene	4300	0.2348

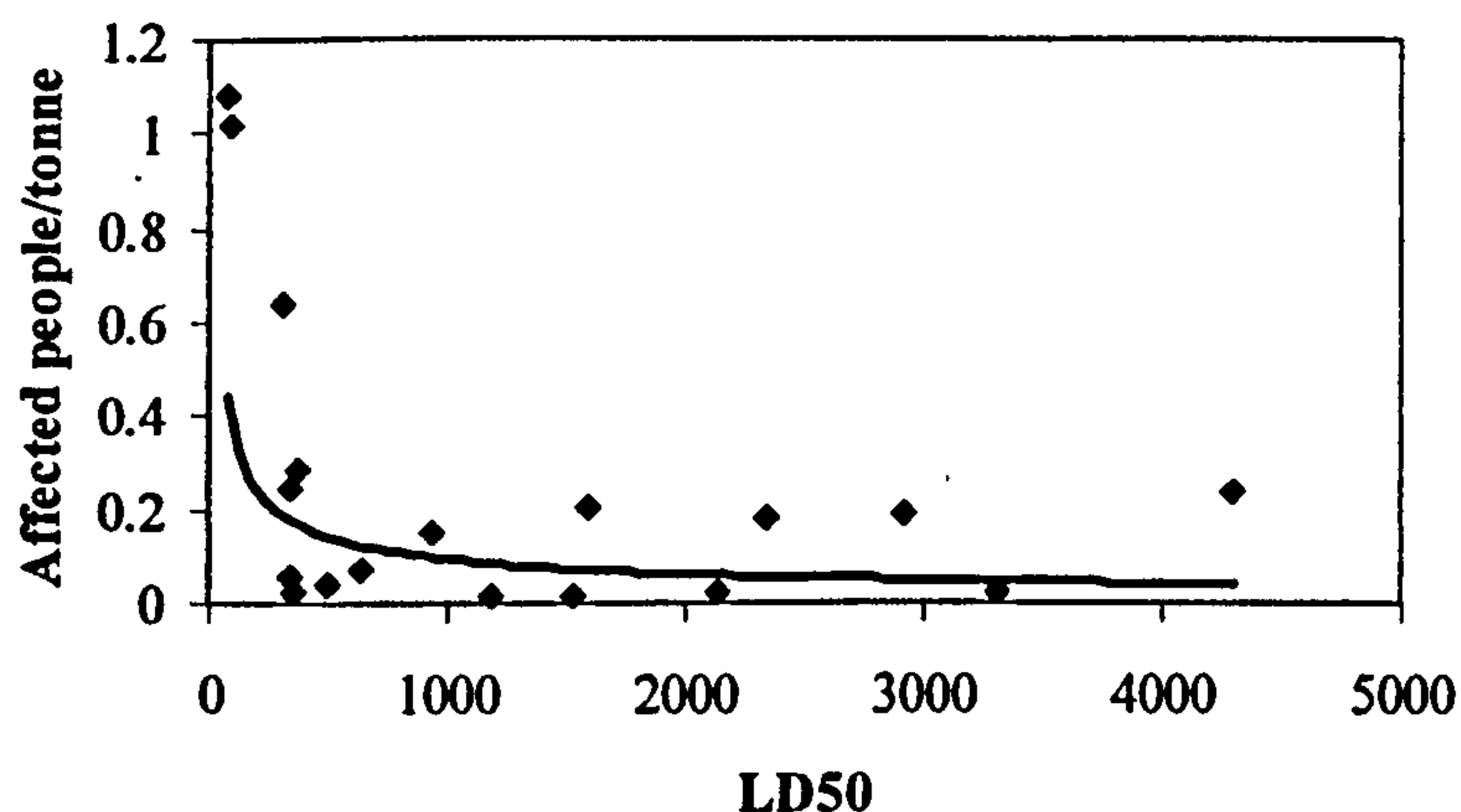


Figure 1: Affected people per tonne of chemical released and the lethal dose

$$\text{Affected people/tonne} = (5.4764) LD_{50}^{-0.5881} \quad (1)$$

The regression of equation 1 is shown in Figure 1 with an R^2 value of 0.2482. Although, the accuracy of the equation is low, Figure 1 shows a clear relation in the form of a power function between the affected people and the lethal dose. Also, the accuracy of the equation is not expected to be very high because the data for affected people and the amount released were taken from a single accidents database, ARIP database. Some incidents in the database have reported the release of a chemical which was not 100% pure and for some chemicals the number of incidents counted was not very high. It is strongly believed that the accuracy of the equation can be drastically increased if a larger number of incidents were included. In addition, It is strongly emphasised that Equation 1 is used to estimate the hazardous effect of a chemical release only in cases where no such data is available.

Accidents reported in the accidents database include toxic, fire and explosion incidents and the number of affected people reported in ARIP and listed in Table 3 is the sum of these three types of accidents. By attributing the number of people affected to a toxic effect only, as in Equation 1, it was assumed that the number of people affected by toxic release dominates over fire and explosion effects. Belke (2000) indicated that the toxic effect of a chemical is far more severe than its fire effect. He stated the following:

- In general, toxic release scenarios result in a greater endpoint distance than flammable worst case scenarios. The distance to the endpoint is the distance from the release location to the point at which toxic vapour cloud, heat from a fire, or blast wave from an explosion cease to have harmful effects that causes a hazard problem
- The median endpoint distance for toxic worst case scenarios is 1.6 miles, while the median endpoint distance for flammable worst case scenarios is 0.4 miles.
- Under the RMP rule, the population potentially affected by a release is defined as the residential population inside a circle with radius equal to the end point distance. The median population for flammable worst case scenarios is 15 people, while the median for toxic worst case scenarios is 1,500 people- two full orders of magnitude greater, whereas the difference in the median value for the endpoint distance is only a factor of four.
- Flammable worst case scenarios are, on average, less severe than toxic alternative scenarios. Notably, most flammable release scenarios would not affect any members of the off-site public.

This was the result of an analysis done on the RMP*info accidents database. This database was also analyzed by Al-Qurashi (2000) and it was found that 81% of the releases reported in the database are from toxic substances.

The above analysis from the accident database indicates that the toxic effect of chemicals is dominant over its fire and explosive effects. Consequently, a simplified relationship, such as Equation 1, to relate the number people affected to LD_{50} only can be acceptable.

Index Structure

Starting from the basic definition of risk, which was the product of the incident probability and the magnitude of the harmful effects, a simple risk index K is proposed that is suitable for use in planning optimization models. It is an index that can be applied to chemical plants using the properties of the major chemicals associated with production. It is an index to quantify risk to human life and falls into the group of simple early stage planning and route selection hazard Indices. The index is:

$$K = Freq \times Haz \times Inv \times Size \quad (2)$$

where

Freq = Frequency of accidents, number of accidents per process per year

Haz = Hazardous effect of the chemical, number of people affected per tonne of chemical released

Inv = Inventory of chemical released, tonne per accident

Size = Size of plant, number of major processes in plant

This gives an overall unit of the index K as number of people affected per year, and it represents the maximum number of people affected if an accident caused the release of all the plant inventory of a chemical. Affected people include fatalities, people injured and hospitalized. The plant is assumed to have major processes in which a major chemical is being treated and an accident in any part of the plant may cause, in an extreme case, the release of the plant inventory.

The general definition of risk includes probability, whereas this work uses frequency. This is because of the availability of frequency data and the difficulty of estimating a probability as discussed previously.

The frequency of accidents (*Freq*) can be taken from Belke (2000) as shown in Table 1. If the chemical is not found in Table 1, an estimate of the frequency is made by analogy with a similar chemical or from Table 2, according to which group the chemical can be related to; in this case, the mean group frequency is used. The hazardous effect of a chemical (*Haz*) is calculated from any accidents database by looking at all the available accidents associated with the chemical and dividing the number of affected people by the amount released; ARIP database is a good source. If no accidents were reported for the chemical or if the reported number of affected people is zero, Equation 1 can be used to

estimate this number. The inventory (*Inv*) is taken as the maximum production inventory in a petrochemical plant; usually it is one month of minimum economic production. Finally, (*Size*) of a plant, in term of major processes, can vary from one plant to another but usually a chemical goes through production stage, purification and a final product storage. Therefore, a general number for *Size* is taken as three. Calculations of the index for some chemicals are shown in Table 4 and values plotted in Figure 2.

The above is a sample calculation for the index and it represents a maximum risk from a single chemical in a plant. The index can also be used in other cases as the following:

1. The index can be applied to a chemical plant including major and non-major chemical. The index in this case is calculated as the summation of individual chemicals indices.
2. The inventory of three months of production is used for calculating a theoretical maximum for the risk. Consequently, a high value for inventory is used. The index can give a more realistic (non maximum) value of the risk if it is applied to existing plants with accurate inventories.
3. The number used for the size is a representative number (an average). The actual number of major processes can be used.
4. The index can be applied for chemicals in the plant which are not stored. In this case, an estimate for their inventory in the process equipment can be used.

Table 4: Risk index results

Chemical	<i>Freq</i> Accidents/process yr	<i>Haz</i> People affected/tonne	<i>Inv</i> Tonne/accident	<i>Size</i> No. of process /plant	<i>K</i> People affected / plant . yr
Acetaldehyde	0.008	0.1202*	5625	3	11.2
Acetic acid	0.038	0.0229	5625	3	14.7
Acrolein	0.064	0.5763*	12.5	3	1.4
Acrylic acid	0.038	0.0561	7500	3	47.9
Acrylonitrile	0.042	0.4224*	7500	3	399.2
Ammonia	0.016	0.1357	8750	3	57
Benzene	0.008	0.1465	8333	3	293
Butadiene	0.013	0.1233*	2083	3	10.0
Carbon tetrachloride	0.056	0.1827	1875	3	57.6
Chlorine	0.022	0.8105	7500	3	401.2
Cumene	0.008	0.0742*	5000	3	8.9
Ethane	0.014	0.1526	4366	3	28
Ethyl benzene	0.008	0.0451*	15000	3	16.2
Formaldehyde	0.009	1.8414	1250	3	62.1
Hydrogen chloride	0.06	0.4273	1666	3	128.1
Hydrogen cyanide	0.064	5.9972	2500	3	2878.7
Hydrogen fluoride	0.064	0.0116	1458	3	3.2
Nitric acid	0.038	0.2298	1875	3	49.1
Pentane	0.013	0.1515*	417	3	2.5
Phenol	0.008	0.0002	3750	3	0.02
Phosphoric acid	0.038	0.0133	14400	3	21.8
Styrene	0.008	0.4484	18750	3	201.78
Sulfuric acid	0.038	0.0149	26666	3	45.3
Toluene	0.008	0.0747	5833	3	10.5
Vinyl acetate	0.042	0.1866	5625	3	132.3
Vinyl chloride	0.042	0.0337	10417	3	44.2
Xylene	0.008	0.2348	5000	3	28.2

* calculated from LD₅₀

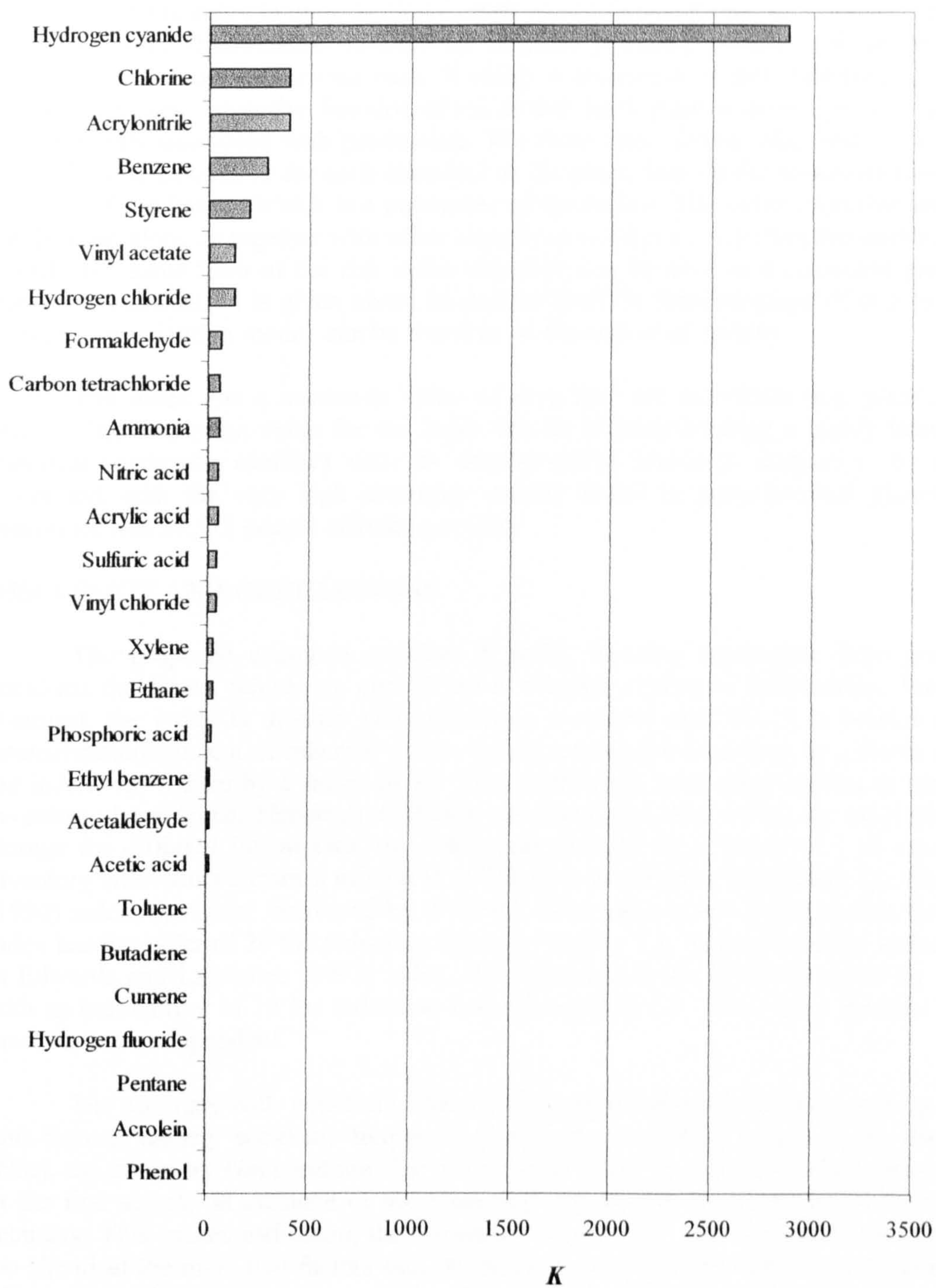


Figure 2: Risk index K for some chemicals

Using the index in optimization models can be in two forms, an objective function or a constraint. Optimization models for industry planning usually look for the best section of plants and production rates. If safety is a concern in that selection, the index can be used as the objective function of the model. Each plant is investigated to identify the chemicals associated with production. The three terms (*Freq*, *Haz*, and *Size*) of the index K , were calculated for each chemical in the plant, leaving the inventory (*Inv*) as a function of production which is a parameter of the model. The index objective function can be used alone or together with other objectives to form a multiobjective optimization model. The same form of the risk index objective can be used as a constraint provided that some information is given about its desired limit. A detailed usage of this index in planning optimization model can be found in Al-Sharrah *et al.* (2006).

The index has a minimum value of zero for safe chemicals (e.g. plastics and resins). The maximum value for the index can be estimated taking a highly hazardous chemical (hydrogen cyanide) with its corresponding accidents frequency, hazardous effect and with the very high inventory usually found in petrochemical plants. The maximum was 57,573 people affected per year.

DISCUSSION AND CONCLUSIONS

The proposed chemical accident K index includes experience from previous accidents databases, which are considered a valuable source of information. For each chemical, the index is directly proportional to inventory and thus it is related to the intensification concept of inherent safety. By decreasing the inventory by a factor of 10, the index will reduce by a factor of 10. This is different from other indices in terms of inventory dependence. Hendershot (2000) calculated the Dow F&EI for ethyl acrylate storage for different inventories; the index was reduced by a factor of 1.16 when the inventory was reduced from 2 million lb to 200,000 lb (10 times reduction). For Heikkila (1999) index, the index decreased by 2 for the same inventories; knowing that Heikkila index has the order of 20 the reduction factor is roughly 1.1. Using the same inventories in Edwards and Lawrence (1993) index, the reduction in the index was only by 1 and with an index order of 15 the reduction factor is roughly 1.1. This makes the new index more inventory dependent.

The accuracy with which the index is determined depends on the accuracy of its four factors, namely accidents frequency (*Freq*), the hazardous effect of the chemical (*Haz*), the inventory (*Inv*) and the size of the plant (*Size*). In any stage of planning, even in the first stages, an estimate of the plant size and inventory can be found with good accuracy. This makes estimating the frequency of accidents and the hazardous effect of the chemical the main two factors that affect the accuracy of the index or estimating the effect of the plant accidents on people. Good values of *Haz* come from good accidents databases, the number of historical incidents has to be as high as possible and the number of affected people has to be accurately counted together with the amount of chemical released. If no data is available, an estimate can be found from Equation 1. The chemical accidents frequencies can also be estimated from accidents databases if the number of

processes using the chemical is listed in the database otherwise Belke (2000) analysis and Table 2 are a good source for estimation.

In developing the index, data from past incidents was analysed and very useful safety 'alerts' were found. Most important of which is the relation between corrosion and plant accidents. Moreover, the toxic effect of a chemical release is dominant over its explosive and flammability effects. These alerts are important because identifying and addressing the factors contributing to industrial chemical accidents is a first step in reducing and hopefully eliminating such accidents. The large number of system components and features in the HSE fields was translated to a representative number as an index.

The new risk index is formulated to represent the theoretical maximum number of people affected if an accident caused the release of the whole of the plants chemical inventory. The merits of this index can be expressed as follows:

- Can be simply used for risk comparison within optimization models.
- Can be applied in initial process assessment, even as early as the conceptual design stage of a plant.
- It uses past experience and data on chemical accidents into the risk evaluation and comparison.
- Can be used for the planning of new plants.

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Paper III

Decision-Making for Petrochemical Planning Using Multiobjective and Strategic Tools

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Decision-Making for Petrochemical Planning Using Multiobjective and Strategic Tools

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Abstract

Decision-making for planning a petrochemical industry is a difficult task, particularly when decisions are required to be made under constraints and different objectives. This paper presents the application of multiobjective optimisation tools for planning of a mixed-integer model of a petrochemical industry to arrive at a small set of good solutions out of the Pareto optimal solutions. The two main objectives are economic gain and risk from plant accidents. Following this optimisation, an economical strategic tool is used to reach the final decision. The proposed procedure has been applied to the petrochemical industry in Kuwait and found to be successful in defining a balanced petrochemical network with acceptable risk.

Key words: petrochemical industry; multiobjective optimization; strategic tool; mixed integer programming.

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INTRODUCTION

Decision-making is the heart of most important activities in businesses and governments. In today's competitive environment, continuous global operations and information management systems are essential tools to improve throughput, maximize yield, and resolve quality problems rapidly. Efficient data analysis, and integration of analytical results into the decision-making process, are critical to maintain profitability, and to achieve world-class quality.

For all industries and especially for the petrochemical industry, decision-making generally involves comparing two or more risky options, with uncertainty being a major factor. Industry decision problems may be divided into three categories (Shah, 2005): (i) infrastructure (network) design; (ii) policy formulation; (iii) planning and scheduling. Following the profit-maximization principle doesn't always necessarily lead to the proper decision because safety, for instance, is another factor which has recently started to have a major and, indeed, decisive influence. The problem with regard to safety usually arises from the toxicity of chemicals which unavoidably accompany the production process. The raw material, the intermediate, and the finished products present the primary independent hazard element (Ward, 2002). The issue of controlling safety in the production of hazardous chemicals is by no means less important than that of controlling the economics of production. Ignoring this increasingly important factor would be a great oversight, since safety and protection of the environment are becoming major forces influencing the shape of the industry.

From the history of chemical accidents, the risk from deliberate acts or large chemical accidents are now considered both real and credible. The risks associated with such accidents must be estimated so that adequate countermeasures are provided that ensure that the risks are as low as reasonably practical. Therefore, good risk quantification, especially due to accidents, and continual improvement in safety planning has become a very important objective for the petrochemical industry. An objective that runs parallel to the economical gain from that industry. Many economical objectives were used in industry planning. Examples are: minimum cost (Fathi-Afshar and Rudd, 1981, De Santiago *et al.*, 1986 and Bagajewicz and Cabrera, 2003); maximum profit (Song *et al.*, 2002 and Bonfill *et al.*, 2004); maximum net present value (Rodera *et al.*, 2002). On the other hand, many safety or hazard indices were used for planning. Examples are: Tyler (1985); Edwards and Lawrence (1993). Tyler (1985) used the Mond index (ICI Mond Division, 1993) that highlights features of plant having a significant toxicity, fire and explosion hazard potential. Edwards and Lawrence (1993) developed an inherent safety index calculated as the sum of a chemical score and a process score. The chemical score consists of inventory, flammability as flash point and boiling point, explosiveness as a difference between explosion limits, and toxicity as the chemical threshold limit value (TLV). The process score includes temperature, pressure and yield.

The focus of the work described in this paper is to perform early planning and decision-making for a number of petrochemical plants producing desired chemicals. It is

aimed at structuring these plants in a network for a maximum economical gain, with long-range economical insight, and for a minimum risk to people due to possible chemical accidents. The two objectives of economics and risk are combined in different forms generating many possible optimum solutions and the final decision is found using a strategic tool. This paper provides tools to support decision-making the most important of which is the incorporation of a new risk index into the objective and the visualization of the industry options on the portfolio of a strategic tool.

TOOLS FOR PETROCHEMICAL PLANNING

Economic Forecasting

Forecasting the future prices of petrochemicals represents a major input to all aspects of production and market planning in the petrochemical industry. The two classes of forecasting techniques are qualitative, which use either experts, salespeople, or customers to make forecasts, and quantitative, most of which use historic data to make the forecasts. An important quantitative forecasting category is causal models.

Causal models, relate statistically the time-series of interest (dependent variable) to one or more other time-series (independent variables) over the same time period if there appears to be a logical cause for this correlation, then a statistical model describing this relationship can be constructed. Knowing the value of the correlated variable (independent variable), the model is used to forecast the dependent variable. The most applied causal model is the regression model. This approach attempts to quantitatively relate a chemical demand (dependent variable), for instance, to the causal forces (independent variables), which determine the chemical demand. Thus regression is a mathematical procedure that takes into account the relationship of the dependent variable and the independent variable(s).

To illustrate this point, one can assume that the demand of a chemical is a function of the Gross Domestic Product (GDP), chemical price and oil price. All three independent variables are assumed to be exogenously determined; they are not influenced by the level of demand itself or by each other.

Forms of models that can be used as causal models are transfer functions. Second Order Plus Dead Time (SOPDT) transfer function model is used extensively in system identification and it can be used as a forecasting model. The model has the form:

$$\frac{\text{dependent variable}}{\text{independent variable}} = \frac{k e^{-\theta s}}{\tau^2 s^2 + 2\zeta\tau s + 1} \quad (1)$$

Where k is the gain, θ is the dead time (delay), s is the Laplace transform variable, τ is the time constant and ζ is the damping factor.

Another useful model, used extensively in forecasting, is the polynomial form of a transfer function. It is explicitly defined as a polynomial between the input u

(independent variable) and the output y (dependent variable). The current output $y(t)$ (dependent variable) is a function of previous na outputs and previous nb inputs delayed by nk together with some noise $e(t)$. The model is named Auto-Regression with eXogenous variable (ARX) model (Ljung, 1999) and is presented as:

$$y(t) + a_1y(t-1) + \dots + a_nay(t-na) = b_1u(t-nk) + b_2u(t-nk-1) + \dots + b_nbu(t-nk-nb) + e(t) \quad (2)$$

Nogales *et al.* (2002) used ARX and a transfer function causal model to forecast the next-day electricity prices. They used the electricity demand as the independent variable. Al-Sharrah *et al.* (2003), also, used SOPDT and ARX models to forecast chemical prices using oil price as the independent variable.

Chemical Accidents Risk

Over the last few decades, the petrochemical industry has reduced its harmful emissions significantly, amongst others via environmental management and technological development (Dijkema *et al.*, 2003). Health, Safety and Environment (HSE) issues are a concern for all industries, but particularly for the petrochemical industry. The consumers, employees, shareholders, legislators and the communities for which the industry operates are all becoming increasingly aware of HSE issues and demand ever-higher standards.

The risk from an industrial process or a technical installation is defined, in the process industries, as the combination of an incident probability and the magnitude of its harmful effects. Thus, this term strongly refers to probabilistic assessment. Risk analysis on a theoretical basis with a full-scope analysis is difficult for the chemical industry. The variety of chemical installations would require too much effort for such a procedure (Hille, 2002). Nevertheless, the question remains as to whether procedures of risk evaluations are available that are not so comprehensive, much easier to apply and yield useful results for risk comparisons.

Recently developed and applied risk analysis tools are Optimal Risk Analysis (ORA) proposed by Khan and Abbasi (1998, 2001) and "risk curve" introduced by Cuny and Lejeune (2003). ORA involves four steps: i) hazard identification and screening, ii) hazard assessment (both qualitative and quantitative), iii) quantification of hazards or consequence analysis, and iv) risk estimation. The "risk curve" results from the combination of the two dimensions of quantitative risk assessment: frequency and severity.

A Simple Risk index

Starting from the basic definition of risk, which was the product of the incident probability and the magnitude of the harmful effects, the simple accidents risk index K (Al-Sharrah *et al.*, 2006) is used. It is an index that can be applied to chemical plants using the properties of the major chemicals associated with production. The index is:

$$K = Freq \times Haz \times Inv \times Size \quad (3)$$

Where

Freq = Frequency of accidents, number of accidents per process per year

Haz = Hazardous effect of a chemical, people affected per tonne of chemical released

Inv = Inventory of chemical released, tonne per accident

Size = Size of plant, number of major processes in plant

This gives an overall unit of the index *K* as people affected per year, and it represents the maximum number of people affected if an accident caused the release of all the plant inventory of a chemical. Affected people includes fatalities, people injured and hospitalized. The plant is assumed to have major processes in which a major chemical is being treated and an accident in any part of the plant may cause, in an extreme case, the release of the plant inventory. This is a simple risk index that can be used for risk comparison.

The frequency of accidents (*Freq*) can be taken from Belke (2000). In his analysis of chemical accidents in the U.S., he used the Risk Management Plans (RMP*info) chemical accidents databases to calculate normalized accident rates and these were used as the frequency (*Freq*) for the index. If the chemical is not found in Belke's study, an estimate of the frequency is taken from a similar chemical mainly in structure

The hazardous effect of a chemical (*Haz*) is calculated from any accidents database by considering all the recorded accidents associated with the chemical and dividing the number of affected people by the amount released. The database used in this work is the Accidental Release Information Program (ARIP) (1999) accidents database. It was the only reliable database available in the internet. The inventory (*Inv*) is taken as the maximum production inventory in a petrochemical plant; usually it is one month of production. Finally, (*Size*) of a plant in term of major process can vary from one plant to another but usually a chemical goes through three major stages: a production stage, a purification stage, and a final product storage stage. Therefore, a general number for size is taken in this preliminary study as three.

Petrochemical Models

Mathematical models of the petrochemical industry have the objective of defining the structure within which the petrochemical industry must function. The structure is formed by the large but linked number of chemicals and by the rigid feedstock, by-products, and energy requirements of these chemicals. The products of one segment of the industry become the feedstock for another segment; thereby defining a network of material and energy flows that constrain business activities.

The model used in this study is a Mixed Integer Linear Programming (MILP) model based on the work of Al-Sharrah *et al.* (2001) with some modifications and is introduced below.

Model assumptions

- The petrochemical network is constructed from plants each contains a number of processes achieving a main chemical transformation between the feedstock and the product.
- The plant inventory of chemicals is mainly in the storage section, having a maximum inventory of one month of production. Equipment inventory is assumed much smaller than storage inventory and hence can be neglected in the calculation of risk of chemical release.
- A number of intermediate chemical are produces and then totally consumed in the petrochemical network; their net production rate is zero.

Model formulation

Let:

N be the number of chemicals involved in the operation of M plants,

X_j be the annual level of production of plant j ,

Q_i be the annual amount produced of chemical i ,

F_i be the annual amount of chemical i used as a feedstock, and

o_{ij} be the output coefficient of chemical i from plant j .

The main constraints that govern the operation of the petrochemical network are the material balance constraints:

$$F_i + \sum_{j=1}^M o_{ij} X_j = Q_i \quad i = 1, 2, \dots, N \quad (4)$$

These constraints ensure that the total quantity produced of each chemical i is equal to the sum of all the amounts produced by all the plants plus its quantity as a feedstock. This constraint applies only to the main chemicals in the plant, not the secondary feedstocks or the by-products.

The final products in the planned petrochemical industry will be governed by their demands in the petrochemical market, according to the country's share in that market.

$$Q_i \leq D_i U \quad i \in I_1 \quad (5)$$

Where D_i is the world demand for chemical i and it is multiplied by the country's share in the petrochemical market, U . The above constraint is only applied for final products group I_1 .

Introducing the binary variables Y_j for each plant j will help in the selection requirement of the planning procedure. Y_j will be equal to 1 only if plant J is selected and

zero if plant J is not selected. Also if only process j is selected, the production level must be at least equal to the plant minimum economic capacity B_j . For each process j we can write the following constraint:

$$B_j Y_j \leq X_j \leq H Y_j \quad j = 1, 2, \dots, M \quad (6)$$

Where H is a valid upper bound.

It is logical that only one plant should be selected to produce a single chemical. The following constraints should be included for each chemical:

$$\sum Y_j \leq 1 \quad j \in J_1 \quad (7)$$

Where J_1 is the group of plants that produces a single chemical. This constraint ensures that a maximum of one plant is selected from each group.

For the final products:

$$\sum Y_j = P \quad j \in J_2 \quad (8)$$

Where P is the number of final products selected from the proposed list of products, and J_2 is the group of all plants that produce a final product. This is a single constraint applied on the group J_2 .

The available supply of some feedstocks will impose additional constraints on selection and planning, i.e.:

$$F_i \leq S_i \quad i \in I_2 \quad (9)$$

Where S_i is the supply availability of feed chemical i . The used feedstock F_i is a function of the optimization variable X_i while the supply S_i is a deterministic input parameter to the model. The above constraint only applies for some feedstock chemicals represented by the group I_2 . Not all the feedstock chemicals are included in I_2 because some are additives and some are needed in small quantities. Also, some petroleum-rich countries have few (if any) limitations on petroleum feedstocks.

An additional economic constraint is required for the limit on the investment budget. If cap_j is the capital investment cost for constructing plant j and Bg is the available budget, then the constraint is formulated as:

$$\sum_{j=1}^M cap_j \times Y_j \leq Bg \quad (10)$$

For simplicity, the objective function used is a maximum economical gain in the selected plants. The economical gain is represented by the overall added value; it is the price of final products minus the cost of feedstock for the petrochemical network. If C_i is the price (or cost) of chemical i , the added-value objective function will be represented by:

$$\max f_1 = \sum_j^M \sum_i^N o_{ij} C_i X_j \quad (11)$$

The second objective function is formulated starting from the risk index K discussed previously. The three terms (*Freq*, *Haz*, and *Size*) of the index K , were calculated for each chemical in the plant (major or minor chemical), leaving the inventory (*Inv*) as a function of production (one month of production). The overall plant index was the summation of all chemical indices, and the risk objective is formulated as:

$$\min f_2 = \sum_j^M \sum_i^N o_{ij} \left(Freq_i \times Haz_i \times Size_{ij} \times \frac{X_j}{12} \right) \quad (12)$$

The two objectives, minimize risk and maximize economic gain, are usually in conflict with one another; some valuable final products of resins and plastics need very hazardous chemicals for production, for example Acrylonitrile Butadiene Styrene (ABS) resins needs acrylonitrile which is very hazardous. Therefore, it is not possible, in many situations, to reduce the industrial risk without any decrease in economic gain. Therefore, one has to use multiobjective techniques to reach a certain trade-off between them. Overall, the model described above is in the form of a deterministic Mixed Integer Linear Programming (MILP) model with multiple objectives. This form will provide a strong selection tool.

Multiple Objectives Optimisation

The notion of multiple objectives or multiobjectives (MO) in planning the petrochemical industry is used extensively due to the number of objectives decision-makers aim to achieve. Most important of these are: profit; cost; environmental concerns; safety. MO programming deals with optimization problems with two or more objective functions. It differs from the classical single objective (SO) optimization only in the number of respective objective functions. In single objective function problems the goal is to identify a feasible solution that gives the best value of the objective function. However, for MO problems the notion of optimality must be dropped because a solution which minimizes (or maximizes) one objective function will not in general minimize (or maximize) any other objective. In other words, what is optimum in terms of one objective is usually non-optimum for another.

The MO optimization problem has a vector (set) of solutions instead of a single solution. Determining the best outcome needs to consider ordering and preference of one solution over another. Optimal MO solutions are defined in terms of these sets by

conditions called Pareto optimality conditions. A feasible solution to a MO optimization problem is Pareto optimal if there exists no other feasible solution that will yield an improvement in one objective without causing degradation in at least one other objective. The Pareto optimal set is usually an infinite set. The decision-maker, therefore, in most cases has to choose the desired solution from the set. The Pareto set usually form a frontier when visualised in the objective function space. In other words, if we have two objective functions plotted in the coordinates of a graph, the Pareto set will form a line in the graph.

There is an abundance of ways in which MO optimization can be solved; some of them are presented below for the objectives $f_1, f_2 \dots f_V$.

Weighted Objective method

In this method, the MO problem with V objectives f is converted to a single objective (SO) problem by using a weighted sum of the original multiple objectives. The equivalent optimization problem is then given by:

$$\min \sum_{m=1}^V w_m \left(\frac{f_m}{f_m^*} \right) \quad (13)$$

And is subject to the model constraints. The w_m is the weighting coefficients satisfying the following conditions

$$0 \leq w_m \leq 1 \quad \text{and} \quad \sum_{m=1}^V w_m = 1 \quad (14)$$

and f^* is the best value of each objective found from single objective optimization and is used in the objective above for normalization due to the use of incommensurable formats and units in those objectives.

A complete set of Pareto solutions can be obtained by varying the weighting coefficients. The final solution is then chosen by the decision-maker. Although the formulation is simple, there is no clear relation between the weights and the obtained solution ; taking an even spread of weights will not result in an even spread of points in the Pareto set making some sections of the Pareto set difficult to populate (Kasprzak and Lewis, 2001). The weighting sum method was shown to work well with convex problems. However, it is not possible to locate solutions at a non-convex part of the Pareto front (Anderson, 2001)

Trade-off Method (ϵ -constraint)

In this method, a trade-off among the multiple objectives is specified by the decision-maker. The original problem is converted to a new problem in which one objective is minimized subject to constraints that limit the value of the remaining

objectives together with the original model constraints. Mathematically, we have the following problem:

$$\min f_r(x) \quad (15)$$

subject to

$$f_m(x) \leq \varepsilon_m \quad m = 1, V; m \neq r \quad (16)$$

Where ε_m is the limiting value of f_m desired by the decision-maker. By varying the values of ε_m a complete set of Pareto optimal solutions can be obtained. This method is not computationally practical if the number of the objective functions is very high. However it is used widely in engineering problems especially when the number of objectives is two.

The distance-based method (L_p norms)

This method is base on minimization of the relative distance from the candidate solution to the best values of the objective functions that were found from single objective solutions. The objective function can be formulated according to equation 17.

$$\min \left[\sum_{m=1}^V \left(\frac{f_m - f_m^*}{f_m^*} \right)^p \right]^{\frac{1}{p}} \quad (17)$$

The exponent p gives different ways of calculating the distance and its value ranges from one to infinity. The most frequently used values for p are 1 for simple formulation, 2 for Euclidean distance, and infinity for Techbycheff norm. This method when used with other methods of MO optimization can generate multiple points on the Pareto front. The most used form is the weighted L_p norm method and the objective function will have the form:

$$\min \left[\sum_{m=1}^V w_m \left(\frac{f_m - f_m^*}{f_m^*} \right)^p \right]^{\frac{1}{p}} \quad (18)$$

The different approaches discussed thus far all require additional input from the decision-maker, which is often subjective. Therefore, MO optimization is as much an art as it is a science. Choosing a method to solve a MO problem depends on the nature of the system and on when the decision-maker articulates his preference concerning the different objectives. Also it is important to choose a MO method that maintains diversity in the Pareto optimal front (Abido, 2001).

Not all methods can be applied successfully with models containing integer variables since the solution space is not convex. If the model contains integer variables, more advanced procedures are used. Most procedures are iterative, have phases, and

require decision-makers preferences. Their aim is to best identify the Pareto optimal solutions. Al-Refai (1993) gave a good collection and description of methods used for MO with integer variables. These solutions, although not being simple, contain in their steps the simple MO methods discussed earlier. However, some authors solved MO with MILP models using simple methods; Chang and Wang (1996) used the weighted L_p norm for a solid waste management system, Song *et al.* (2002) used the ϵ -constraint for scheduling a refinery, Bagajewicz and Cabrera (2003) used the ϵ -constraint for design and upgrade of instrumentation network and Bonfill *et al.* (2004) used the weighted method for scheduling batch plants. Identifying different methods for solving MO optimisation is essential to best populate solutions for the Pareto optimal curve, especially if the model is complex or contains integer variables.

Products Selection and Manufacturing Strategy

Manufacturing strategy is an area of growing concern in most industries. It is simply an effective use of resources for a strong competitive position in the market. For any manufacturing firm to stay competitive in the more globally oriented market of today, the understanding of strategic, tactical and operational issues concerning the link between markets, products and production is fundamental (Olhager and Wikner, 2000). The main step in developing a strategy is to prepare a list of all the products that are in the portfolio of the industry for which a strategy is being prepared. It is then necessary to identify the development and competitive advantage the industry is able to achieve through these products.

One strategic tool used in planning and product selection is the General Electric (GE) / McKinsey matrix developed in 1971 and shown in Figure 1. This matrix is known as the "Industry Attractiveness" – "Business Strength" matrix or the nine-box matrix. To use the matrix, a firm would determine the values of each dimension for each of its products and when placed in the matrix this would provide an overview of the company portfolio. It would indicate whether the status of parts of the business were located unfavourably.

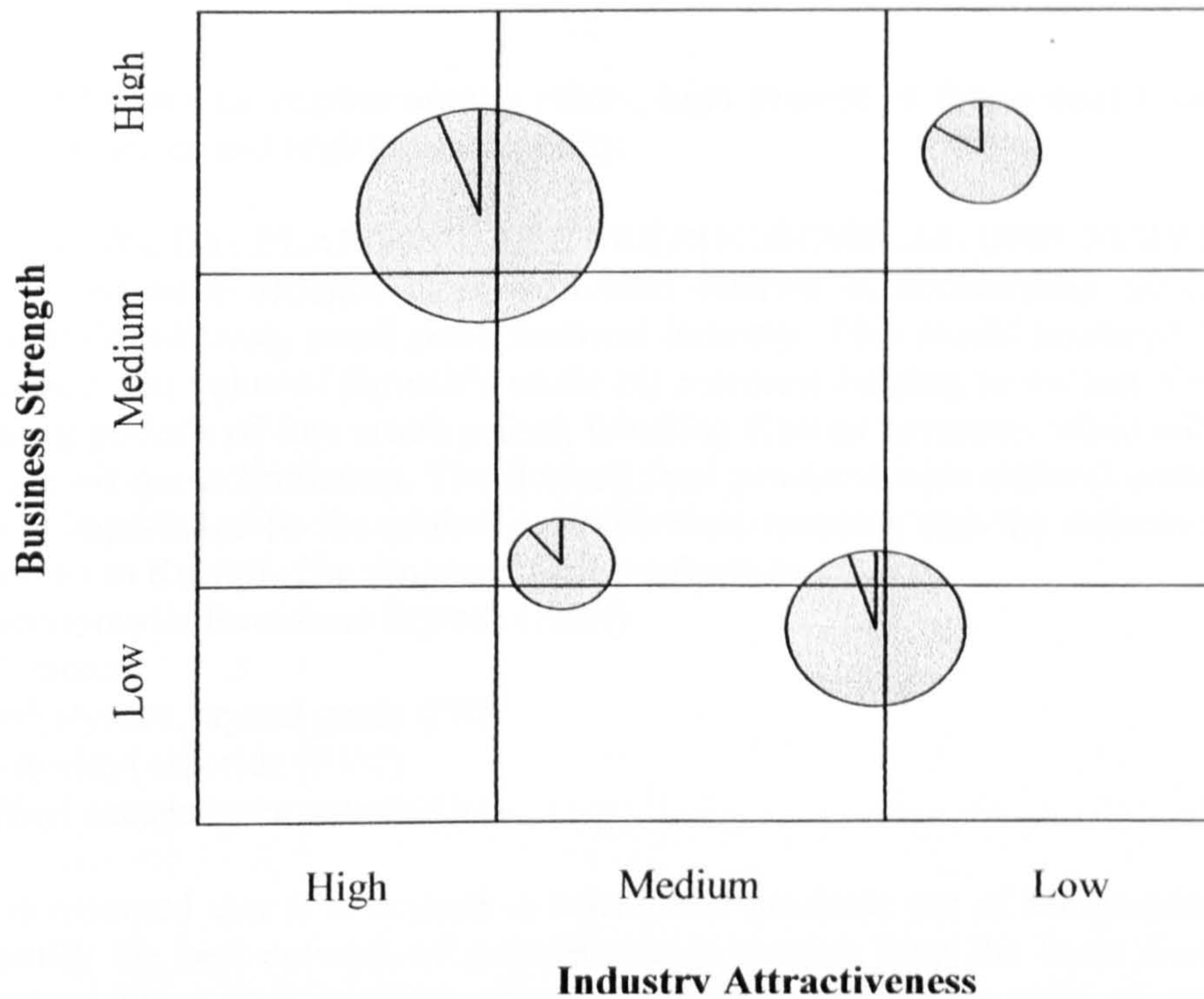


Figure 1: The General Electric / McKinsey matrix

In the GE / McKinsey matrix, business strength is plotted on the vertical axis; the industry attractiveness on the horizontal axis and the size of the circle represents the size of the industry with a shaded wedge representing the firm's current share of the industry. The matrix is divided into nine cells.

1. The three cells at the top left hand side of the matrix are the most attractive and require a policy of investment for growth.
2. The three cells running diagonally from left to right have a medium attractiveness, and the management of businesses within this category should be more cautious.
3. The three cells at the bottom right hand side are the least attractive, and management should follow a policy of business rejection unless the relative strengths can be improved.

A market or industry is considered to be attractive if its potential for providing a significant growth and return on investment is judged to be high. Different strategists and consultants have devised different sets of variables for industry or market attractiveness; typical factors that affect market attractiveness are market size, market growth rate and market profitability. For the other matrix dimension, business strength,

it is a factor that implies among others, high present or future cash flow, high relative profit margins and high product quality.

CASE STUDY: PLANNING THE PETROCHEMICAL INDUSTRY IN KUWAIT

Kuwaiti officials have expressed interest in accelerating development of the country's relatively small petrochemical industry. This would accomplish several goals: boosting the value of Kuwait's crude oil reserves; helping to protect Kuwait's revenues during periods of low crude prices; boosting Kuwait revenues while adhering to OPEC crude oil quota limitation. The desired final products were defined under the criteria of their importance to the global petrochemical industry and the relevance of each final product to Kuwait. The proposed final products are:

- Acrylonitrile Butadiene Styrene (ABS)
- Cumene
- Polystyrene, crystal grade (PS)
- Polyvinyl chloride (PVC)
- Vinyl acetate monomer (VAM)

It is assumed that it is desired to select four products out of the proposed ones, and to identify the best network of petrochemicals starting from the basic feedstocks that can produce these final products together with the production rates of each plant in the network.

The Modelled Network

To construct a petrochemical network, for the desired final products. The routes from the basic feedstock to the final products were determined by selecting a number of manufacturing plants and taking all the possible alternatives of producing the desired products. At the end a network of 62 plants linking the production and consumption of 51 chemicals was formed. Some of the chemicals are catalysts, additives and inorganic reagents and some are considered as intermediate feedstocks and intermediate products in the petrochemical network. A simplified network of the chemicals is shown in Figure 2 with numbers on the figure indicating the 62 plants.

Model Data

The heart of the model is the material balance constraints. Hence, estimation of the output coefficients, o_{ij} , is a key step in constructing the model. For this purpose, yield data for each chemical transformation is required. In many cases, plant yields are variable and depend on what product mix is desired or on what capital expenditure can be afforded. The model uses average yields reported at commercial installations and were taken from Stanford Research Institute (SRI) reports (1992).

The supply of feedstock and demand for final products are needed to complete the construction of the model constraint set. Since the industry must compete for its feedstock and markets, supply and demand data were taken from different sources mainly from recent SRI reports and Kuwait's Petrochemical Industries Company (PIC) annual reports.

The constraint on the final products demand, Equation 5, uses a value for Kuwait's share in the petrochemical market. An overview of Kuwait's exports of some chemicals like methanol and fertilizers have shown that Kuwait share is roughly 1% of the total world petrochemical market. However, Al-Sharrah (2000) recommended that, after a development, Kuwait must increase its share in the petrochemical market to at least 4%, so as to get a good economical utilization of the industry and its products. Therefore, U in Equation 5 will take the value of 4%. The next constraint, Equation 6, needs the minimum economic production rates B_j . These values were taken for all plants in the model from SRI reports (1992). In the constraint equation, Equation 6, H is a valid upper limit for production rates X_j . The importance of assigning a reasonable value for H came from its effect on the model solution. A low value for H resulted in excluding some good high production rates from the model solution. A high value for H resulted in increasing the solution space and hence, higher computation time.

The P in Equation 8 is the number of final products needed to be selected from a set of proposed final products. For this study we have a case for selecting four products and therefore, P will take the value of four.

Chemicals price forecast

The data needed for the economic objective function in the model are prices of final products and main feedstocks; these were presented and then forecasted together with oil prices using causal models following the procedure of Al-Sharrah *et al.* (2003). Results for VAM are shown in Figure 3.

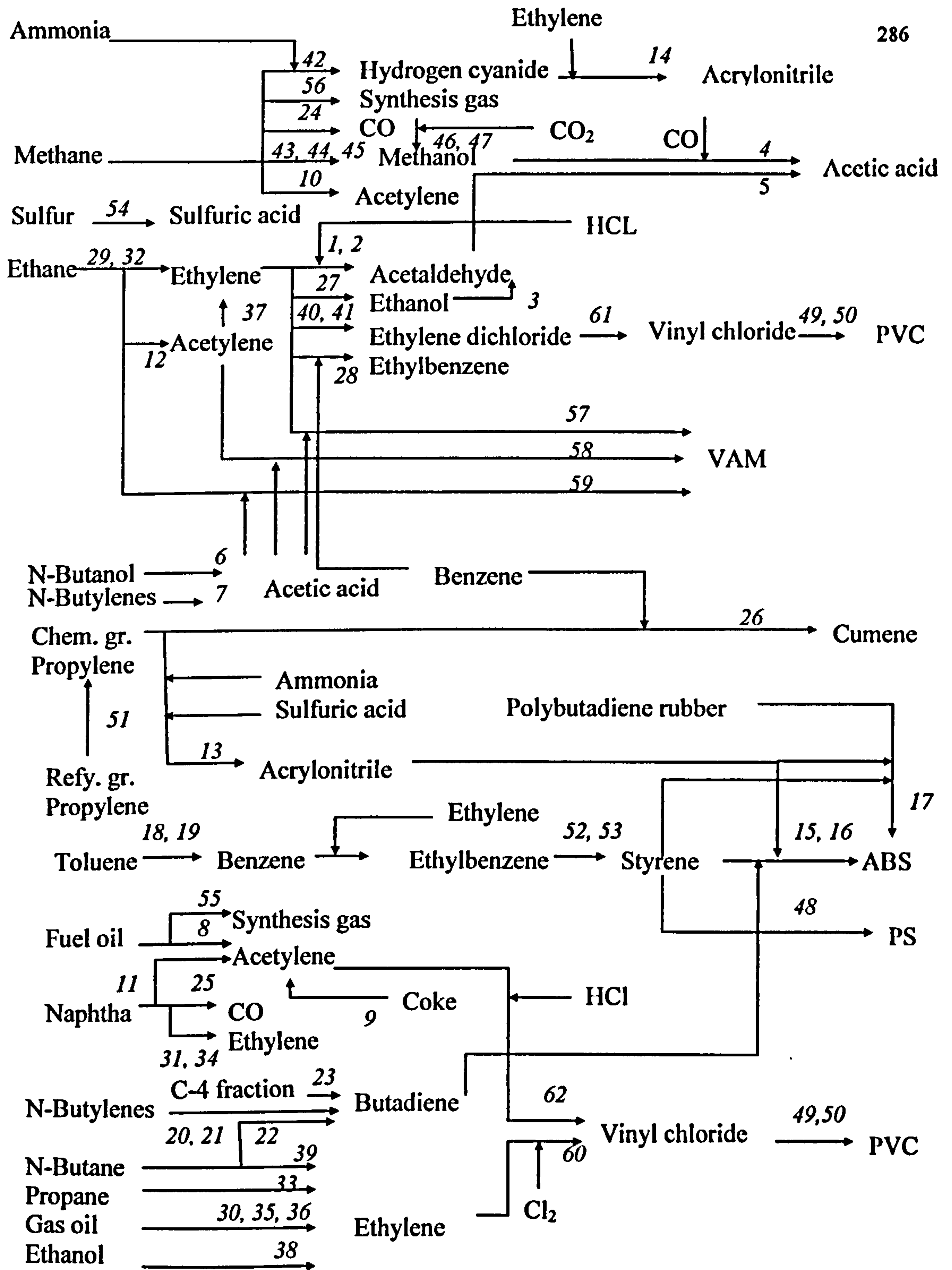


Figure 2: A simplified network of the chemical transformation in the model (numbers on network indicate plants indices)

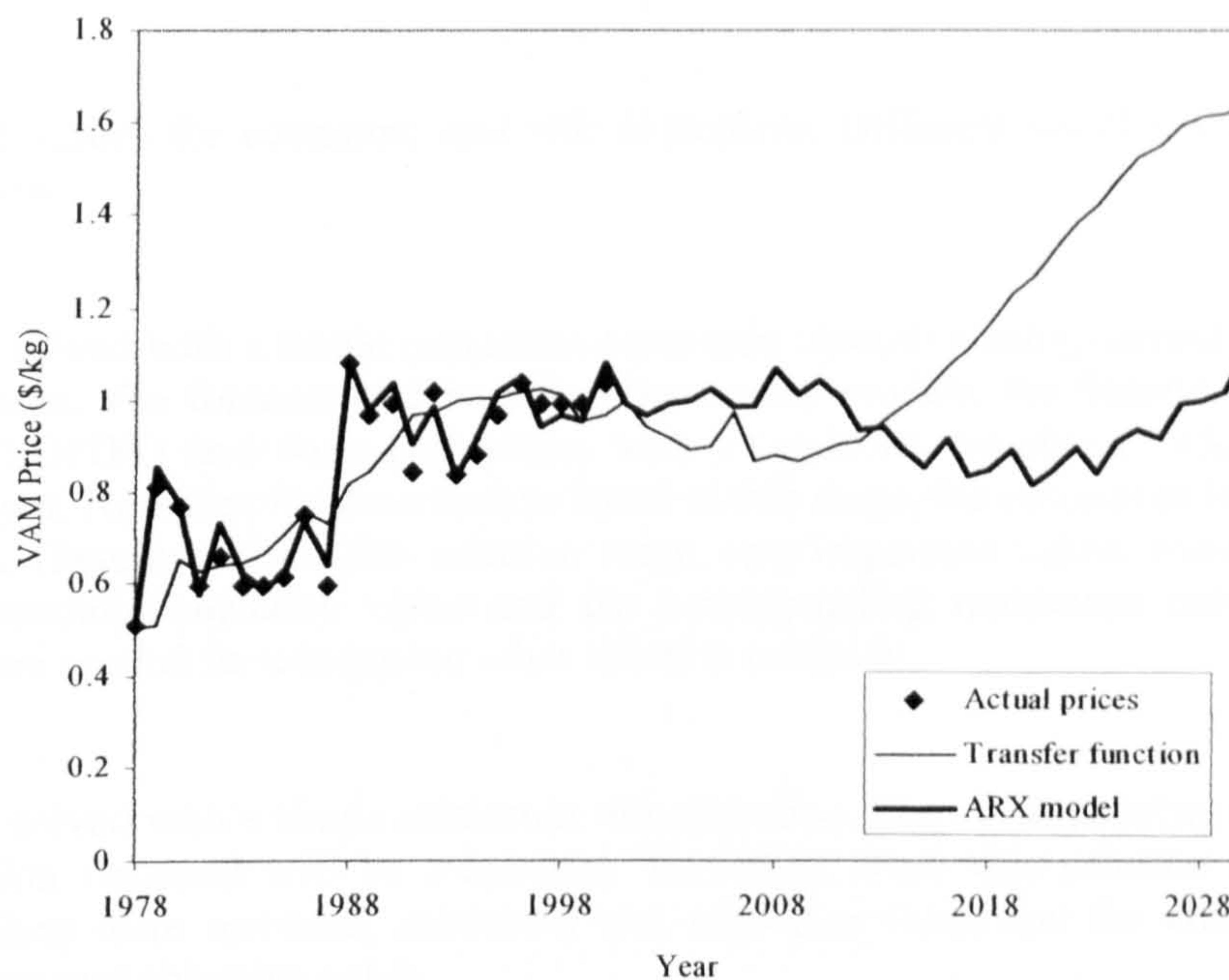


Figure 3: VAM actual and forecasted prices

Model Solution

The MILP petrochemical model was solved using the commercial optimization package GAMS (Brook *et al.*, 1992) with CPLEX (7.5) solver on Pentium 4. Overall, the model is composed of 70 continuous variables, 62 binary variables and 185 constraints. The model in this form is moderate in size and was solved in seconds. However, it was noticed that using a very high unrealistic value for H in Equation 6 increased the computation time. Some problems concerned with obtaining a solution of the model were encountered when using the Lp norm method due to its non-linear form ($p > 1$). For this method, the computational difficulty increased when the value of p was increased, the function becomes more non-linear and sometimes with very high numerical values. The solver used for the non linear objective was SBB solver in GAMS.

Both risk and economic objective functions were tested with the model separately. The model was solved using a single objective function to get the industry bounding structure. The economic objective was also solved with forecasted prices of chemicals. The solution was obtained several times with different final product prices taken for the planning horizon (forecasted prices for the years 2010, 2020, and 2030). The forecasted prices were taken from causal models. Other solutions were found from MO methods. At this stage a set of solutions for the model was being generated.

The model solution gives the selected final products (four out of five chemicals), the corresponding petrochemical network of plants from the basic feedstock to final

products, and values for economic and risk objectives. Different solution methods are explained below.

Method 1:

The model is solved with a single maximum economic objective using current prices and forecasted prices. The forecast is done using two causal models, the Second Order Plus Dead Time (SOPDT) and Auto-Regression with eXogenous variable (ARX), with oil price as an input. Note that for the solution found at this stage, the corresponding risk will be very high. Therefore, from this solution stage, two important values were recorded, maximum economic objective value and the corresponding maximum risk objective value which are needed for computing other solution methods.

Method 2:

The model is solved with a single minimum risk objective. The corresponding economics for the solution obtained will be minimum. Therefore, from this solution stage, two important values were recorded, minimum risk objective value and the corresponding minimum economic objective value.

Method 3:

The model is solved using the multiobjective ϵ -constraint method. The model has a single maximum economic objective with an additional constraint stating that the risk objective is between its maximum and minimum values. The maximum risk objective is found by solution method 1 and the minimum risk objective ($Risk_{\text{minimum}}$) by solution method 2. The ratio between the maximum and minimum risk is 15.3. Therefore, the constraint on risk objective is:

$$Risk \leq M1 * Risk_{\text{minimum}} \quad \text{and} \quad 1 < M1 < 15.3$$

Method 4:

The model is solved using the multiobjective ϵ -constraint method. The model has a single minimum risk objective with the additional constraint that the economic objective is between its maximum and minimum values. The maximum economic objective is found by solution method 1 (taking current prices) and the minimum economic objective ($Economic_{\text{minimum}}$) by solution method 2. The ratio between the maximum and minimum economic objectives is 6.2. Therefore, the constraint on economic objective is:

$$Economic \geq M2 * Economic_{\text{minimum}} \quad \text{and} \quad 1 < M2 < 6.2$$

Other MO methods were tested with the model, the weighted method and the weighted L_p , but their results were not satisfactory. An even spread of weights did not produce an even spread of points in objective values. The model selection was poor and it is very similar to single objective, therefore their results were excluded from the final decision. Abido (2001) favoured the ϵ -constraint over the weighted objective after identifying a number of difficulties in its application.

The solutions obtained so far are plotted to obtain the Pareto optimal curve. This curve helps to visualize the set of optimal solutions and to identify regions of the solution that should be investigated. The curve is a plot of one objective versus the other as shown in Figure 4 and clearly indicates the conflict between these two objectives which was indicated in many studies (see Fathi-Afshar and Yang, 1985 and Steffens *et al.*, 1999). The Pareto curve has two frontiers, the bottom one is formed from all solutions (single and multiple objective) when using current prices of chemicals and the top frontier is formed when using forecasted prices. The forecasted prices are relatively higher than current prices, therefore a higher value of the economic objective is found. The curve with its two frontiers shows good continuity with some gaps. To try to cover the gaps in the Pareto curve, many solution trials for the model with different combinations of objectives were performed, but no new solutions were generated. Possibly no solutions exist for some ranges of the objective functions. Similar discrete Pareto curves from MILP model were used efficiently by Bagajewicz and Cabrera (2003) and Bonfill *et al.* (2004) for decision-making.

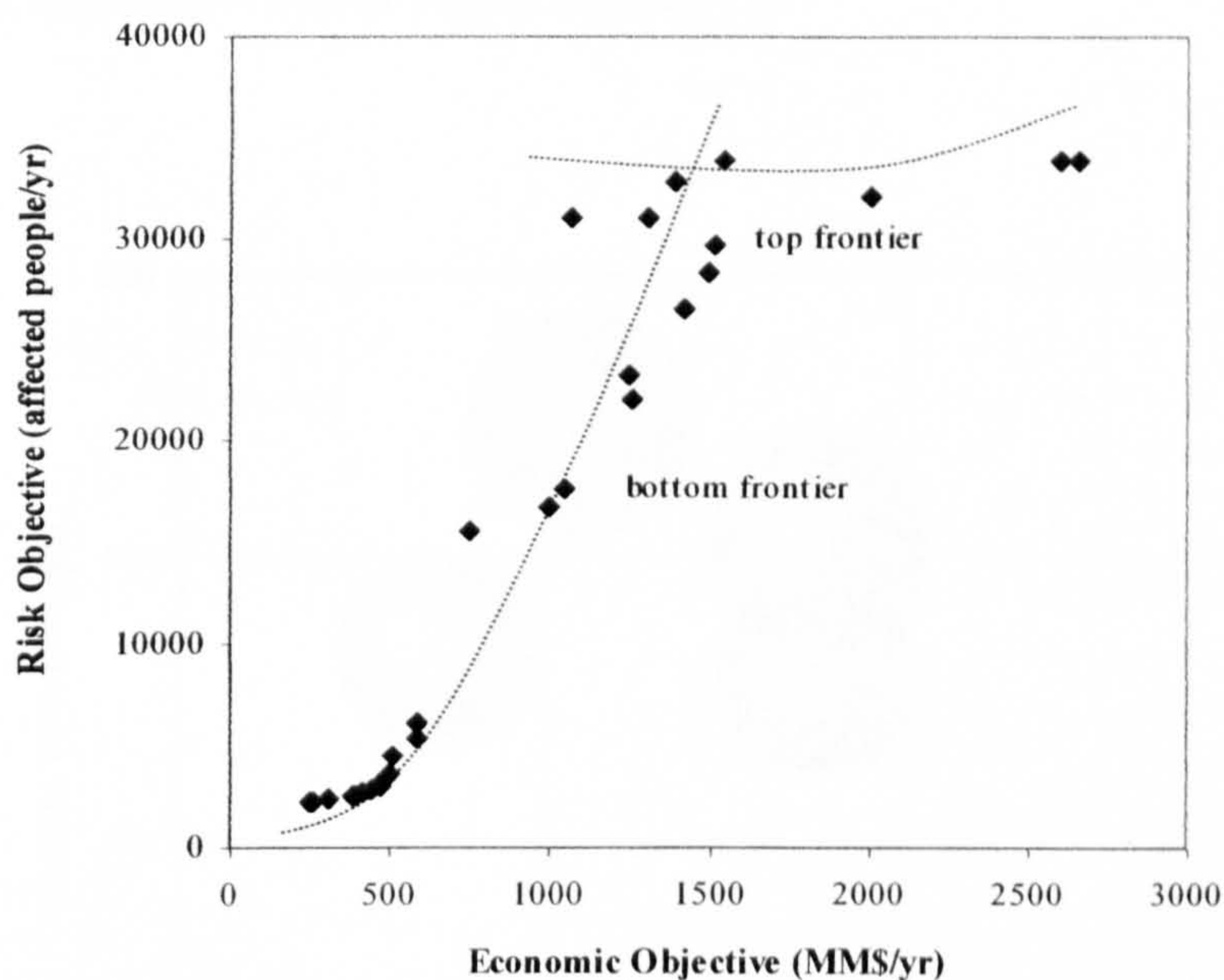


Figure 4: The Pareto optimal curve

From all the results, minimizing risk recommended the rejection of ABS while maximizing economics with current prices recommended the rejection of Cumene. Between risk and economic objectives and with forecasted prices, the model will mostly reject polystyrene. From the solutions of the model, five different networks were proposed for the rejection of polystyrene. The final decision on the best network can be determined from the values of the economic and risk objectives or using another tool, a

strategic one. The strategic tool to be used is the GE / McKinsey matrix with "Industry Attractiveness" presented as the average growth rate of all chemicals in the solution network and "Business Strength" as the present value of the network with a 10% interest rate. This interest rate is the number used for most future plans in petrochemicals. The size of the circles is the average production rate of the final product chemical from the petrochemical network.

Solutions, rejecting PS, are located in the GE / McKinsey matrix and shown in Figure 5. Figure 5 indicates that some model solutions will give a petrochemical network that is not strategically attractive and not strong enough to keep its position in the world market. The best solution is chosen to be the highest leftmost circle in the matrix. This is considered as the best strategic solution and it is a network of 14 plants listed with their production in Table 1 and forming a network plotted in Figure 6. The network has the following features:

- Network chemicals average growth rate = 2.9071 %
- Network Present value (10% interest rate) = 987.6 10⁶ \$
- Economic objective = 2,002.04 10⁶ \$/yr
- Risk objective = 31,878 people affected / yr

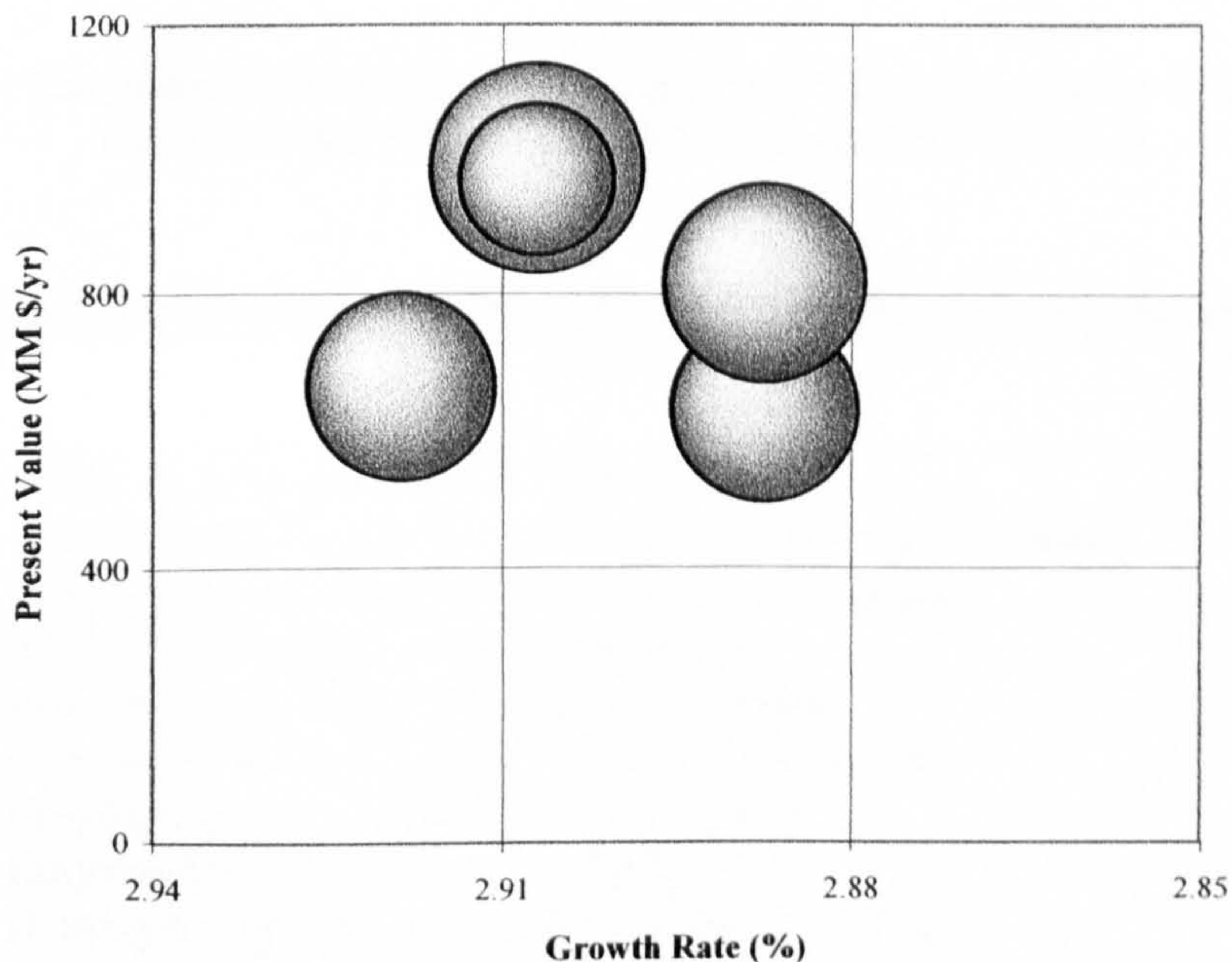


Figure 5: Model solutions on the GE / McKinsey matrix

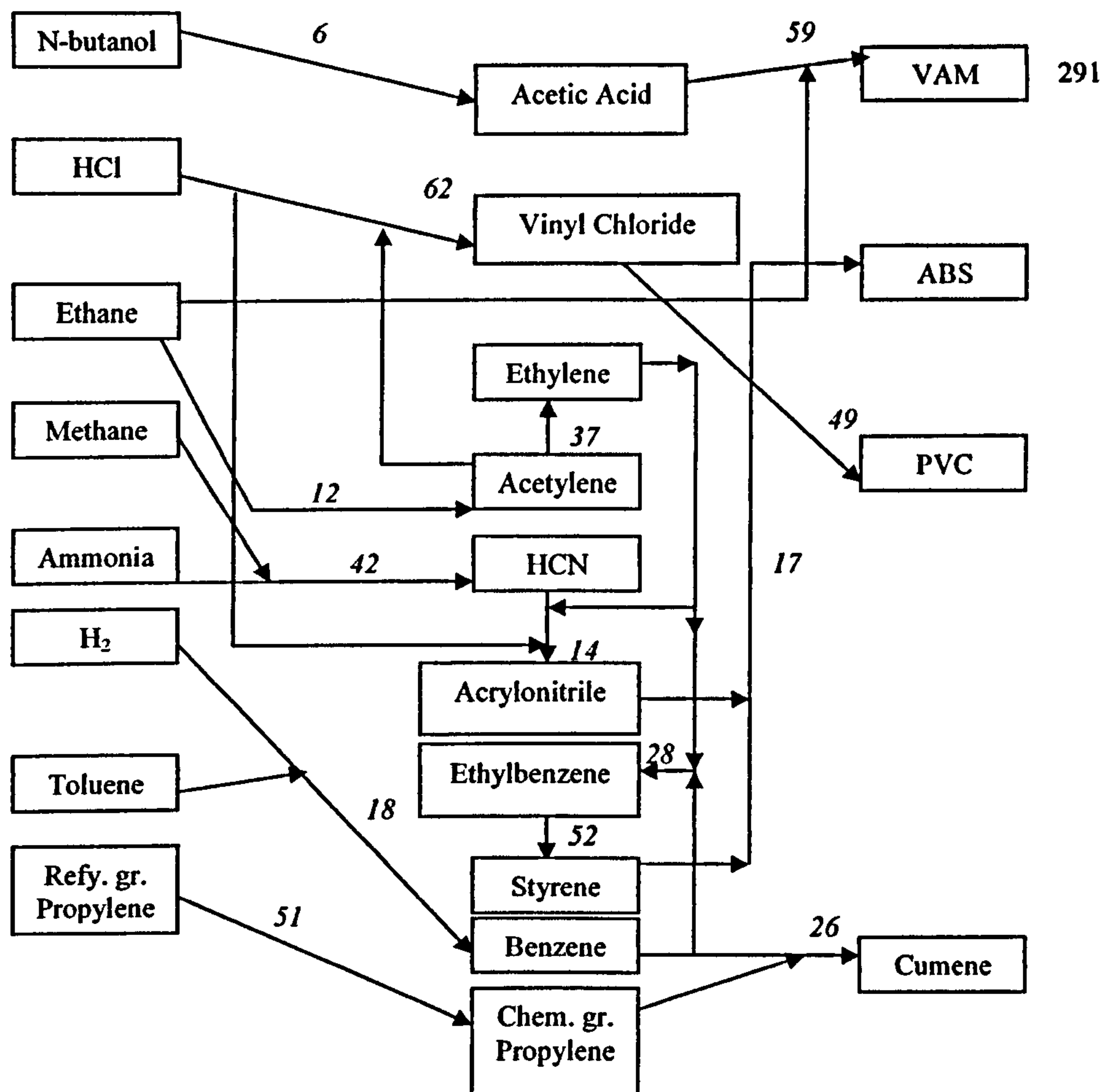


Figure 6: The planned petrochemical network from basic feedstock to final product chemicals (numbers on network indicate plants indices)

Table 1: Plants Recommended by the Best Strategic Solution of the Petrochemical Model

Plant Index, <i>j</i>	Plant	Production Rate (10 ³ tonne/yr)
6	Acetic Acid by oxidation of N-butanol	121.6
12	Acetylene by the pyrolysis of ethane (Regenerative process)	446.8
14	Acrylonitrile by the cyanation/oxidation of ethylene	176.0
17	ABS by bulk/suspension polymerization	800.0
18	Benzene by the hydrodealkylation of toluene	632.5
26	Cumene by the reaction of benzene and propylene	288.7
28	Ethylbenzene by the alkylation of benzene	615.3
37	Ethylene by hydrogenation of acetylene	299.9
42	Hydrogen cyanide by the ammoxidation of methane	105.6
49	Polyvinyl chloride by bulk polymerization	272.2
51	Propylene (chemical grade) from propylene refinery grade	109.2
52	Styrene by dehydrogenation of ethylbenzene	536.0
59	Vinyl acetate by the reaction of ethane and acetic acid	160.0
62	Vinyl chloride by the hydrochlorination of acetylene	279.0

The risk objective value obtained is industrial risk on people. Determining the acceptability of this risk is often the most challenging aspect of risk assessment. Some regulators provide guidelines or criteria that can be used to interpret whether the facility under study is considered below the level of acceptable risk. The risk from the selected model solution, representing the planned petrochemical network, is 31,878 people affected per year and this includes people hospitalized, injured or dead. This risk is a theoretical maximum, or potential, risk for a chemical release accident and must be examined against the current standards and risk criteria in industrial risk assessment.

The most important question on risk acceptability is: If a petrochemical network is working with the current acceptable safety standards, what maximum risk is expected to result? There are many international and national standards about this aspect. One useful and clear example is in the state of Queensland, Australia. The "Guidelines for Major Hazard Facility" (2002), prepared by the Chemical Hazard and Emergency Management (CHEM) unit in association with the Queensland Government, presents numbers for acceptable risk criteria. In the guidelines, the target for individual fatality risk for residential and industrial sites were 1 and 50 in a million per year respectively. Squire (2001) also, gave a hierarchical statistical nature of injures; he indicated that for each fatality, there are 30 lost-time injuries, 300 recordable injuries and 30,000 near misses injuries. These numbers add up to give an approximate theoretical maximum for affected people accompanying a fatality. Evaluating a theoretical maximum risk takes into consideration all types of incidents, not only recorded chemical incidents but possibly "Near Miss" incidents. A "Near Miss" is defined as an unplanned event, where a serious or minor incident would probably have occurred had circumstances been only slightly different or had the activity been continued. Moreover, Kammen (2005) gave an estimation of the number of plant workers that are expected to be in industrial areas, he estimated 20 engineers per plant and an employee to engineer ratio of 20 to 10. The above mentioned numbers and estimates are useful for risk calculation in industrial sites.

The planned petrochemical network will be established in one of Kuwait's industrial areas. There is one problem with Kuwait's demographic nature; most of the inhabited areas are near the seaside and some are surrounding industrial areas. Moreover, many studies about the demographical and meteorological parameters and their relation to risk of plants emissions indicated that plant releases may cover all of Kuwait; see for example (Elkilani and Bouhamra 2002). From all of the above risk criteria and facts, if the industrial and residential population is taken as all Kuwait population, 2,335,648 in 2005, and the planned industry of 14 plants is operating within acceptable safety standards, the following can be calculated:

- Estimated total number of workers for the plants = 5880
- Acceptable fatality rate on industrial sites = 0.294 per year
- Acceptable fatality rate in residential areas = 2.330 per year
- Total acceptable fatality rate = 2.624 per year
- Maximum affected people = 79,589 per year

The last number is the potential maximum risk on people according to Squire (2001) accident analysis and according to the current industry standards and criteria. Compared to the results of risk for the selected network which was calculated from the proposed risk index, 31,878 people affected per year, the planned petrochemical network is expected to work, in Kuwait, below current industry risk standards.

DISCUSSION AND CONCLUSION

Single objective solutions and the final strategic solution are shown in Figure 7 in the form of selected plants; each plant is assigned a number. Thirteen plants were selected by the economics objective and eleven by the risk objective. Seven plants are shared by both objectives; however, it was observed that 2 out of the 7 plants have been selected merely due to the lack of alternatives. After eliminating two such cases there remains only 5 plants which are favoured by both objectives. However, these observations suggest that if a safer industry is desired, about 55% of the plants (with alternative routes) which have been proven to be cost efficient will have to be abandoned. Fathi-Afshar and Yang (1985) reach to similar conclusion with 45% plant abundance. Figure 7 indicates that more than 70% of the plants favoured by the two objectives were selected by the strategic solution also. This proves the validity of the proposed decision-making method to give a balanced solution between risk and economics.

The set of solutions for the strategic tool were considered as the best solutions from the Pareto optimal solutions. Usually in MO optimisation, the selection is based on the values of objective functions but in this work another issue is taken into consideration which is the selection or rejection of plants. The plant or chemical that is rejected the most often in the Pareto optimal solutions should be removed from the planning process.

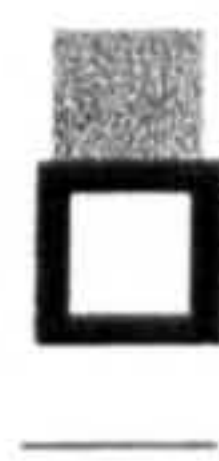
A general overview of this work is a decision based on four requirements; two objectives for the MILP model and two metrics for the strategic tool. Decomposing the overall problem into two levels with two requirements (objectives) in each level is done to provide good visualization of the results leading to easier decision-making. The Pareto curve and the GE / McKinsey matrix were the visualization tools for the first and the second levels respectively. Combining the four requirements as objectives for the model, i.e. economic gain, risk, growth rate and present value, will make results visualisation more complex.

The proposed approach and the decision-making tools can be applied for more than two objectives. The steps will be similar with a difference only in generating the solutions for the MO optimisation stage. When the number of objectives increase, the procedure for generating the Pareto optimal solutions will be more comprehensive.

This work uses modelling, quantification, forecasting and other analytical techniques for decision-making. Although, a great part of the decision-making will always be intuitive, analytical techniques, modelling, and optimization can be of great value and can permit vast improvements in the planning process.

1	2	3	4	5	<u>6</u>
7	8	9	<u>10</u>	11	<u>12</u>
13	<u>14</u>	15	16	<u>17</u>	<u>18</u>
19	20	21	22	23	24
25	<u>26</u>	27	<u>28</u>	29	30
31	32	33	34	35	36
<u>37</u>	38	39	40	41	<u>42</u>
43	44	45	46	47	<u>48</u>
<u>49</u>	50	<u>51</u>	<u>52</u>	53	54
55	56	<u>57</u>	58	<u>59</u>	60
61	<u>62</u>				

Figure 7: Comparison between single and final strategic solution.



■ Process selected by the risk objective function
 □ Process selected by the economic objective function
 — Process selected by the strategic tool

NOMENCLATURE

- a_{na} : coefficient for the previous na output variable in ARX forecast
 Bg : budget available for the development, \$
 B_j : minimum economic production rate of plant j , kg/yr
 b_{nb} : coefficient for the previous nb input variable in ARX forecast
 cap_j : capital investment cost for plant j , \$
 C_i : price (cost) of chemical i , \$/kg
 D_i : world demand of chemical i , kg/yr
 e : noise in data for ARX forecast
 F_i : annual amount of chemical i used as a feedstock, kg/yr
 f_m : objective function number m
 $Freq$: frequency of accidents, number of accidents per process per year
 H : valid upper bound on production rates, kg/yr
 Haz : hazardous effect of a chemical, people affected per tonne of chemical released
 Inv : Inventory of chemical released, tonne per accident
 K : risk index, people affected per year
 k : transfer function gain
 M : total number of plants
 N : total number of chemicals
 na : number of previous output variables used in ARX forecast
 nb : number of previous input variables used in ARX forecast
 nk : number of delay in input variables used in ARX forecast
 o_{ij} : output coefficient of a chemical i from plant j

- p : exponent for the distance-based method
 P : number of the desired final product
 Q_i : annual amount produced of chemical i , kg/yr
 S_i : supply availability of feedstock chemical i , kg/yr
 $Size$: size of plant, number of major processes in plant
 s : Laplace transform variable
 t : time, yr
 U : country's share in petrochemical market, %
 u : input variable (independent variable)
 V : total number of objective functions
 w_m : weighting coefficient for the objective function number m
 X_j : annual level of production for plant j , kg/yr
 y : output variable (dependent variable)
 Y_j : binary variable for selecting plant j ($Y=1$ if selected $Y=0$ if not selected)
 ζ : damping factor
 θ : dead time for transfer function, yr
 τ : time constant for transfer function, yr

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