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

Ghanima K. Al-Sharrah,[†] Imad Alatiqi,^{*,‡} and Ali Elkamel[§]

Chemical Engineering Department, Loughborough University, Loughborough LE11 3TU, U.K., Chemical Engineering Department, Kuwait University, P.O. Box 5969, Safat 13060, Kuwait, and Chemical Engineering Department, University of Waterloo, 200 University Avenue West, Waterloo, Ontario N2L 3G1, Canada

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 autoregression with an exogenous variable 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 routes in the network are selected for different final product prices. It is found that including the market cycles and using the causal models for forecasting petrochemical product prices will provide possible scenarios for chemical price forecast, and then a risk-adjusted present value can be calculated.

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 byproducts 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 of 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 an 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 the planning model for the 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 includes 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 processes of biological or social nature.¹

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

* To whom correspondence should be addressed. Tel.: (965) 4811188 ext. 5599. E-mail: imad@kuc01.kuniv.edu.kw.

[†] Loughborough University.

[‡] Kuwait University.

[§] University of Waterloo.

Table 1. K-Wave Dates and Forces

K-wave	1st wave (1785–1843)	2nd wave (1843–1894)	3rd wave (1894–1941)	4th 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

progressing 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: 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 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 wave.²

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 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.³ Market dynamics of natural gas suggest also future cycles, as is indicated by the U.S. Department of Energy.⁴

Kondratieff was not the only person to notice long-term cycles within the economy. In 1939, the great economist Joseph Schumpeter, author of the concept "Creative Destruction", hypothesized that technology runs in 50-year waves. Schumpeter notices that bursts of technical transformation coincide with upturns in economic activity.⁵ He assumed that they were the causes of that activity: new technology drives faster the economic growth, and then 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, but 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 of 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 global.⁷ In his paper⁸ he showed that economic models for capital goods—the metals, machines, chemicals, concrete, etc.—can generate long-wave cycles of about 50 years in length. Forrester's work has inspired a group of researchers at MIT to follow him; most notable is John Sterman. In his work he showed how interaction between multiple time scales in a nonlinear model can

lead to long-wave cycles of about 50 years in length, on top of shorter wave cycles.^{9–11}

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".

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 mainstream 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 indexes such as the 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.¹² 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 anomaly.¹³ Recovery of demand was predicted for base chemicals, and oil prices were predicted to remain weak.¹⁴ Other prominent forecasters predicted declining prices for oil from 2000 until 2003 in different scenarios around and below \$20/bbl.¹⁵ In fact and as already known, oil prices remained strong from 1999 until early 2003. Students of the long wave had different calls at about the same time.^{16,17} Finally, a caution is in place. Neither is the cyclic phenomenon new nor is its discussion 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 that 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 forward.¹⁸ Market analysts know that the cycles of human progress are based on a psychology that takes a long time to manifest and will not accrue in a strict periodic rhythm.¹⁹ 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.^{20–22}

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 decisions.² Yimoyines²³ explained this by recognizing that the petrochemical industry is characterized by large plants that take several years to build; finally, they come to stream, together creating oversupply and thus the bottom of the cycle.

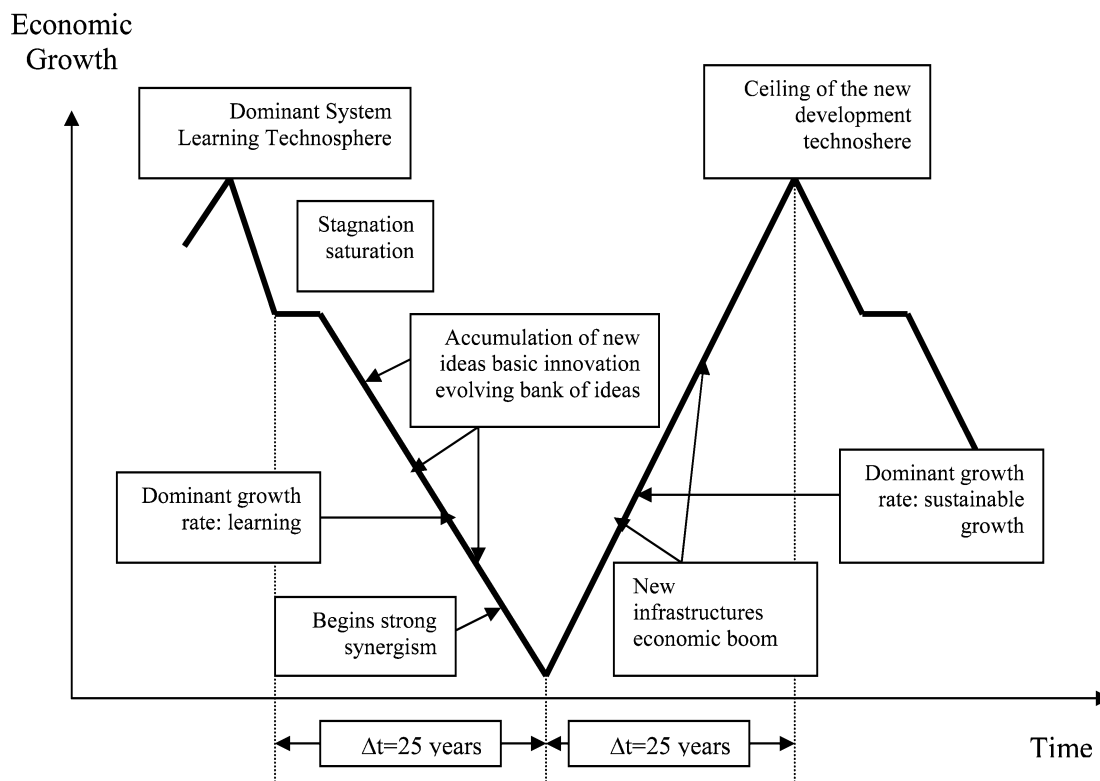


Figure 1. Learning dynamics of succeeding generations.

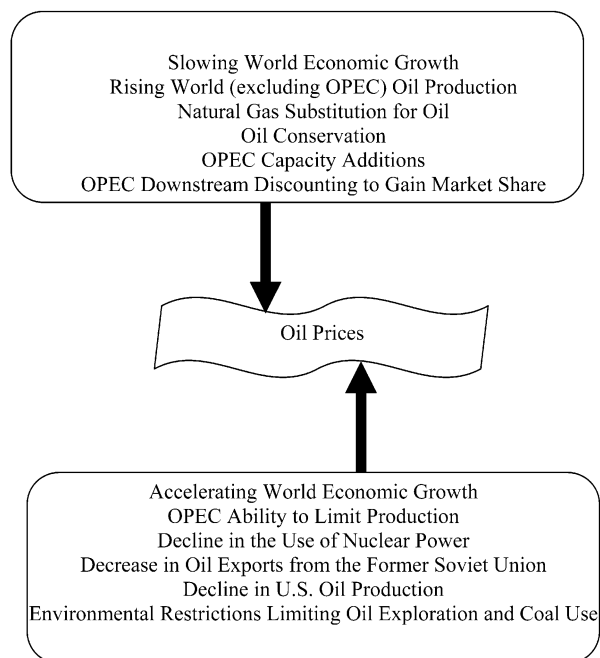


Figure 2. Variables determining oil prices in the short range.

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 2 shows a representative diagram of variables affecting oil prices and consequently causing short-term disturbances to the petrochemical industry.²⁴

Short-term disturbances occur also in the form of cycles. A famous short cycle is the "Kitchin" 3.5–4-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 time-series techniques have been employed to model short-cycle features. Simpson et al.²⁵ forecasted the U.K. quarterly index of production using a model of the business cycle. He adopted both linear and nonlinear approaches. Kontolemis²⁶ also analyzed the U.S. 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 worldwide 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, byproducts, 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 an 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 feedstocks into final products. These technologies are characterized by technical coefficients of consumption of raw materials, chemicals, utilities, labor, byproduct production, and 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 the total production cost as an objective.

Other different researchers presented variants to the linear programming model of Rudd with different objective functions. Al-Fadli et al.²⁸ and Fathi-Afshar et al.²⁹ selected the minimization of the total production cost; in other studies, Sokic and Stevancevic³⁰ and Stadtherr and Rudd^{31,32} selected minimization of feedstock 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 because 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. 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 the Jimenez model with a small modification in the process capacity constraints. The objective function was the maximization of the total annual profit. A 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 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 Sahinidis⁴⁵ 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 Rekalitis,⁴⁶ Grossmann and Sargent,⁴⁷ Halemane and Grossmann,⁴⁸ Straub and Grossmann,⁴⁹ Novak and Kravanja,⁵⁰ Pintaric and Kravanja,⁵¹ and Rooney and Biegler.⁵² Uncertain demand only was included in the models of Acevedo and Pistikopoulos^{53,54} and Ahmed and Sahinidis.⁵⁵ 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 chemical prices will be considered in this study and is treated with forecasting tools.

4. Forecasting

Forecasting of future prices of petrochemicals is 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 historical 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 the 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 as likely that the next value of the series will be above the mean value as it is that it will be below it. The kinds 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 because 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 1

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, follows 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 pattern, 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 the 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 Yahyai,⁶⁰ and it is identified (in a form called "dynamic harmonic regression") as useful to the investigation of periodic phenomena for forecasting.⁶¹ Ierapetrinou 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 a 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 increases (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 International Ltd.⁶³ 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 the 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 interdependencies. In an econometric model, one is faced with many tasks similar to those in regression models. These tasks include the following:⁶⁴

- (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 the causal model is transfer functions or polynomials. The 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 n_a outputs and previous n_b inputs delayed by n_k together with some noise e . The model is named autoregression with an exogenous variable (ARX)⁶⁵ and is presented as

$$y(t) + a_1 y(t-1) + \dots + a_{n_a} y(t-n_a) = b_1 u(t-n_k) + b_2 u(t-n_k-1) + \dots + b_{n_b} u(t-n_k-n_b) + e(t) \quad (1)$$

Noglaes 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 reintroduced below. Let N be the number of chemicals involved in the operation of M processes, X_j 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} 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 of 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 is multiplied by the country's share in the petrochemical market and U represents valid 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 the petrochemical industry is directed toward building new plants to produce petrochemicals. It is logical, therefore, that only one process should be selected to produce a single chemical. The 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 processes that produce a final product.

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

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

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 of 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 B_g is the available budget, then the constraint is formulated as

$$\sum_{j=1}^M \text{cap}_j Y_j = B_g \quad (7)$$

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 the feedstock for the petrochemical network. If C_i is the price of chemical i , the added-value objective function will be represented by

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

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

Because 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 of historical data on a chemical price are collected, and they are correlated with time. When a reliable correlating function is found, a forecast of the 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 transfer function and ARX models, where the oil price is the input and the chemical price is the output. Historical data of the oil prices and chemical prices were used to find the best causal models. The 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 the 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 limitations.

The desired final products were defined under the criteria of their importance to the global petrochemical industry and its relevance to Kuwait. The proposed final products are acrylonitrile-butadiene-styrene (ABS), cumene, polystyrene, crystal grade (PS), poly(vinyl chloride) (PVC), and 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.

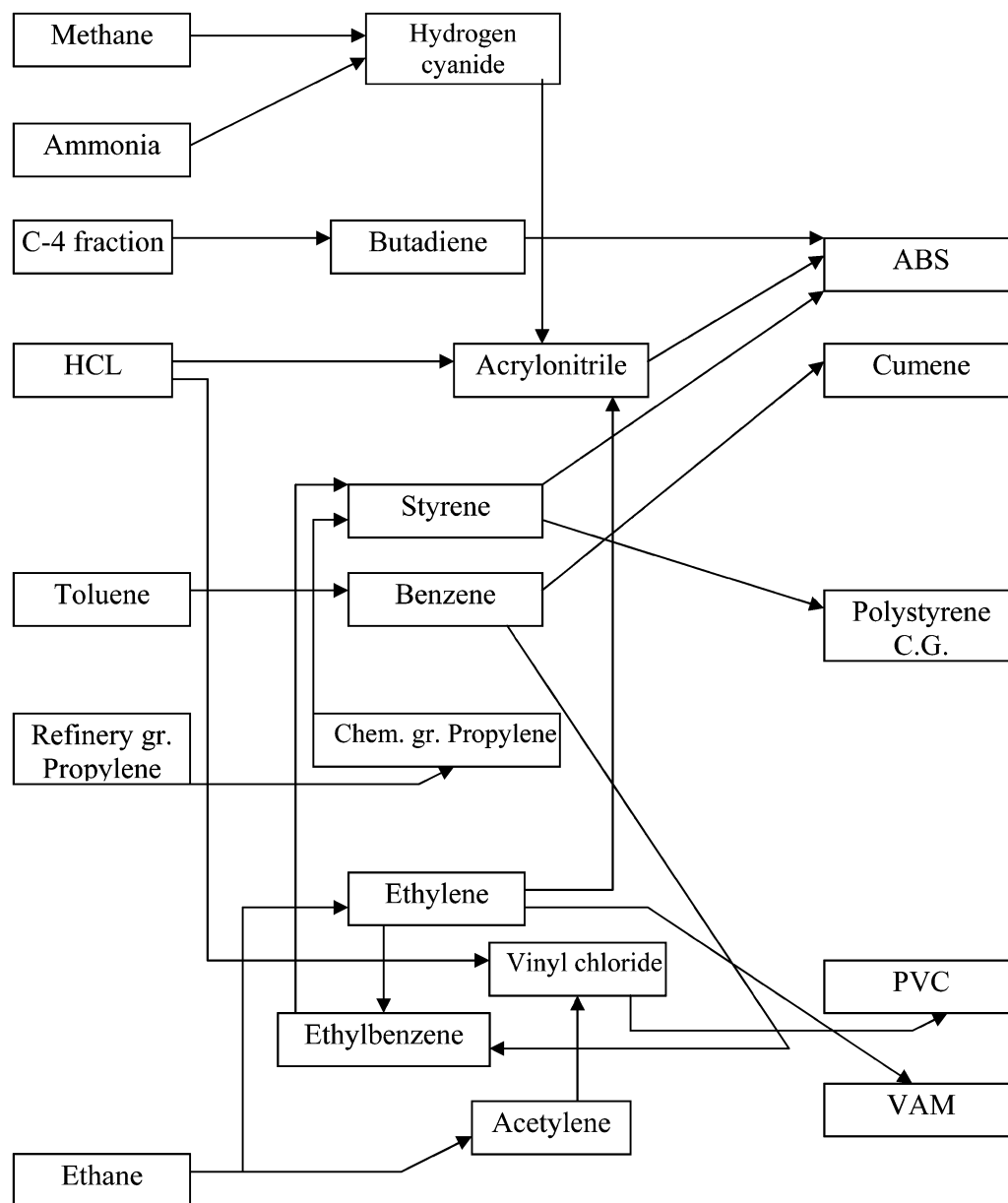


Figure 3. Simplified petrochemical network for the proposed products.

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 are 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 the demand of final products. Because 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

the journal *Chem. Mark. Rep.* 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 55-year-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.

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 fits the chemical prices data. First, a simple third-order polynomial of price with time was used. However, its results were very poor because it indicated some negative prices or very high prices when used in the forecast. Second, because the price data are cyclical, Fourier analysis is applied

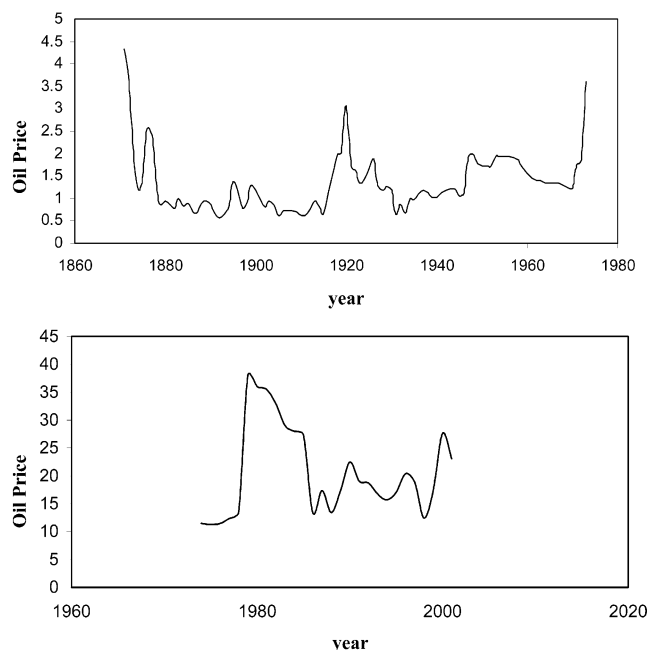


Figure 4. Historical data of oil prices (\$/bbl).

with only one frequency together with a trend term. Results are presented as follows:

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

$$\text{cumene (¢/kg)} = 0.005t + 4.324 \cos(5.500t) + 4.872 \sin(5.500t) + 37.672 \quad (9b)$$

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

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

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

The previous 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

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

where t is the time in years. A plot of the 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 until 2030; for the petrochemical industry, the long-range horizon is considered as the time for building and then running the plant through its expected life; this time is around 3 decades. Therefore, all forecasts were done to the year 2030. Oil price prediction suggests the next bottom in oil prices to be in the year 2006 at a price of 16.88 \$/bbl. This is consistent with the predictions for Kuwait Export Crude⁶⁸ and Dubai crude;¹⁵ their bottom was in 2006 and at 17 \$/bbl for Dubai crude. However, this

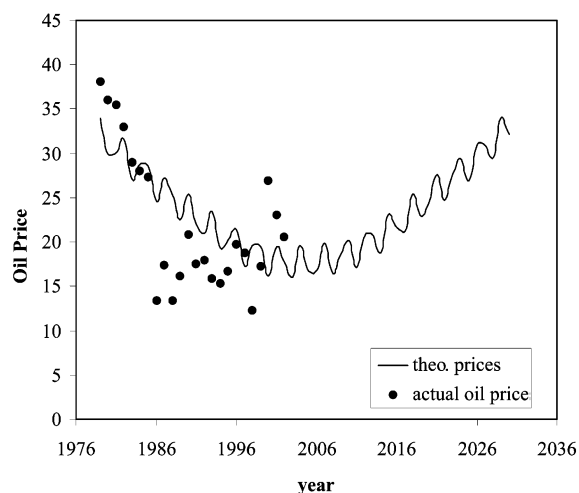


Figure 5. Oil prices (\$/bbl).

Table 2. SOPDT Transfer Function Parameters Relating Chemical Prices and Oil Prices^a

	gain K (¢/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	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

^a The transfer function is a relation between the change in prices of products and the change in oil prices.

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 rates in the long-wave sense by 3–4 years, which is logical with the role of oil as a driver of inflation.

The second stage in the forecasting stage is finding the causal model between oil prices and product prices. The first causal model is represented by a transfer function relating oil prices as an input and product prices as an output. The transfer function is found in the form of a SOPDT. The transfer function 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 (1–3 business cycles) for the chemical prices to respond to oil price changes, but as soon as they respond, they respond relatively fast. This result is consistent with the fact that downstream industry takes several years to be operational. The damping factor for all chemical prices was very small, indicating a high oscillatory underdamped response. The third stage in the forecasting is using the forecasted oil price and the transfer functions to forecast product prices.

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

Equations 9 and 10 and data in Table 2 were obtained using Nelder–Mead simplex direct search optimization

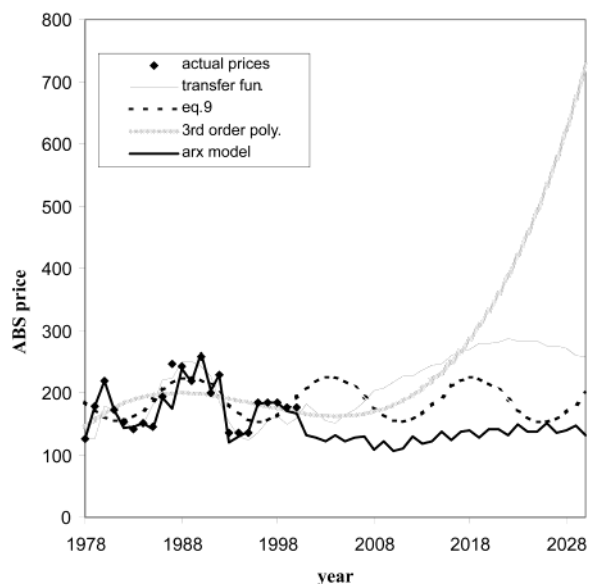


Figure 6. ABS actual and forecasted prices (¢/kg).

in 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 (eqs 9a–e). Results show an average absolute error of 14.8% with the transfer function model, 1.82% with the ARX model, and 24.5% for the time-series model (eq 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 an unrealistic forecast. Inspection of Figure 6 reveals an interesting trend for the ABS price pattern, with long-term topping action between the years 2022 and 2024. The transfer function and ARX models both exhibit this phenomenon, which implies the possibility that the long wave may apply to petrochemicals in addition to commodities.

Model Solution. The petrochemical MILP model was solved using the commercial optimization package GAMS.⁷⁰ The solution was obtained several times with different final product 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; the solution gave the selected final products (four out of five chemicals) and the corresponding petrochemical network of plants from the basic feedstock to the final products. Analyzing the 13 model solutions with the corresponding “rejected” chemical indicated that cumene was rejected seven times, PS four times, and VAM two 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 from the basic feedstocks to the final products will be found from the model solution.

Risk Assessment. At this stage of planning, it is possible to introduce some risk concepts. 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.⁷¹ The second type of risk can be well handled by variance techniques such as the variance of expected monetary value (EMV)⁷² or the risk-adjusted-return family of methods such as the Sharpe ratio.⁷³ 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 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 of some factors affecting the oil prices, some of which started in recent years; these include environmental factors, reduced cost of production, and alternative energy 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, \$3.4, and \$5.5 b for the transfer function, ARX, and transfer function with oil price models, respectively. An EMV can be calculated from the PVs as the following:

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

The PV of each scenario is multiplied by its probability of accordance p . The variance can be calculated from

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

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, EMV will be \$4.8 b. This number represents a risk-adjusted PV 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 from allocating money in a new capacity. This inaction results in demand increase and supply stability. After a 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 onstream, prices go down again because of the competition. Thus, the boom–bust and cyclic phenomena exist.^{23,74}

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 suggest that prices would be stronger than what 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. The most notable example is the Equate Chemicals Co. A joint venture of PIC with Dow Chemicals commenced production in 1997 for ethylene, polyethylene, and ethylene glycol. With 4 months delay in startup, prices were at the bottom of the business cycle. In 1998, the Asian crisis hit markets and product 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 meantime, PIC and Equate Chemicals Co. sponsored a conference on investment opportunities in PIC in Kuwait in Oct 1998. At this conference a critical analysis of the Asian crises from the perspective of the long wave was presented. It was suggested² that the crisis 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 Chemicals Co. required 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 led 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 Aug 2001, phase 2 of the olefin complex (U.S.\$2000 million capital) was approved. In addition, a much delayed and debated aromatics complex of U.S.\$1400 million capital was also approved.⁷⁵ 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 Mar 2003, Dow Chemicals signed a strategic partnership with PIC (the parent of Equate Chemicals Co.) for the realization of the expansion. The proposed processes in this paper 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.

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 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 the purpose of studying 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 rates in the long wave by 3–4 years.

From the tested forecasting models, the causal models in the form of SOPDT and ARX models were able to model the past prices and well forecast future prices. A risk-adjusted PV was found from the PV of all possible price forecast scenarios. The large variance of the EMV emphasizes the need for disturbance analysis in the decision making.

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