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**MULTIPERIOD OPTIMISATION
AND STRATEGIC PLANNING
FOR CHEMICAL PROCESSES**

Relatore: Prof. Fabrizio Bezzo
Correlatore: Dr. Maarten Nauta

Laureanda: ELEONORA BUFFOLO

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Abstract

The topic of this thesis is the implementation in a commercial process simulation software (gProms by Process Systems Enterprise, Ltd.) of a new resolution method for a multiperiod optimisation. The main issue of this type of optimisation is the size of the model, which is tackled by the new method by splitting the problem into smaller subproblems that can be solved independently using multiple processors.

Two types of multiperiod problems are considered: with inventory levels and with strategic planning decisions.

To achieve the objective, a prototype resolution software, mostly written in the programming language python, is assessed. This test is carried out in the first part of the thesis, where a number of multiperiod problems are solved using both the prototype structure and the standard gProms implementation. Results show that the prototype software still cannot cope with large problems, but is adequate for small-medium problems.

The second part of the thesis is dedicated to strategic planning multiperiod problems. Since the prototype software used for inventory levels cannot be applied in this case, the design of a second prototype software is initiated. A general structure for the problem is defined and written in an xml file. Three instances are considered: contract stipulation, revamping and building of new plants. Preliminary results demonstrate the potential of the proposed software architecture.

Riassunto

Il tema di questa tesi è l'ottimizzazione multiperiodale in relazione a processi chimici.

L'ottimizzazione multiperiodale è un tipo di ottimizzazione per cui il funzionamento di un impianto viene modellato per un lungo periodo di tempo, che è suddiviso in periodi più corti. Ogni periodo è risolto separatamente, e collegato agli altri per mezzo di alcune equazioni che modellano delle decisioni a lungo termine. In particolare, due tipi di decisioni sono prese in considerazione: i livelli delle scorte da mantenere alla fine di ogni periodo oppure decisioni riguardanti la pianificazione strategica dell'impianto. Lo scopo di un'ottimizzazione multiperiodale è individuare le condizioni operative ottimali per un impianto durante ogni periodo e allo stesso tempo prendere le decisioni a lungo termine.

Il vantaggio di questo approccio è che considera le interazioni tra decisioni prese a breve ed a lungo termine, per cui il profitto dell'impianto risulta maggiore. D'altro canto il modello, che generalmente non è lineare, ha un costo computazionale elevato che ne limita le applicazioni. Per questo motivo ci sono vari studi che puntano a semplificare i modelli oppure a trovare delle nuove strategie risolutive per l'ottimizzazione.

L'obiettivo finale del lavoro svolto in questa tesi è quello di implementare un nuovo metodo risolutivo in gProms, un software per le simulazioni di processo legate all'ingegneria chimica sviluppato dall'azienda Process Systems Enterprise, Ltd. Il nuovo metodo consentirebbe di risolvere le ottimizzazioni multiperiodali considerando un periodo alla volta. Sarebbe possibile risolvere i periodi in parallelo o in serie, e sarebbe possibile sfruttare processori multipli. Nel complesso, il metodo consentirebbe un risparmio di memoria o di tempo.

Per raggiungere questo obiettivo è necessario passare attraverso vari livelli di sviluppo. All'interno dell'azienda era già stato svolto del lavoro per quanto riguarda l'ottimizzazione multiperiodale relativa ai livelli delle scorte. Una nuova struttura risolutiva, implementata principalmente nel linguaggio di programmazione python, era già stata messa a punto. Questa struttura consente di risolvere separatamente i periodi, ed è uno stadio intermedio verso l'implementazione in gProms. L'obiettivo della prima parte di questa tesi è testare questa struttura. Per fare ciò, il modello generale dell'ottimizzazione multiperiodale relativa ai livelli delle scorte è stato applicato a tre processi chimici: un semplice processo di miscelazione, una rete interconnessa di impianti ed un impianto per la produzione di etilene. L'ottimizzazione è stata risolta utilizzando sia gProms che la struttura in python, e i risultati sono stati confrontati. Sono stati ottenuti gli stessi risultati con entrambi i metodi per il processo di miscelazione e per

la rete di impianti, mentre non è stato possibile risolvere l'impianto di produzione di etilene con la struttura in python a causa di un problema nel solver. Il risultato è quindi che al momento la struttura è in grado di risolvere ottimizzazioni multiperiodali su modelli di media grandezza, mentre non riesce a gestire modelli molto complessi.

Per quanto riguarda l'ottimizzazione riguardante la pianificazione strategica, non era presente nessun lavoro precedente all'interno dell'azienda. Per questo motivo l'obiettivo è applicare il modello generale per questo tipo di ottimizzazione ai casi specifici del processo di miscelazione e della rete di impianti, e di raggiungere una soluzione utilizzando esclusivamente gProms. In particolare, tre tipi di pianificazione strategica sono stati considerati: la stipulazione di un contratto, la costruzione di un nuovo impianto ed il rimodernamento (*revamping*) di parte dell'impianto o delle apparecchiature. Questi esempi hanno permesso di individuare una struttura generale che potesse essere applicata a questo tipo di problemi, cosa necessaria per arrivare a costruire la struttura in python. Il passo successivo per quanto riguarda la pianificazione strategica è la messa a punto della struttura in python, che dovrà essere seguita dal confronto dei risultati usando python e gProms.

Quando i risultati delle ottimizzazioni multiperiodali ottenuti con la struttura in python e con gProms saranno uguali per ogni tipo di impianto, sarà possibile procedere all'implementazione esclusivamente in gProms, che è l'obiettivo finale del lavoro.

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Introduction

The topic of the thesis is a multiperiod optimisation, which is a type of optimisation performed considering that a plant will work for a long time horizon. The problem is general, but it has been studied in relation to chemical processes. The solution of a multiperiod optimisation has some advantages over a standard optimisation, but its applications are limited by the complexity of the problem, since the models are usually big and highly non-linear. In literature, there are many articles which try to simplify specific models or to develop new resolution strategies.

As the developer of a platform for advanced process modelling for chemical processes, Process Systems Enterprise, Ltd. is interested in introducing in the general modelling platform gProms, a new strategy to solve multiperiod problems. The new strategy will allow to solve the single parts of the problems, the periods, independently, to save time or memory. In particular, the company is interested in two types of problems: multiperiod problems which focus on the inventory levels, and multiperiod problems which focus on strategic planning decisions such as contract stipulation, revamping and building of new plants.

The implementation of the new resolution strategy requires many stages of development. A first objective of this thesis is to validate an intermediate prototype resolution structure for multiperiod problems with inventories. In order to do so, the general structure of the multiperiod problem is applied to the models of three different plants, and some examples are solved using both gProms and the prototype structure. A second objective is to extend the new resolution strategy to strategic planning multiperiod problems. Some examples are solved with gProms in order to define a general structure of the strategic planning multiperiod problem.

The thesis is articulated into two main parts. In the first part the focus is on the formulation and solution of a multiperiod optimisation with inventories, while in the second part the multiperiod optimisation is extended to strategic planning.

The thesis is divided into four chapters, which include a literature review, the formulation of the multiperiod problem and the solved examples.

Chapter 1 introduces the multiperiod optimisation problem and contains the literature review related to both inventory levels and strategic planning. In particular, the strategic planning problem is articulated in three different examples: the signing of a contract, the building of a new plant and the revamping of an existing plant.

Chapter 2 contains the mathematical formulation of the problem. The first part is related to the multiperiod problem with inventories. First, the equations which lead to the objective functions formulations are explained, then the resolution structures is described, considering in particular the solver, and the xml to insert the data. The second part of the chapter is related to the strategic planning multiperiod problem, where the changes in the model and in the solver are explained. Chapter 3 contains all the numerical examples relative to the multiperiod optimisation with inventories. In particular the problem is solved for a blending problem, a network of plants and an ethylene plant.

Chapter 4 contains all the examples related to strategic planning. In particular the optimisation is applied to the blending problem and to the network of plants.

Some final remarks and a discussion on future work conclude the thesis.

Chapter 1

Motivation and literature review

This chapter introduces the multiperiod problem in simple terms and explains its importance in chemical processes. The difference between the two types of multiperiod problem tackled in this thesis, the one related to inventories and the one dealing with a more complex strategic planning, is explained. An overview of the existing literature on the subject is given, with a focus of the most frequent applications and resolutions strategies. In the end the purpose of this work is discussed.

1.1 Problem introduction

The multiperiod optimisation problem is a very general problem that can be applied to a variety of different processes. Its peculiarity is that the operation of a plant is considered over multiple distinct periods of time. The purpose is to optimise the operating conditions of a process together with other long term considerations, such as the trading of raw materials and products or the construction of a new section of the plant.

Two main situations are considered in this work. The first is a multiperiod optimisations where the focus is on the inventories, while in the second case operations like the construction or rebuilding of a new plant and the signing of contracts are taken into account.

1.1.1 Multiperiod problem with inventories

Even if the problem can be applied to a number of plants, it is possible to identify some fundamental characteristics. In general, the plant transforms given raw materials into products. It is assumed that some or all of the raw materials and products can be stored and that the amount stored during one period is available during the next period. In addition, during each period raw materials can be bought and products can be sold. Prices for raw materials, products and utilities can vary from period to period.

As an example, it is assumed that a new plant is built. The first month of operation is taken into account.

It is possible to perform an optimisation to find the ideal operating conditions for this plant, such as the ideal raw materials flowrates or the ideal utilities consumption. At the end of the month, part of the products is stored

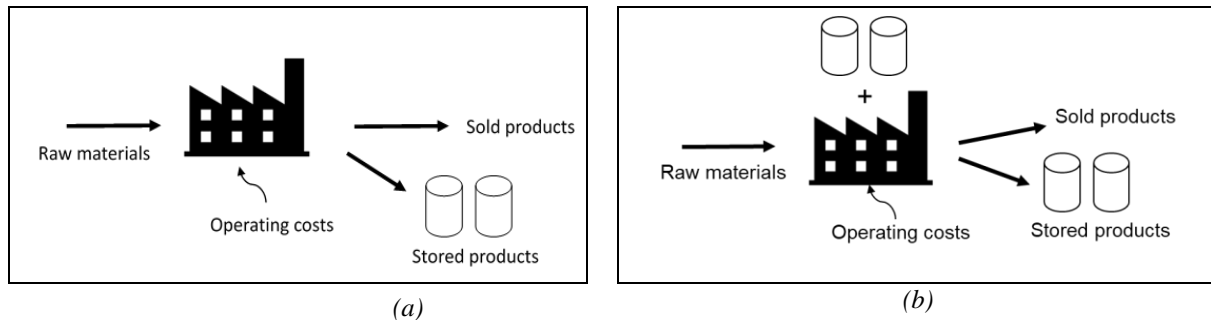


Figure 1.1. The two figures illustrate the operation of a plant during (a) the first month and (b) the second month of operation.

At the beginning of the second month, the situation is different from the beginning of the operations, because part of the product is stored in the inventory.

The presence of the inventory affects all the decisions taken by the optimisation. Since part of the product is already available, it is possible to process a smaller raw material flowrate and to have less operating costs. An alternative is to produce the same amount of products as in the first period and to store the surplus, but in this case the maximum capacity of the warehouse should be taken into account. A different solution is to sell everything that is produced during the second month and to keep the inventory levels unchanged.

In every single one of the solutions proposed, the decisions taken during the first month of operation have an impact on the second month of operation. For this reason, solving the two months simultaneously allows to reach better results than solving them separately. This consideration can be extended to a longer time horizon if more months are taken into account, and the problem can be generalized for periods of time of every length.

The results that are required from the optimisation are the optimal selling schedule and the optimal operating conditions which that schedule can achieve. The decisions are taken considering the prices fluctuations of product and raw materials. It is more profitable to sell the products when the prices are higher, and it is also an advantage to produce when the prices of the raw materials are lower. For this reason, it is expected from the optimisation results that the production would be very high when the raw materials costs are lower, and that the products would be stored and sold when the price would be at the highest.

1.1.1.1 Literature review

In general, a multiperiod problem is articulated into a series of optimisation problems, each one considering a single period, which are coupled by constraints in order to link one problem to the next. It is applied in the following cases:

- Network of plants. The plants are linked through the products, which are taken from a plant to the next one.
- Single plant over multiple periods of time. The periods are linked through the storage, since the materials stored in one period are used in the next.

This is the case of the multiperiod problem with inventory levels, and will be tackled in this section.

- Strategic planning applied to a single plant or to a superstructure over multiple periods of time. The periods are linked because strategic decisions taken during one period of time affect the following periods.

This case is typical of strategic planning multiperiod problems, so it will be discussed in §1.1.2.1.

Since the problem is general, it can be found in literature in many different situations, such as a cutting stock optimisation for wood processing (Reinders, 1992), a multiplant complex in food industry (Corsano et al., 2007), a multi-plant polymerization (Jackson et al.), an oil refinery (Chen et al., 2015), a cryogenic air separation system (Zhu et al., 2011), a catalytic chemical reaction (Bizet et al., 2005), etc.

The aim of the process is to optimise the plant operation for a long period of time, taking into account variations in the operating conditions, prices and demands. To reach this objective, the operation span of the plant is divided into shorter periods of time. Usually the problem is formulated as the optimisation of a single objective function, which can be modelled in different ways as summarized by Li et al. (2004). The simplest model has the objective of minimizing the total cost, which includes all the costs of the plants, such as utilities, inventory and raw materials, changing the operative conditions. A more general approach is to maximize the profit of the plant, which includes the revenues calculation. It is possible to assume that everything produced by the plant is sold in the market, or it is possible to distinguish between production and sales taking into account an inventory. The last approach is the more general because it is possible to find the optimal production schedule to satisfy the market fluctuations.

A different approach is to define multiple objective functions and to take them into account individually, as proposed by Chen et al. (2003). The article starts from the consideration that if the optimisation focus on only one objective function, the global optimal results may be disadvantageous for the single parts of the plant. To solve this problem, the model presented in the article uses a multiple-objective optimisation, maximizing the overall profit along with other functions such as the customer service level or the safe inventory level. The objectives can be conflicting, so the final solution will be a trade-off between the different aspects of the plant. This approach is not much used in multi-period optimisation because of the complex resolution strategy required.

The multiperiod problem is articulated in two levels. At the lower level, the solver controls the operating conditions to reach the optimal profitability in each single period, while at the upper level decisions variables as the inventory levels to be maintained and the amount of products to be sold and produced are decided. The single periods may be steady state or dynamic simulations, and the operative conditions of each of them can be changed independently. The periods are linked together by some key variables, usually the inventory levels of each product. One important distinction between the multiperiod problems are the estimation of the market fluctuation, which could be predicted using deterministic or stochastic programming (Li et al., 2004). In the case of the stochastic programming, the main difficulty is evaluating uncertain functions and their expectations, because the methods are difficult or slow. For this reason the functions are usually approximated as linear integrals.

Jackson et al. applied the multiperiod approach to a real world polymer plant that produces multiple products. The key feature of the optimisation is the use of empirical models based on real data to predict the production. The model considers a multi-plant including two different types of plant. Type I plants can produce only one product at the time, while Type II plants produce continuously a fixed set of intermediate products, which are later post-processed and blended to obtain the final products. The plants are interdependent because of the shared resources and of the intermediate products, so an inventory has to be considered. The aim of the optimisation is determining the monthly production, the final inventory levels of each product, the number of days dedicated to each product in each plant and the key operating parameters. Extending the problem to multiple periods is possible to adjust these parameters to the fluctuations of the market. The model includes three Type I plants and two Type II plants and has several thousand variables and constraints, so a web interface was built to allow multiple users to access the optimisation.

Zhu et al. (2011) tackled the topic of the optimisation of a cryogenic air separation system. They studied a classic double distillation column with the addition of a side column for the awangrgon separation, and included compression and pre-purification of the inlet gas in the model. The single period model is extended to a multiperiod formulation adding an inventory for the products and considering uncertain demand and contractual obligations. An important feature of this study is the use of a loss function to take into account economic losses when the demand is not met by the production rate and the inventory. The purpose of the optimisation is to find the optimal inventory level, which is a trade-off between profitability and customer-satisfaction levels. In fact, a higher inventory level results in both higher inventory costs and in a higher probability of meeting the demand. The result of the multiperiod optimisation could be useful for contract development, because it shows which long-term strategies meet the contractual obligations and how much could be renegotiated before seeing a loss in profit.

Bizet and Grossmann (2005) presented a mixed-integer nonlinear programming optimisation model to schedule catalyst changeovers. A chemical process involving the use of a decaying catalyst is taken into account. The time horizon of the process is divided in multiple periods, where it is assumed that the reactor works in steady state. It is assumed that the characteristics of the catalyst, such as expected minimum and maximum life, cost and time required for the turnover, are known. A kinetic model to calculate the production and the catalyst deactivation is required. Using these information, it is possible to model the reactor and to perform an optimisation. The demand is predicted considering seasonal figures, and it is not necessarily met. The multiperiod approach allows not only to determine the best process parameters to delay the deactivation of the catalyst, but also to calculate the optimal number of catalyst loads to be used in the time horizon, the appropriate times for the changeovers and the levels of production and inventories.

There are many examples of multiperiod optimisation applied to a refinery. Chen et al. (2015) studied the optimal procurement and operation of an oil refinery that is assumed to perform three representative processes: separation, mix and blending. The main purpose is to integrate a stochastic model for oil price estimation in a multiperiod optimisation of the process, in order to find the optimal values of the operating variables in different periods and of the purchase and selling schedule. Zhao et al. (2014) formulated a model to optimise simultaneously the production system and the utility system of a refinery, showing that this integrated approach obtains energy savings, emission reductions and an improvement of the profit. The main advantage of this kind of approach is that the interaction between the production and the utility systems are taken into account. For this reason, situations in which the demand for utilities

exceeds the capacity of the plant are avoided, and it is possible to evaluate how the by-products of the plant are used as fuels for the utility system.

A similar study was carried out by Wang et al. (2016), who proposed a model for the optimisation of both the processing and the utility system of a plant for polyvinyl chloride. The production of the polymer require the use of power-intensive equipment, which has to be shut down or restarted to save energy when it is not necessary. It is not possible to use frequent start-stop switches because they have an effect on the electricity quality in the supply system. For this reason the purpose of the optimisation is to take into account the energy consumption of various process operations and determine a global production arrangement plan to meet the product demand. The results are a trade-off between the electricity consumption, the production and the switching operation cost.

Apart from this singular studies, common problems that required a multi-period optimisation are the pooling problem, the supply chain problem and the multiproduct batch plant design.

The pooling problem is commonly found in refinery, where there is the necessity to blend different streams to obtain a product which fulfils determined concentration constraints. An important decision is the selection of the raw products to buy from a set of supply streams. The optimal blend must satisfy the quality constraints and the demand, while maximizing the profit. The optimisation has to decide the schedule of the filling and emptying of the storage and charging tanks, taking into account the connections between the tanks. Often the transportation costs of the raw materials and the time of arrival are considered. Other complications due to the multiperiod formulation are the inventory levels and the change of prices and demand over time. It is proved that the economic performance of a refinery can be improved in an inexpensive way optimising the schedule of the operations (Kelly et al., 2003). For this reason, many articles tackled this problem (Castro, 2016; Lotero et al., 2016; Kulkarni-Thaker at al., 2013; Luo et al., 2007; Luo et al., 2009). The optimisation can be extended to the plant design, in order to find a model for integrated scheduling and planning of the plant.

The supply chain problem can be found in many different situations. In a plant, it denotes the handling of the product from the manufacture to the selling point. It includes transportation operations, storage and current and future sales. The purpose of the optimisation is to find the best schedule for the plant operation and the transportations, in order keep efficient custom delivery, to meet the plant necessities and to maintain the inventory levels within their bounds. Problems linked to the transportation have to be taken into account, such as the exclusive use of the employed dispatchers companies, the allocations of the products to assure full loans and the use of intermediate warehouses. The problem can be solved for the single period or for

multiple periods, and can include deterministic or stochastic demand. (Engau et al., 2015; Yi et al., 2011; Chen et al., 2003; Rahim et al., 2013).

Another plant where a multiperiod optimisation is often used is a multiproduct batch plant. In this type of plant there are multiple reactors operating sequentially or in parallel to produce multiple products. The intermediate products can be moved from a tank to another. The purpose of the optimisation is to find the optimal allocation of each product in the batches and to schedule the transfer from a piece of equipment to another. When the problem is extended to multiple periods, the change of the prices of raw material and products and the inventory levels are taken into account and the optimisation has to plan the production accordingly. Often the problem is extended to include also plant design. Moreno and Montagna worked extensively on that problem, first proposing a model for deterministic demand that takes into account the interaction between design decisions and commercial, production, sales and inventory policies simultaneously (Moreno et al., 2007). They then extended the model proposed considering that the units are available only in discrete sizes for the design (Moreno et al., 2009) and taking into account uncertain demand (Moreno et al., 2009). A similar work was presented by Petkov et al. (1997), who extended Birewar and Grossmann's model (Birewar et al., 1990) to stochastic demand. Deterministic demand was taken into account by Fumero et al. (2015).

When an optimisation is extended to multiple periods of times, the size of the problem increase and the resolution is difficult. For this reason, many different articles focus on the resolution of the problem, proposing both approximations of the model and the resolution strategies.

An important distinction between models is the linearity of the objective function and of the constraints, since the resolution of a linear problem is easier.

For this reason a common resolution strategy is to linearize the model. Moreno and Montagna in their studies (Moreno et al., 2007; Moreno et al., 2009; Moreno et al., 2012) propose a strategy to simplify the bilinear terms in the objective function and in the constraints, and then solve the optimisation using the commercial solver GAMS. It is worth noting that the computational effort needed for the model is further lowered eliminating the dependence of the discrete variables from the time periods.

Yi et al. (2011) proposed a realistic size model for a multiproduct, multistage and multiperiod production. Since the model was non-linear, the optimisation solver required a good initial guess. In order to find a good starting point, a separable programming technique to approximate the linear function with pieces of linear functions is used. The linear model is solved using GAMS, and then the solution found is improved by the non-linear solver.

The computational expense could be too expensive even for linear problems if the length of the planning horizon increases. Dogan et al. (2006) studied a multiperiod mixed-integer linear problem optimisation model and proposed a rigorous bilevel decomposition algorithm to reduce the time needed for the resolution. The hierarchical structure of the problem is exploited to divide the problem into an upper-level problem and a lower-level problem. The upper-level is solved first, and determines the most important decision variables for each week, such as the type of product, the production levels and the inventories. The lower-level is solved next. The advantage of this solution method is that it is possible to exclude from the lower-level problem the products not chosen from the upper-level optimisation. The two levels are solved at each iterations until a solution is reached.

The two levels decomposition strategy is widely used in non-linear multiperiod optimisation problem. Luo et al. (2007) proposed an optimisation model for a pooling problem, with the purpose of finding the optimal short term schedule for the refinery operations. They successively extended the resolution method to a longer period of time (Luo et al., 2009) adopting the rolling horizon approach. The time period is divided into planning periods of a week, which in turns are divided in scheduling periods of a day. The two-level decomposition algorithm is applied to the first planning periods, and a solution is found. At the end of the period the state of the system is updated, and the solving algorithm is applied to the following period. The computational cycle is repeated with the horizon advancing one period by one period until the solution is reached. It is possible to use the rolling horizon approach when the periods are linked to each other just through few variables, such as the inventory levels. It is worth noting that the periods are solved sequentially, not in parallel.

The two-level decomposition is exploited also by Lotero et al. (2015), who proposed a new formulation of the problem for obtaining solutions in few minutes. A source based formulation is used to determine the composition of the streams from the initial raw materials. Since the compositions of the sources are known parameters, the constraints are linear. Other linear constraints are added to improve the relaxation. An important assumption for the optimisation is that the tanks can not charge and discharge simultaneously. The model is then solved sequentially using a two-level algorithm.

Since the size of the model is big, relaxation techniques are often used. Rahim et al. (2014) tackled the supply chain problem and proposed to divide the inventory allocation from the vehicle routing and to solve the two problems separately. In order to divide the problems, a Lagrangian relaxation procedure is proposed. Since the demand rates are stochastic, an additional algorithm is applied to the inventory allocation problem. To reduce the number of

unfeasible solutions found at each iteration, a Lagrangian heuristic algorithm is proposed. The resolution is sequential.

A relaxation procedure is also used by Castro (2016), who proposed a two stage procedure to find the optimal solution. At the first stage, a McCormick relaxation is exploited to transform the function into a convex one. The simplified problem is solved to calculate a lower bound for the global optimisation. The binary variables are then fixed, and the optimisation is solved to obtain the upper bound. If the values of the lower and upper bounds are close enough, the global optimal solution is found. If the gap between the bounds is too high, a normalized multiparametric disaggregation technique (NMPD) is used instead of the McCormick envelope, and the calculations are performed until a solution is reached.

Chen et al. (2015) tried to find a suitable approximation for a stochastic dynamic programming problem, using sampling and approximations. The profit is calculated for every period of time using a set of steady state points. The results are used to calculate the approximate objective function using a MARS algorithm, which minimize the distance between the origin and the approximate function.

Often the resolution strategies proposed are tailored for the considered process. Bizet et al. (2005) used two approaches, a partitioning of the time horizon and a strategy that uses the Generalized Benders Decomposition (GBD). In fact if the problem is solved considering long time horizons, high non-linearity can lead to suboptimal solutions. To overcome the problem, a partitioning search strategy is proposed. The time horizon is divided in periods of one year and a local minimum is found for each period, then the optimum minimum is selected as the best one. The method is not rigorous, but is able to find global solutions near to the optimal one and requires less computational effort than the global search. An additional difficulty is that the size of the problem increases with each additional time period. For this reason, a decomposition technique is used. The solution is reached solving iteratively a subproblem and a master problem. The subproblem corresponds with the global problem in which the binary variables are fixed, and from its resolution it is possible to calculate the Lagrangian multipliers. The solutions are then used to solve the global master problem.

Zhao et al. (2014) proposed a strategy that can be applied when the nonconvex terms are mostly related to the blending model and the blending problems. The initial estimations of the production model and of the utility system are obtained fixing the quality of the final products according to the production experience and the solutions are used as initial estimates for the rigorous model. However the proposed method is not able to solve large-scale problems because of the possible multiple optimal points.

This issue was tackled by Kulkarni-Thaker et al. (2013), who proposed an algorithm to find a set of optimal solutions for the gasoline blending problem. The starting point for the study was the observation that different solvers reached different solutions for the same model, and that there was not the possibility to search for multiple solutions in commercial software. In order to find a single solution, a two-level search algorithm is built. The top level searches for the blend volume for each grade and each period, while the lower level individuates the optimal blend recipes. A useful feature of the model is that, if the blend volume is fixed at the top level, the lower level problem is linear. The multiple optimal solutions are found using a Differential Evolution Algorithm, which is an algorithm with the ability to “move” across the region where the objective function is flat. A set of populations is generated by the algorithm, where each member of the population corresponds with a solution. The final result is a population where each member is an optimal solution. The advantage of the method is that it is possible to choose between equivalent solutions taking into account additional considerations, such as preferred inventory profiles or source material. The algorithm requires extensive computations, but it would be possible to solve the optimisation using parallel computations, saving time.

This approach was exploited by Zhu et al. (2011), who tackled the topic of the optimisation of a cryogenic air separation system. The main problem of the model is that the separation process contains highly integrated flowsheets with strong nonlinear interactions between different process variables and production rates, and it is not possible to simplify the equations. For this reason the single period problem is solved using a primal-dual interior-point NLP solver, which handles variable bounds using a barrier term in the objective function. The solution for the single period is found solving iteratively the barrier problem. The multiperiod problem is solved using a tailored parallel nonlinear programming algorithm. The solver exploits a decomposition method to decouple the single period blocks, which are linked together by some coupling variables. This solution approach has good scalability and computational efficiency.

An important feature of the model is the use of a loss function to quantify the customer satisfaction. When the demand is not met by the inventory levels, the satisfaction level decreases, and that is represented as an economical loss.

The problem is more difficult when a multi-objective multi-period optimisation is required. Chen et al. (2003) proposed a decision-making method in two phases to assure a compromise solution between the objectives. The first step of the proposed resolution method is the direct maximization and minimization of each objective function, with the purpose of calculating the bounds for the global optimisation. The next step is to define membership functions for the fuzzy objectives. In the articles a linear membership function is used, corresponding to a scaling of

all objective values onto the interval [0, 1]. Successively the profit of the worst situation is maximized and the result is used as a lower bound for the overall problem.

An interesting approach to Multi-period Steam Cracking was proposed by Zhang et al. (2015). The article tackles the optimisation of a steam cracking plant in order to increase the ethylene yield. The plant is simulated in details through an accurate multi-scale modelling. The feedstock component prediction is achieved through Shannon entropy method, while the reactor is simulated as a plug flow. The reaction model is divided into two main submodels: a light hydrocarbon part and a heavy hydrocarbon part. The physical properties of species such as radicals or not-common substances are estimated through the group contribution model, since they are difficult to estimate. The most interesting feature of the model is the construction of the multi-period simulation. The periods are linked together just through the coke thickness, and the purpose is to find the optimal COT (coil outlet temperature) for each period. It is assumed that the other operative conditions are constant.

To perform the simulation it is necessary to apply an accurate model for the coke deposition. It is assumed that the coke thickness is only related to the furnace running time and to COT, then a model is obtained through regression from experimental data. An equation to relate the measured temperature to the COT is also derived.

The optimisation is solved using a parallel computing method, the pool parallel job partitioning method. The single period simulations are stored in the work pool and solved individually. The processors fetch jobs from the work pool as long as it is not empty. The product yields and outlet wall temperature for all the periods are evaluated by the solver until the optimal solution is reached. This type of computing method has many advantages, such as velocity, possibility of handling smaller models in one processor and the possibility of using a warm start. In fact if the iteration information of the first simulation is stored, it can be used as a warm start for the next ones, reducing CPU time.

The parallel computing method used in this article is the most promising technique, so this work will focus on its implementation in gProms, which is a platform provided by PSE for advanced process modelling, targeted at chemical processes. The parallel computing method allows for multiprocessing and for a consequent saving of time or of CPU. The multiperiod optimisation will be applied as an example to the steam cracking plant, but in principle the method could be applied to every type of plant in which the single periods are almost independent.

1.1.2 Strategic planning multiperiod problems

The second type of multiperiod problem tackled in this thesis is related to strategic planning. As in the previous case, the operations of one or more plants over a long period of time are considered and the decisions taken in a determined moment affect the following periods.

The difference between this case and the multiperiod problem related to inventory levels is the type of decisions that the optimisation has to make. In this type of problems, the optimisation has to answer specific questions, such as the following:

- Should we build a new plant in 2020?
- Shall we increase the capacity of the current plant next year?
- Should we sign a contract for one product next month?

In general, the optimisation has to provide a yes/no answer to these questions, and at the same time it has to find the optimal operating conditions of the plant. These two aspects of the optimisation are related, which makes a multiperiod approach to the problem useful.

For example, the construction of a new plant will increase the overall capacity of the network, and a higher demand would be satisfied. After that the plant has been built, if the demand decrease, it would be possible to decrease the production of one of the plants, changing the operating conditions. If instead a piece of equipment is revamped, the plant operating conditions would change as a consequence. The signing of a contract would bind the production to reach a minimum value, which has also an effect on the operating variables.

All of these decisions are taken considering the prices of products and raw materials during the time horizon. For example, it would be reasonable to increase the production of the most profitable product, in the period when the price is at the highest. The possibility of taking these factors into account is the advantage of performing a multiperiod optimisation.

Since the decisions taken by the optimisation, for example the building of a new plant, may require years of time to be realized, the time horizon covers a period of 10-20 years. For this reason the inventory levels are not considered in the model, because it is assumed that everything that is produced is sold during the period.

1.1.2.1 Literature review

An overview of the literature on strategic planning multiperiod problems is given, in order to identify the fundamental characteristics, solving methodology and issues related to it.

A multiperiod strategic planning problem is a model which can be applied to one or more plants and that is solved considering multiple periods of time. The solution of the problem has to show how to operate the existing plants and to decide raw materials sources and products destinations, taking into account long term decisions. Typical examples are articles considering the possibility of building and revamping a new plant, or more rarely, the signing of a multi-year contract. The time frame usually covers at least 10 years.

The longer time horizon requires the introduction of economical consideration, so the profit is usually calculated in terms of Net Present Value, which takes into account inflation and the risks of long term investments. The optimisation aim of the process is usually the maximisation of the NPV.

Since it is difficult to predict how the prices will behave in a long time span; stochastic models are more effective than deterministic ones, but the computational cost is higher.

There are many articles in literature which discuss the strategic planning problem, both with a continuous and a discrete time approach. This review takes into account only the discrete time approach, since it is the formulation adopted in this thesis.

As for multiperiod problem with inventory levels, there are two aspects that the articles focus on. Some articles focus on modelling, presenting more general and complete models, while other articles focus on the resolution procedure, since a multiperiod planning problem is usually difficult to solve in a short time.

The structure of the problem is general and can be applied to many different situations, so the articles focused on modelling deal with many different problems. The supply chain problem is the most studied situation, in particular in the applications related to the petrochemical industry. Examples are the articles of Meshalkin et al. (2017), Cafaro et al. (2014), Andersen et al. (2013), and Gargalo et al. (2017).

Meshalkin et al. (2017) in their article provide a model for a gas condensate stabilization plant. The aim is to evaluate two possible restructurization projects of the existing supply chain, since an increase of the natural gas production is expected. The first option is to introduce a new gas chemical plant to convert pre-processed gas into polyethylene into the supply chain, while the second option is to introduce a plant to produce polyethylene and polypropylene. The plants are characterized by their capacity, cost and construction time. Additional information is the price of raw materials and products. The results of the optimisation are the optimal functional organization structure of the supply chain and the estimation of the optimal operational

parameters of each unit within different time periods. The single periods may be solved both using a dynamic and a steady state formulation.

Another model is proposed by Cafaro et al. (2014) for a gas supply chain for natural gas production from shale formations. The key decisions that the optimisation has to take are size, number and location of the new shale gas drilling sites, since their costs are the highest. Other results of the optimisation are the section and length of the pipelines, the compressors power and the necessary amount of freshwater for the hydraulic fracturing. The model assumes that the gas extraction can only start after the drilling is completed and that the production of an active drill can not be interrupted. A correlation is found for the productivity rate, together with some assumptions about the gas composition. It is possible to drill in multiple sites during the same time period, but there is an upper bound due to technologies limitations. The model handle pipelines diameters as continuous variables, which are then rounded considering the commercially available pipes. The objective is to maximise the Net Present Value of the supply chain.

Andersen et al. (2013) propose a bigger model for integrated ethanol and gasoline supply chain. The model follows the distribution of the products from the harvesting and production to the retail gas stations. The units which are modelled are harvesting sites, ethanol plants, gasoline distribution centers and retail centers. It is possible to decide the location, capacity, technology and operating conditions of each type of units. In particular, the gas stations are divided into two categories: stations which sells only one type of blends, and stations which can sell every type. A superstructure is modelled using those units with two different levels of details, in order to simplify the resolution. Two models are proposed: a rigorous one which considers the number of gas stations needed to satisfy the fuel demand as an optimisation decision variable, and an aggregated simplified one which considers the fuel demand per country. The aim of the optimisation is to minimise the total costs over multiple periods of time.

A model for a biorefinery supply chain is proposed by Gargalo et al. (2017). The model, called GlyThink, is multiperiod, multistage and multiproduct and considers both production and logistics aspects of the supply chain. It is possible to build a superstructure with given glycerol suppliers and potential products. The aim of the optimisation is to decide location, capacity and technologies together with inventory levels, production and transportation. The technologies are characterized by yield and upper and lower capacity bounds. It is possible to build the plant in multiple countries, and the distance between the units is taken into account. The model takes into account also government incentives, taxation, depreciation and other financial data, which

are important for the calculation of the net present value. The period corresponds with the usual lifetime of the refinery.

Other examples of supply chain not related to the petrochemical industry are the articles of Saif et al. (2014) and Hong-Choon Oh et al (2004).

Saif et al. (2014) studied a supply chain for water desalinisation and production, using a time horizon of 15 years. The objective is to optimise the expansion capacity of the supply chain, together with operational decisions such as production, consumption, brine disposal and CO₂ emission. Deterministic demand is assumed. It is possible to decide to build a new plant, considering also what would be the optimal location, or to expand the capacity of plants, pipelines and storage tanks which are already present. Other choices are the optimal pipeline configuration and the optimal desalinization technology for new and old plants, which is characterized by cost, operational requirement and environmental impact. These decisions are taken in order to assure the water demand at the end of each period and to maximise the net present value. It is proved how running the optimisation for a longer time horizon leads to better results.

A very general approach is followed by Hong-Choon Oh et al (2004) to model a supply chain in countries around the world. The purpose of the article is to address the problem on a general scale, including also distributions centers, outsourcing and uncertainty, and to account the effect of the key regulatory factors on expansion and capacity planning. In particular it focus on the effect of corporate tax and import duty. It is assumed that the construction of a new plants does not affect the capacity of the existing ones and that the fixed number of periods is necessary before the new plant is available. It is not possible to build a new plant if another one is already in construction. It is also assumed that it is not possible to shut down a plant once it has been built. One important feature of the model is that the size of capacity expansions and the capacity of new facilities are decision variables. For this reason the cost for an expansion is calculated adding the fixed costs to the variable ones. Inventories are not taken into account, since a time horizon of one year is adopted.

Even if the supply chain problem is the most studied, there are many articles tackling other situations, as the ones written by Iyer at al. (1998) and Mitra et al. (2014).

Iyer at al. (1998) propose a model for the planning and scheduling of investment and operation in offshore oil field facilities. It is assumed that there are some sites available for the drilling, and that in each site there is a certain number of reservoirs, which in turn contains one or more wells. The plant is articulated into well platforms, where the oil is collected, and production

platforms, where gas and oil are separated and sent to the sales. The platforms are connected through pipes. The optimization has to decide which reservoir to develop, the sites to use from among the candidates, the schedule of the well drilling and of the platform installation, the capacities of wells and platforms and the production rates of fluid. The model takes into account nonlinearities in the performances of the reservoirs, constraints on surface pressure and on resources. It is possible to optimize a selected economic indicator, which is usually the Net Present Value.

Another problem which was solved using a multiperiod model was the planning of power-intensive continuous processes, which was studied by Mitra et al. (2014). The aim of this article is to optimize the planning of power-intensive processes, where the electricity prices are very relevant for the final profit. The difficulty of this situation is that the integration of the time scales, since the electricity prices change between night and day, but the time horizon covers year. The problem is solved dividing a year into four seasons, each with a different price. The model is formulated both with a deterministic and a stochastic demand, and the results are compared in order to find out when they are more appropriate to use. The planning decisions taken by the solver are the upgrade and purchase of the equipment. In particular the model is applied to an air separation system.

As seen with these examples, the most studied planning problems are the ones which consider an expansion, the construction or the purchase of a plant or of equipment. Another issue which is less studied in multiperiod planning problems is the possible signing of a contract during one of the period, tackled in the articles by Tay et al. (2005), Li et al. (2012), Devalkar et al. (2011), Zhang et al. (2010) and Lutze et al. (2007). All of these articles are related to supply chain problems, since it is the most common situation where this issue is important. Mostly these articles are specific for a type of contracts.

Tay et al. (2005) includes contracts selection in their model of a chemical supply chain. They focus on terminaling and tank storage of liquid chemicals, operations which are common occurrences during the transport, use and trading. The article proposes three different formulations for selecting contracts and allocating tanks to contracts in a typical storage terminal to maximize profit. The models are formulated as Mixed Integer Linear Programming. The first model, called M1, represents rigorously a terminal containing 27 tanks and takes into account 40 contracts. The second model M2 assumes that a new period starts only when there is the possibility of a new contract; this hypothesis reduces drastically the number of variables and consequently the computational time, even if the final profit is smaller than the one calculated

using M1. These two models assume that it is possible to meet the contract only in part. A third model M3 is elaborated assuming that a contract is binding. The article applies the models to the same problem, and concludes that M2 offers the best trade-off between velocity and accuracy of the results.

Another study was published by Devalkar et al. (2011). They develop a model to optimise both the operation and the selling schedule of the products, including forward contracts. They consider the integrated procurement, processing and trade decisions for a firm dealing in commodities. In particular they assume that it is possible to produce multiple outputs from one input. The article shows the benefits of the integrated optimisation approach, proving also that the inventory level is price-dependent. For this reason the price estimation for the contracts is calibrated using past data, and assuming that there is no seasonal variation. Capacity constraints are also implemented for each period.

Zhang et al. (2010) focus on short-term contracting in conditions of asymmetric inventory information. It is assumed that at the beginning of each period it is possible to sign a contract to purchase a determined amount of raw material, which is instantaneously received. At the end of the period part of the purchased material will remain in the inventory because the demand is uncertain. It is not possible for the supplier to know if the raw material had been used or not, and the contract can be designed only considering the previous purchases. For this reason the model developed is able to describe how the observable action of the retailer influences the following periods. A peculiarity of this model is that they consider an infinite time horizon. The results show how this type of model is more effective than simpler ones.

Another typology of contracts, the lead-time contracts, are studied in the article of Lutze et al. (2007). They consider a two level supply chain in a finite time horizon under demand uncertainty, which implies inventory uncertainty. The proposed typology of contract reduces the risk of demand uncertainty on the supplier and the risk of uncertain inventory availability on the retailer. The contract binds the supplier to guarantee on-time delivery of complete orders of any size after a promised lead time, which is decided by the optimisation. The purpose is to minimize the inventory cost. The article solves the problem with two different hypotheses: full information and asymmetric information. The results show that the risk for the supplier is higher when the information is kept private from the retailer, which is an usual occurrence in practice, or when the retailer is located far. It is defined a cutoff level on the retailer's service level that shows when it is convenient for the supplier to sign the contract.

Li et al. (2012) focus their article specifically on supply chain contracting. It is assumed that there is one manufacturer with two competing suppliers. The signing of a contract is decided

taking into account the current performance outcome and the change in the ratings. Their model takes into account also the effect of asymmetric information on the decisions.

A classification of the many types of contracts is proposed by Bansal et al. (2007). They defined two types, the quantity-commitment, when the buyer agrees to purchase a minimum quantity of each material, and the dollar-commitment, when the buyer agrees to a minimum dollar amount of purchase. The commitment is in turn divided into total, when the contract lasts for the complete time horizon, and periodic, when the contract lasts for a set of periods. The result is the classification of the contracts in four main classes. They are then further divided considering price discounts and flexibility on purchase commitment. Each type of contract is modelled using a MILP formulation. The aim of the main optimisation is the selection of the best contracts and suppliers together with the optimal distribution of materials from various suppliers to plant sites.

Two articles deal with expansions, revamping at contracts at the same time. They were written by Guptas et al. (2012a, 2012b), and the first details a model for a offshore oil and gas field planning problem, the second includes contracts into the study. The first article presents a mixed integer non linear programming to solve the strategic planning problem. The three components (oil, water and gas) are included using higher order polynomial. The model includes production, storage, installation, expansion, connections, well drilling and production rates. It is formulated as a multisite model. The objective is to maximize the net present value. The problem is then reformulated as a linear one in order to simplify the resolution. This first article is generalized in a following publication, which adds explicit fiscal calculations to the model. The financial rules are reduced to a variety of contracts. Contracts are also taken into account. The aim of this article is to have a general model the more adherent to reality as possible.

The articles which tackle the resolution of the problem focus on the peculiar mathematical formulation of the strategic planning problem, which uses binary variables to express planning decisions. For this reason it is necessary to use mixed-integer programming techniques to solve the optimisation.

Since the problem usually covers a long time horizon, the solution of the optimization may take a long time. For this reason, many resolution strategies are proposed in literature.

Grossmann et al. (2002) individuated the Branch and Bound method and the Generalized Benders Decomposition as the major resolution strategies to solve a MINLP problem. Different possibilities are the linearization of the model or a logic-based optimisation, for which the main

possibilities are Generalized Disjunctive Programming and Constraint Programming. These methods can be employed for models of a moderate size, but if the size of the problem increase it is necessary to adopt other techniques. The most common approaches for big models are decomposition, bilevel decomposition and aggregation. In literature there are many articles discussing an effective strategy for the solution of a specific model or proposing a specific algorithm.

A recent article by Cafaro et al. (2014) propose an algorithm tailored for a shale gas supply chain optimisation. Since the objective function includes nonconcave terms and unbounded derivatives it is not possible to solve the problem with implemented methods. The nonconvex power law expressions are handled both using a piecewise linear approximation and a logarithmic approximation. The first method partition the domain of a variable into intervals and introduce binary variables to determine to which interval the variable belongs. The resulting model is reduced to a MILP model; a key variable is the division of the domain, that is a trade-off between an accurate representation of the model and the necessity to reduce the computational cost.

Another resolution strategy is proposed by McLean et al. (2013) to tackle MILP problems which include uncertainty. They assume that the problem is solved using a two-level strategy, where the first level is related to the development of the supply chain and the second level to the operations. Two robust scenario formulations are elaborated. In the first one, called naïve robust scenario formulation, the infinite number of uncertainty realizations are grouped into a finite number of scenarios. In the second formulation, called affinely adjustable robust scenario formulation, the first formulation is expanded. While in the first method the same second-stage decision is applied to all the different uncertainty realizations of one scenario, in the second formulation it is possible to adjust second-stage decisions according to the realizations of uncertainty. Both formulations can be transformed into a deterministic optimisation problem if the uncertainty is bounded, without relying on assumptions about the uncertainty region. The two methods are tested and it is proved that they generate a smaller number of scenarios and shorter solution times.

Gupta et al. (2012) propose some reformulation and approximation techniques that could be used to simplify their model of an offshore oil and gas infrastructure. These strategies can still be applied to other similar models. In particular the article concentrates on formulating alternative models. If the function is monotonically increasing, it is possible to add some additional constraints. It is also possible to use an alternate formulation for the fiscal rules which does not include binary variables.

Kostin et al. (2011) proposed an algorithm for supply chains in the sugar cane industry. The method can be applied with linear models. The method is based on a rolling horizon strategy, which is based in dividing the problem into subproblems and solve them sequentially. In the first iteration, the problem is completely solved, but only the solutions of the first period are implemented. The state of the system is updated, and in the next iteration only the remaining periods are solved, and only the solutions of the second period are implemented. The algorithm proceeds until all the variables has been calculated. The article proposes to approximate the binary variables with continuous ones, which can reduce the computational cost without sacrificing the quality of the solution. Only the variables related to the period which is solved in that moment are bound to be integers, while the binary variables included in the other periods are approximated. The proposed methodology was tested, and the optimal solution reached was similar to the one calculated in the rigorous way.

Ryu et al. (2007) in their articles described a modelling framework based on a two-level optimization. It is assumed that the model is linear. The resolution method that they propose is divided in two parts. First, it is necessary to allocate a demand to each plant. To do so, demands in different locations during the whole time horizon are aggregated, and then distributed to the single plants using three different operation policy. These policies, which are coordination, cooperation and competition, are explained in a previous article by Ryu et al. (2005). The second step of their method is to define the operation planning of the individual plants in order to minimize the total operating cost during all periods. The aim of the complete algorithm is to maximize the total profit during all periods.

1.2 Purpose of the work

Even if multiperiod problems are usual in chemical processes optimisations, currently gProms has not a library that specifically handles them. It is still possible for the customers to perform these types of optimisation if they write their own scripts, but there are some limitations, which would be removed in an ad-hoc built feature.

In order to introduce this new possibility in gProms, it is necessary to carry on a number of tests. While some work has already been done inside the company to introduce in the program problems related to inventories, nothing had been done for problems related to contracts, building of new plants and revamping. For this reason the purpose of the tests is different in the two cases.

Since part of the program related to the inventories had already been written, the aim is to check if the implemented solving method gives the same results as the currently available gProms resolution. It is also necessary to check the effect of using this method on complex flowsheets. For the strategic planning problem a number of examples, each one detailing one of the most frequent problems, was set up in gProms. The aim was to identify the necessary data and the key equations, which link the periods in order to reduce this type of problems to a common structure easy to implement. Additionally, since there were no previous examples solved using the same methodology, it was also necessary to check if the solver reacted as expected to price fluctuations.

In the next chapters the old and the newly implemented resolution methods will be explained in details; afterwards, the examples elaborated for the two cases will be explained.

Chapter 2

Multiperiod optimisation: formulation

This chapter tackles the mathematical formulation of the multiperiod problem and the procedure used to solve it. The first part deals with the inventory problem, explaining the modelling equations, the objective function calculation and the structure of the solver in details. The second part shows how equations and solver can be adapted to take into account strategic planning multiperiod problems.

2.1 Multiperiod problem with inventories

As stated in the introductory chapter, it is possible to apply a multiperiod optimisation to a variety of different processes. In order to solve them, it is necessary to have a general set of equations, which should be applicable to every type of process, and a resolution strategy.

The purpose of this part of the work is to finish to set up the resolution strategy and to check its functioning on a number of examples.

Both the equations needed and the resolution strategy are detailed in the next paragraphs.

2.1.1 Equations

In general, the solver requires an objective function and a set of constraints in order to find a solution. In this section it is explained how it is possible to calculate them, passing through the formulation of the single period equations and of the inventory level equations.

2.1.1.1 Single period equations

In a multiperiod problem the aim is to optimise both the operating conditions of the plant and other long term considerations. The operating conditions are included in the single period formulations, which for this reason become the basis of the problem.

In general, it is assumed that the single period process can be modelled by the following equations $f_{j,t}$.

$$y_{j,t} = f_{j,t}(u_{1,t}, \dots, u_{l,t}) \quad (2.1)$$

The equations return J outputs y_j for each period t of time, starting from I inputs u_i for each period t .

During each period t , it is possible to divide the inputs u_i into two categories:

- a number M of inputs μ_m that are present in each period, such as with the operative conditions of the process, the inlet flowrates etcetera;
- a number N of inputs θ_n that are not always present, representing unexpected occurrences.

The outputs y_j are divided into two categories:

- a number P of materials that can be stored, indicated as M_p ;
- a number Q of utilities that can not be stored, indicated as U_q .

In general, the inputs and the outputs could have upper and lower bounds, as written below.

$$u_{i,t}^{min} \leq u_{i,t} \leq u_{i,t}^{max} \quad (2.2)$$

$$y_{j,t}^{min} \leq y_{j,t} \leq y_{j,t}^{max} \quad (2.3)$$

where $u_{i,t}^{min}$ and $u_{i,t}^{max}$ are the lower and upper bounds of the inputs, and $y_{j,t}^{min}$ and $y_{j,t}^{max}$ are the lower and upper bounds of the outputs.

The possible single period constraints are represented by the following equations $g_{f,t}$.

$$g_{f,t}(u_{1,t}, \dots, u_{I,t}, y_{1,t}, \dots, y_{J,t}) \geq 0. \quad (2.4)$$

The constraints are relative to both inputs and outputs, and can be summarized in the following equation.

$$c_{f,t} \geq 0. \quad (2.5)$$

Having defined inputs, outputs and constraints of a single period, it is possible to move on to the inventory levels calculation.

2.1.1.2 Inventory levels

In a multiperiod problem the single periods are linked together through some long term decisions. In this particular case, they are coupled through the inventory levels of the raw materials and of the products.

The equation used to link them is based on a simple physical consideration: if a material is stored at the beginning of a process and nothing happens, it will still be available at the end of

a determined period of time. The stored amount can vary if a part of the material is sold or purchased or if the material is produced or consumed in a process.

Following this reasoning, the raw material inventory balance is defined by the equation below.

$$IR_{k,t} = IR_{k,t-1} + A_{k,t} - CR_{k,t}D_t \quad (2.6)$$

The raw material in storage IR_k at the end of a period t is equal to the amount stored at the end of the previous period plus the amount bought A_k and minus the amount consumed by the production. The production is expressed as a product between the production rate $CR_{k,t}$ and the period length D_t , to allow for periods of different length. The subscript refers to the raw material k .

The inventory level of the raw material and the amount purchased have upper and lower bounds.

$$IR_{k,t}^{min} \leq IR_{k,t} \leq IR_{k,t}^{max} \quad (2.7)$$

$$A_{k,t}^{min} \leq A_{k,t} \leq A_{k,t}^{max} \quad (2.8)$$

The maximum inventory level $IR_{k,t}^{max}$ is related to the physical space that is possible to assign to the storage of the material, while the minimum level $IR_{k,t}^{min}$ has the purpose to assure that the production can continue even if there is a shortage in the raw material supply. The limit of the purchase A of raw material is instead constrained between the upper limit $A_{k,t}^{max}$ and the lower limit $A_{k,t}^{min}$ by economical consideration.

The product inventory level is defined by the following equation.

$$IP_{p,t} = IP_{p,t-1} + PR_{p,t}D_t - S_{p,t} \quad (2.9)$$

The equation means that the inventory level IP of a product p at the end of period t is the inventory level at the end of the previous period, plus the amount produced PR_p and minus the amount sold S_p during that period. As in the raw material equation, the production of products takes into account the period length D_t .

Both the inventory level of the product and the sales have upper and lower bounds.

$$IP_{p,t}^{min} \leq IP_{p,t} \leq IP_{p,t}^{max} \quad (2.10)$$

$$S_{p,t}^{min} \leq S_{p,t} \leq S_{p,t}^{max} \quad (2.11)$$

The maximum inventory level $IP_{p,t}^{max}$ is related to the physical space that is possible to assign to the storage of the material, while the minimum level $IP_{p,t}^{min}$ has the purpose to assure that it is possible to sell the product to the customers even if the production is stopped for a while. The constraints on the sales (the lower limit $S_{p,t}^{min}$ and the upper limit $S_{p,t}^{max}$) of product are related to the quantity that is demanded by the customers.

The inventory levels and their constraints are additional data, which are required for the objective function calculation and for the solver.

2.1.1.3 Objective function

The last and more important element required for the optimisation is the objective function, which is used by the solver to find the most profitable conditions for the plant. In the examples solved in this thesis, the objective function to maximize is the total profit made during the complete time horizon.

To calculate the total profit, it is necessary to provide an equation to calculate the profit during the single periods. In particular, the structure of the equation would be the following one.

$$\begin{aligned} \text{profit} = & \text{revenues} - \text{production cost} - \text{raw material cost} \\ & - \text{inventory cost} \end{aligned} \quad (2.12)$$

It is assumed that the only income derives from the sales of the products, while the costs are due to the purchase of the raw materials, the operating costs of production and the costs related to the storage of material.

It is possible to calculate the profit of the time period t using the following equation.

$$\begin{aligned} P_t = & \left[\sum_j \alpha_{q,t}^U U_{q,t} + \sum_l \beta_{p,t}^S S_{p,t} - \sum_i \alpha_{i,t}^u u_{i,t} - \sum_k \beta_{k,t}^A A_{k,t} \right. \\ & - \sum_k \gamma_{k,t}^{IR} \frac{1}{2} (IR_{k,t} + IR_{k,t-1}) \\ & \left. - \sum_l \gamma_{p,t}^{IP} \frac{1}{2} (IP_{p,t} + IP_{p,t-1}) \right] D_t \end{aligned} \quad (2.13)$$

In this equation P_t is the profit at the end of period t , which is calculated including inputs and outputs from the single periods and other variables from the inventory calculations. In the equation, the terms $U_{q,t}$ and $u_{i,t}$ are related respectively to the utilities produced and consumed. $U_{q,t}$ represents the output Q , which can not be stored, and it is sold with a price $\alpha_{q,t}^U$. The utilities consumed are expressed in terms of input $u_{i,t}$, and have a cost $\alpha_{i,t}^u$. The raw materials and the products, which can not be stored, are represented by $S_{p,t}$, which is the sale of product I , and by $A_{k,t}$, which is the purchase of raw material K . Their values is expressed respectively through the coefficients $\beta_{p,t}^S$ and $\beta_{k,t}^A$. These variables are used in the first four terms of the equations to calculate revenues and costs of production and raw materials. The approach distinguish between

materials that can be stored and the materials that can not be stored. The revenues derives from both the types of material, but it is assumed that it is only possible to decide the sale of the products that are stored, while the utilities are completely sold. Using the same reasoning, it is possible to decide the amount of raw material that can be stored, but it is not possible to decide the amount of purchased utilities.

The remaining terms calculate the costs of keeping an inventory. $\gamma_{k,t}^{IR}$ and $\gamma_{p,t}^{IP}$ are respectively the inventory cost of the stored raw materials and the stored products. It is assumed that the cost of storage is directly proportional to the amount of material that is stored, so these costs are multiplied for $IR_{k,t}$ and $IP_{p,t}$. Since the inventory levels are calculated at the end of each period, while the profit is calculated for the complete period, it is necessary to use the average value of the inventory between the beginning and the end of the period.

It is worth to notice that it is assumed that the prices for all the periods are known: the model works using deterministic prices.

The objective function is calculated as the sum of the profits of the single periods.

$$obj = \sum_t P_t \tag{2.14}$$

Since the objective function depends both on the products and raw materials flowrate (related to the single periods) and on purchase and sale (related to the inventory level), it is possible to optimise both the operating conditions and the selling schedule.

2.1.2 Resolution structure

After modelling the multiperiod problem, it is necessary to adopt a resolution structure in order to solve it. In particular, the purpose of this work is to solve the multiperiod problem with a

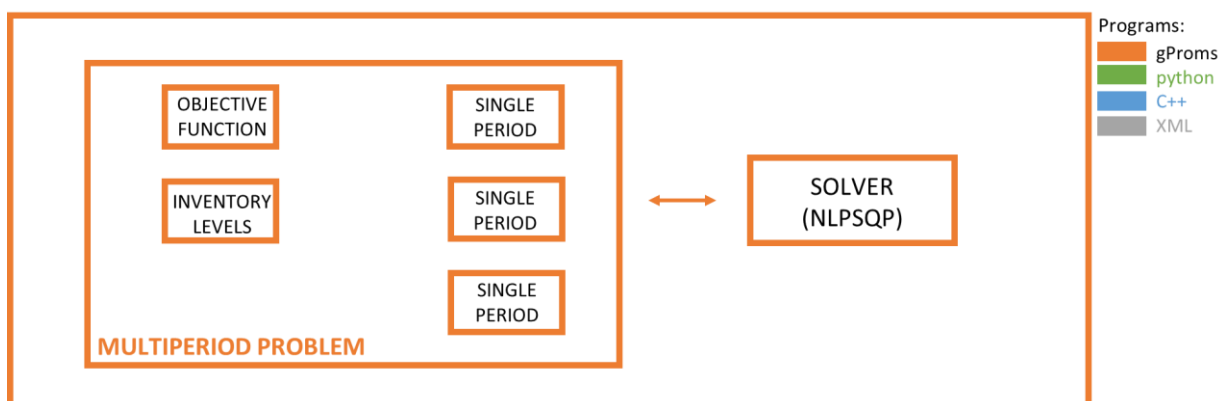


Figure 2.1. Current resolution scheme.

The scheme shows how in gProms the multiperiod problem is a single block containing the single periods, the objective function and the inventory levels.

The problem is processed in his entirety by the solver, which is a Sequential Quadratic Programming for Non-Linear Problems (NLPSQP).

new, more effective, resolution method. Currently, gProms is able to handle multi-period optimisations with the structure depicted in the Figure 2.1.

As shown in the scheme, currently it is possible to create a model for the multiperiod problem and to solve it using exclusively the program gProms. The model is articulated in multiple small functions containing the single period processes, the inventory levels and the calculation of the objective function. These pieces are combined in a bigger function which contains all the data relative to the multiperiod problem. The solver is applied to this complete function, and the solution is reached.

The drawback of this resolution strategy is that it is not possible to solve the single periods independently, because they are all included in the bigger multiperiod problem function. The solver has to receive all the data contained in this function before proceeding with the resolution, and this means that it needs to store all the data relative to all the periods in memory.

The aim of this work is to solve the problems using a new resolution strategy that would allow to solve the periods separately. Since the elaboration of this function directly using gProms is difficult, another prototype resolution method is used first, as shown in figure 2.1. This method is relatively easy to set and allows to solve the periods independently.

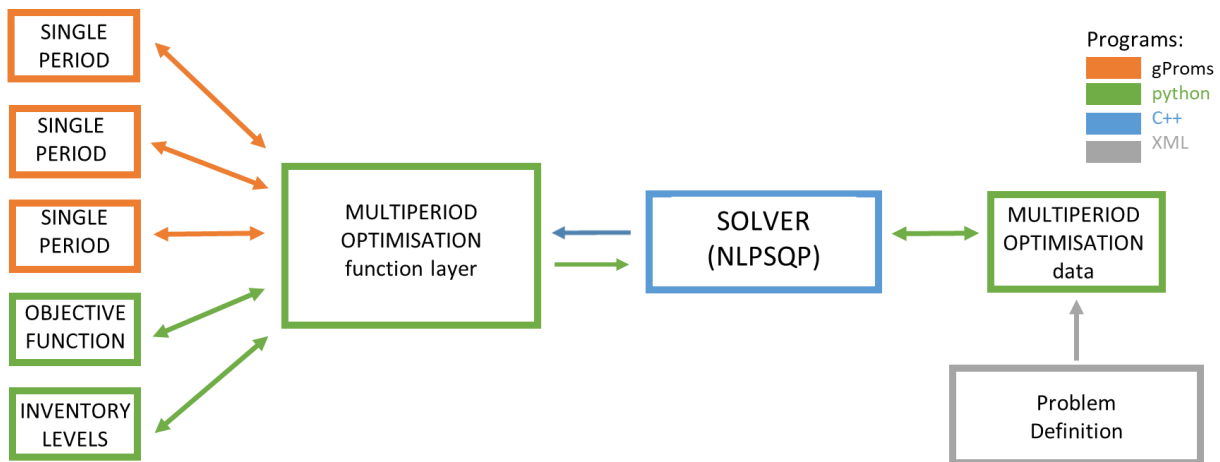


Figure 2.2. *Prototype Resolution Method.*

The scheme shows how the single periods, the objective function and the inventory levels are calculated using different programs and recalled by one python function layer.

The data are inserted through an XML file called "Problem Definition", which is read by another python function. The solver is connected with the two main python function.

This configuration relies mostly on python functions to connect together the parts of the problem. The advantage is that it is possible to keep the single periods, which are the basis of the multiperiod problem, in gProms, and to define in an explicit way the connection with the rest.

The central part of the structure is a Multiperiod Optimisation function layer written in python, which calls back to all the other parts of the problem. The use of python allows to recall separately each single period, and also to solve the periods in multiple processors.

The objective function and the inventory levels equation, which link the periods together, are calculated in two separate python functions and recalled by the function layer. The data required for those calculations and the inputs of the single periods are introduced through a xml file called “Problem Definition”, which is read by another python function. The data are recovered by the python function layer, which passes them to the other functions.

The function layer collects the data from the single periods, the inventory levels and the objective function calculation and sends them to the solver, which is written in C++. For the multi-period problem, the solver used is a Sequential Quadratic Programming for Non-Linear Problems (NLPSQP) solver. This solver is the same one that is used inside gProms with the current resolution structure. The results of the optimisation are sent again to the python function layer.

The prototype structure is the first step towards the final structure, which is shown in Figure 2.3. The problem is not implemented directly using this structure because of the complexity of the set up.

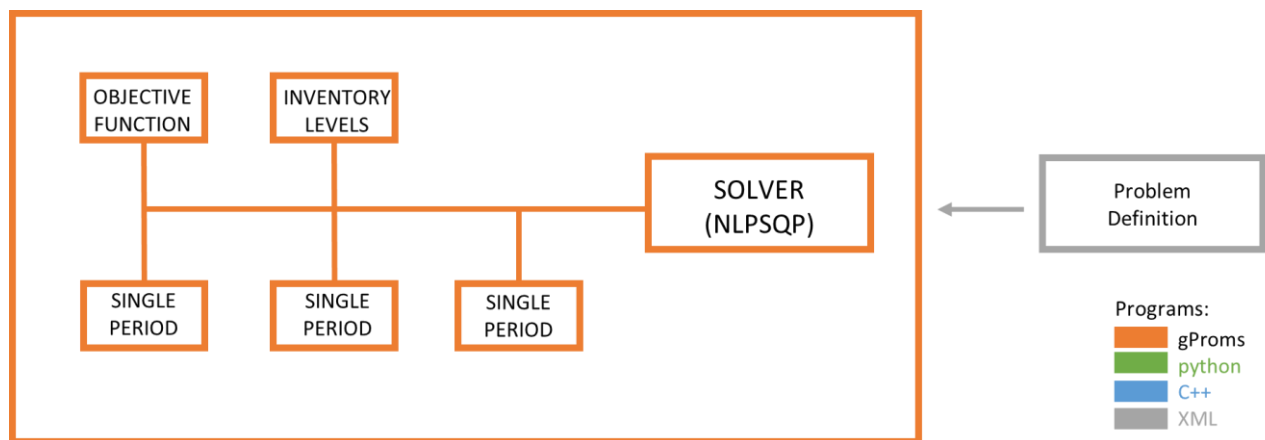


Figure 2.3. Final resolution structure.

The objective function, inventory levels and single period calculations are directly processed by the solver. Every piece of the model is defined in python, except for the multiperiod problem data, which are inserted through an XML file.

As in the current resolution method, the multiperiod problem is defined in a single gProms model, which calls back to the single periods, the objective function and the inventory levels equation. The data of the problem can be introduced through the xml file, or directly in gProms. The difference with the current resolution is that the structure would be rewritten as to allow the solution of the single periods independently, as in the prototype structure.

Part of the work of this thesis was to finish to set up the prototype structure, fixing some minor problems in the functions. After that, the files were adapted to work with some specific examples, described in §Chapter 3, in order to test the structure.

The next paragraphs will describe in details the features of the prototype function, in particular the xml file, the solver and the python function layer.

2.1.2.1 NLPSQP solver

The possible presence of non-linearities in the single model periods makes the multi-period optimisation a non-linear problem. One of the most effective resolution methods for nonlinearly constrained optimisation problem is the Sequential Quadratic Programming for Non-Linear Problems, which is the one used in this case. The methods can be considered an extension of the Newton's method and use a quadratic model of the process.

2.1.2.1.1 Mathematical formulation

The general constrained optimisation problem can be written as

$$\min_x f(x) \quad (2.15)$$

subject to

$$c(x) = 0 \quad (2.16)$$

$$d(x) \leq 0 \quad (2.17)$$

The problem has both equality and inequality constraints, respectively written as $c(x)$ and $d(x)$. For this reason it is necessary to use the Karush-Kuhn-Tucker (KKT) conditions, which are an extension of the method of Lagrangian Multipliers that are able to deal with inequality constraints.

The Lagrangian of the problem is

$$L(x, \nu, \lambda) = f(x) + \nu^T c(x) + \lambda^T d(x) \quad (2.18)$$

where ν and λ are the KKT multipliers.

From the previous equation it is possible to derive the KKT conditions for optimality.

$$\nabla L(x, \nu, \lambda) = \nabla f(x) + \nabla c(x)\nu + \nabla d(x)\lambda = 0 \text{ (stationarity)} \quad (2.19)$$

$$c(x) = 0 \quad (2.20)$$

$$d(x) \leq 0 \quad (2.21)$$

$$\text{diag}(d(x))\text{diag}(\lambda) = 0 \quad (2.22)$$

$$\lambda \geq 0. \quad (2.23)$$

Each iteration is solved as a quadratic programming problem, which means that the objective function is replaced with the quadratic approximation, as in the equation below.

$$\min_{\Delta x} m(\Delta x) \tag{2.24}$$

$$m(\Delta x) = \frac{1}{2} \Delta x^T H \Delta x + \nabla f(x)^T \Delta x \tag{2.25}$$

The constraints are substituted with a linear approximation, as in the following equations.

$$c(x) + \nabla c(x)^T \Delta x = 0 \tag{2.26}$$

$$d(x) + \nabla d(x)^T \Delta x \leq 0 \tag{2.27}$$

$$\|D\Delta x\|_p \leq \delta. \tag{2.28}$$

The final inequality constraint is known as a “trust region”, while δ is the trust region radius which can be set to aid the convergence. The purpose of this parameter is to limit the step size of the optimisation, so as to stay in a region where the approximation of the function is good. If the approximation of the function is good, the trust region radius would be long, while if the approximation is poor the radius would be short.

2.1.2.1.2 Iterative procedure

To reach the solution of the optimisation, it is used an iterative procedure that starts from the single periods. The optimisation can be performed for every number of periods, each one taken into consideration separately.

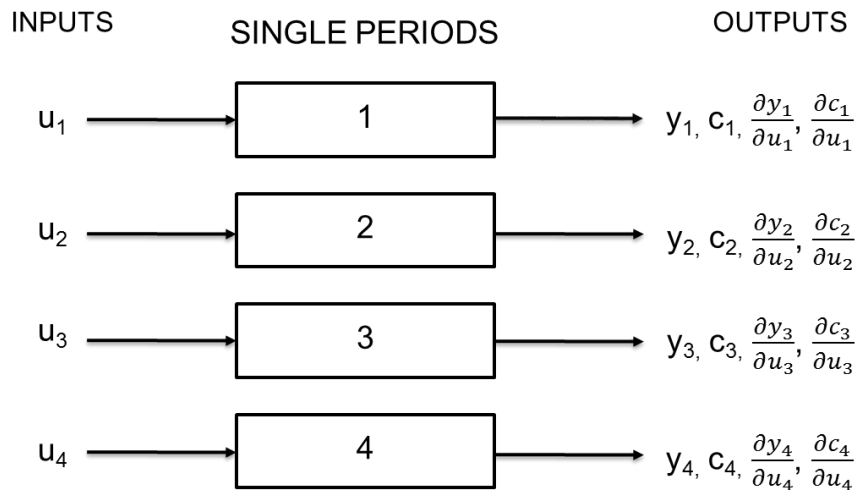


Figure 2.4. Inputs and outputs of the single periods

As showed in Figure 2.4, the optimisation starts when the vectors of inputs u_i are fed to each single period. These inputs are values used as a first attempt. All the single processes are solved (in parallel or in series) for those inputs, and the results are a vector of outputs y_j , a vector of constraints c_i and the gradients of outputs and constraints calculated with respect to the inputs.

Once the single periods have been solved, the results are collected and used to calculate the objective function, as shown in Figure 2.5.

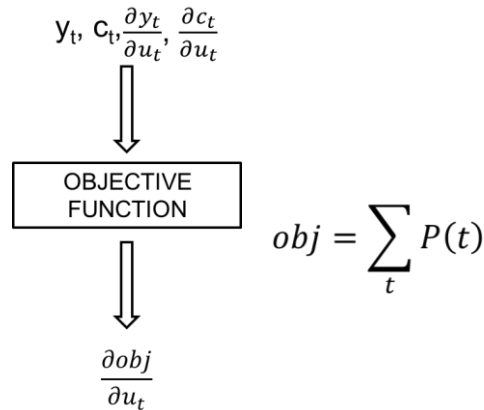


Figure 2.5. Objective function calculation

The results of this passage are the objective function value and its gradients with respect to the inputs. The next step is to send these results to the solver, as in Figure 2.6.

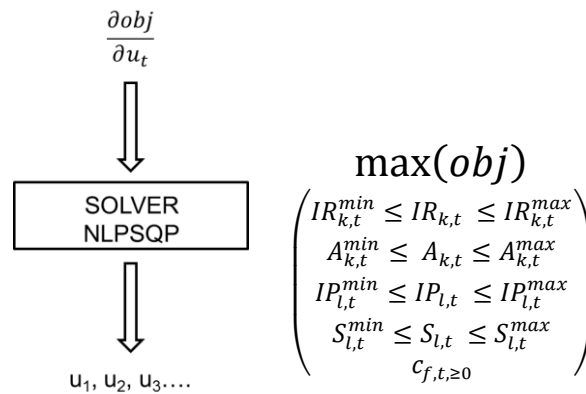


Figure 2.6. Problem resolution

The solver is a Sequential Quadratic Programming (SQP) for Non-Linear Problem. The solver searches for the values of the inputs which maximize the objective function and respects the constraint on sales, purchases, inventory levels and the single periods.

The results of this step are the inputs of the single periods. If the maximum value of the objective function is reached, those results are the global results of the optimisation. If the maximum value is not reached, the inputs are sent again to the single periods, and the cycle starts again.

The complete optimisation structure is shown in Figure 2.7.

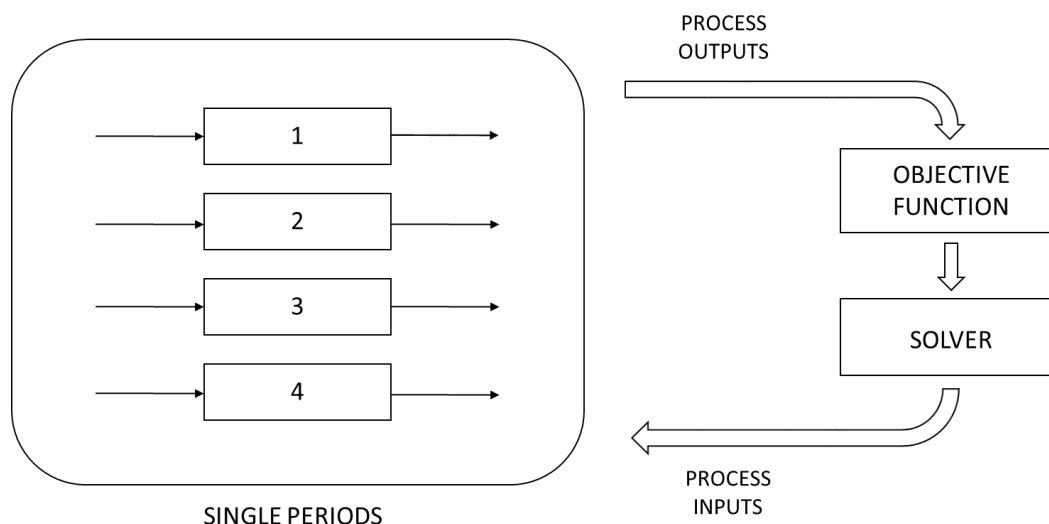


Figure 2.7. Complete iterative procedure.

This resolution method allows to solve the periods separately. They can be solved in sequence, saving memory, or in parallel, taking advantage of multiple processors.

2.1.2.2 XML file

While the data relative to the single periods are inserted directly into the gProms files, the data necessary to the multiperiod calculation are inserted through an xml file. The file provides the data relative to the objective function calculation, the inventory levels, the constraints and the variables that can be manipulated by the solver.

The xml file is articulated in 5 main sections:

- Units
- Periods
- External Materials
- Operation
- Model

The data written in this file are read using a python function which is called by the Multiperiod Optimisation function layer and by the solver.

Part of the work was to modify the xml file and the python function to read it, in order to have more flexibility. In addition, the xml file needs to be modified every time that a new example is solved using the prototype resolution structure.

The xml sections will be illustrated taking the xml file relative to the blending problem solved in §3.1.3 as an example.

2.1.2.2.1 Units

This section shows the unit of measurement that are used in the calculations.

```
<Units>
  <Unit name="Time" value="seconds"/>
  <Unit name="Currency" value="euros"/>
  <Unit name="Amount" value="kilograms"/>
  <Unit name="Flowrate" value="kilogram/second"/>
</Units>
```

In this part of the code every unit of measurement is associated as a name and its dimensions. This section is not passed to the solver, but it is used as a reminder for the user. In fact the unit of measurement have to be consistent, since the solver does not allow for internal conversions.

2.1.2.2.2 Periods

In this sections it is possible to insert the number of periods that the optimisation will take into account.

```
<Periods>
  <Period name="first" duration="1"/>
  <Period name="second" duration="2"/>
  <Period name="third" duration="1"/>
  <Period name="fourth" duration="3"/>
</Periods>
```

The information is basilar to define the multiperiod problems, because it gives the indication of the number of single periods required.

It is possible to define a name, which is used as a reminder, and a different duration for each one of the periods.

2.1.2.2.3 External materials

The External Material section is relative to sales, purchases and inventory levels of products and raw materials, and takes also into account the utilities consumption. Prices fluctuations during the periods are taken into account, together with possible constraints on storage space, sales and purchases limits.

```
<ExternalMaterials>
  <Product name="S4 flowrate" PathName="M.outlet_mass_flowrate">
    <Sale>
      <Period name="first" minvalue="0" maxvalue="10000" price="65" initialguess="0"/>
      <Period name="second" minvalue="0" maxvalue="10000" price="72" initialguess="300"/>
      <Period name="third" minvalue="0" maxvalue="10000" price="72" initialguess="100"/>
      <Period name="fourth" minvalue="0" maxvalue="10000" price="70" initialguess="300"/>
    </Sale>
    <Inventory initial="5">>
      <AllPeriods minvalue="0" maxvalue="50000"/>
    </Inventory>
  </Product>
  <Utilities>
    <Utility name="S1 flowrate" PathName="M.mass_flowrate(1)">
```

```

    <Purchase>
      <Period name="first" minvalue="0" maxvalue="50000" price="3" initialguess="6"/>
      <Period name="second" minvalue="0" maxvalue="50000" price="6" initialguess="6"/>
      <Period name="third" minvalue="0" maxvalue="50000" price="5" initialguess="6"/>
      <Period name="fourth" minvalue="0" maxvalue="50000" price="4" initialguess="6"/>
    </Purchase>
  </Utility>
  <Utility name="S2 flowrate" PathName="M.mass_flowrate(2)">
    <Purchase>
      <Period name="first" minvalue="0" maxvalue="50000" price="60" initialguess="92"/>
      <Period name="second" minvalue="0" maxvalue="50000" price="65" initialguess="92"/>
      <Period name="third" minvalue="0" maxvalue="50000" price="63" initialguess="92"/>
      <Period name="fourth" minvalue="0" maxvalue="50000" price="62" initialguess="92"/>
    </Purchase>
  </Utility>
  <Utility name="S3 flowrate" PathName="M.mass_flowrate(3)">
    <Purchase>
      <Period name="first" minvalue="0" maxvalue="50000" price="8" initialguess="2"/>
      <Period name="second" minvalue="0" maxvalue="50000" price="7" initialguess="2"/>
      <Period name="third" minvalue="0" maxvalue="50000" price="10" initialguess="2"/>
      <Period name="fourth" minvalue="0" maxvalue="50000" price="6" initialguess="2"/>
    </Purchase>
  </Utility>
</Utilities>
</ExternalMaterials>

```

This section defines and passes to the solver the data relative to purchases and sales. The code is divided into two different parts: utilities and products.

The products are defined with a name and a reference to their gProms name, so that it is possible to associate the data with the variable in the single periods. The data are both related to the sales and to the constraints. In the first case, it is possible to define a different price for the product for each period, together with a first guess for the sales. It is possible to define a maximum and minimum sale for each period and a minimum and maximum inventory level to be maintained at the end of the period.

It is worth noticing that it is possible to define different values for each period or to use the same values for all the periods. This possibility was one of the main addition to the code.

The second part of the code is related to the utilities, which are defined, as in the previous case, with a name and a reference to gProms. The data to be inserted are similar to the ones used for the products section, with the exception that there is not an inventory.

Originally the code allowed only to sell the products and to purchase the utilities, but it was then changed to permit also the purchase of raw materials and the sales of utilities.

2.1.2.2.4 Operation

This operation section contains all the information about the variables that can be manipulated and their constraints.

```

<Operation>
  <DecisionVariable name="S1 flowrate" PathName="M.mass_flowrate(1)">
    <AllPeriods minvalue="0" maxvalue="200000" initialguess="6"/>
  </DecisionVariable>
  <DecisionVariable name="S2 flowrate" PathName="M.mass_flowrate(2)">
    <AllPeriods minvalue="0" maxvalue="200000" initialguess="92"/>

```

```

</DecisionVariable>
<DecisionVariable name="S3 flowrate" PathName="M.mass_flowrate(3)">
  <AllPeriods minvalue="0" maxvalue="200000" initialguess="2"/>
</DecisionVariable>
<Constraint name="Outlet mass flowrate" PathName="M.outlet_mass_flowrate">
  <AllPeriods minvalue="0" maxvalue="100"/>
</Constraint>
<Constraint name="Mass fraction of A" PathName="M.outlet_mass_fraction('A')">
  <AllPeriods minvalue="0.9" maxvalue="1"/>
</Constraint>
<Constraint name="Mass fraction of B" PathName="M.outlet_mass_fraction('B')">
  <AllPeriods minvalue="0" maxvalue="0.05"/>
</Constraint>
<Constraint name="Mass fraction of C" PathName="M.outlet_mass_fraction('C')">
  <AllPeriods minvalue="0" maxvalue="1"/>
</Constraint>
</Operation>

```

This section is related to the single periods and to the operating conditions of the process. It is divided into three sections: decision variables, constraints and disturbances.

The first part is needed to define the variables which can be manipulated by the solver. As in the previous case, they are defined by a name and a gProms reference. It is then needed to give an initial guess for the variable values and to give an upper and a lower bound to the solver. These variables coincide with the operating conditions of the process, which are optimised at the end of the process.

The constraints section is used to give an upper and a lower bound for some process variables. For example, in this case there are some quality specifications that the final product should satisfy. The constraints are defined as the decision variables, with the exception that an initial guess is not needed.

There is a third section, which was not used for this problem, which allows the user to define any disturbance of the process that may occur during the periods. The disturbance is defined by its name, the gProms reference and a value, which the variable will be forced to assume during the period.

2.1.2.2.5 Model

The last section contains the references to the gProms single period process, which are necessary to access the gProms files using python.

```

<Model gPROMSfilename="Single_Process" process="Single_Process" password="Single_Process">
</Model>

```

The gProms files are identified by their name and opened using a password chosen by user and set in gProms.

2.1.2.3 Multiperiod Optimisation function layer

The main function, which references all the other parts of the problem, is the multiperiod optimisation function layer. This function is the one which starts the resolution process, taking the data from the xml file, receiving and sending data to the single processes in gProms, calling the other python functions for the calculation of objective function and inventory levels and referencing the solver. In particular, in this function it is possible to choose if a single processor or multiple processors are used.

While the calculation progresses, the information are printed on the screen. In the end a summary of the process appears, together with the final results of the optimisation.

The following paragraphs will detail the two most important python function which are referenced by the function layer: the function which calculates the objective function and the one which calculates the inventory levels.

Both the function needed some minor adjustment before been used in the prototype structure.

2.1.2.3.1 Objective function

The purpose of this function is to calculate the objective function from the outputs of the single period process. The results will be sent to the solver in order to perform the optimisation. The gradients of the objective function are also calculated and sent to the solver.

```

Inputs          u
                  class MPO_info

Step 1
u_plant, u_market <- split inputs(u)
u_plant_operation <- stack(u_plant, MPO_info.u_disturbances)
for w in workers do:
    y_wi = f(u_plant_operation_wi)

Step 2
util_plant = f(y, MPO_info.no_utilities)
obj = -sigma(MPO_info.periods.duration*MPO_info.utilities.purchase.price*util_plant)
      +sigma(MPO_info.products.demand.price*u_market)

Step 3
grad_market <- stack(MPU_info.products.demand.prices,
                    MPO_info.products.purchase.price)
grad_plant = f(MPO_info.utilities.purchase.price, MPO_info.periods.duration,
              MPO_info.no_utilities, MPO_info.no_decisionvariables)
grad <- stack(grad_market, grad_plant)

Outputs        obj
                  grad

```

The inputs required for the calculation are the single period inputs and the data inserted through the xml file. The process can be divided into three steps.

In the first step the inputs are reorganized in a different vector, which is then processed in order to obtain the single period outputs. In this phase it is possible to use one or multiple processors, depending on the instruction given in the function layer.

In the second step the objective function is calculated as the sum of the purchases and sale of products and utilities. The calculation is the one described in equation (2.13).

Step three consists in the collection of the gradients, using the single period outputs and the xml data.

The outputs of the process are the value of the objective function and a vector of gradients, which are needed by the solver to perform the optimisation.

2.1.2.3.2 Inventory level

The aim of this function is to calculate the inventory levels, as required by the solver.

Inputs u
 class MPO_info

Step 1

```
u_plant, u_market <- split inputs(u)
u_plant_operation <- stack(u_plant, MPO_info.u_disturbances)
for w in workers do:
    y_wi = f(u_plant_operation_wi)
```

Step 2

```
prod_plant, constr_plant = f(y, MPO_info.no_utilities, MPO_info.no_products)
grad_prod_plant, grad_constr_plant = f(y, MPO_info.no_utilities, MPO_info.no_products,
                                       MPO_info.no_decisionvariables)
```

Step 3

```
I = np.zeros((MPO_info.no_periods, MPO_info.no_products))
I[0, :] = MPO_info.products.inventory.initial
        + MPO_info.periods.duration[0]*prod_plant[0, :]
        - u_market[0, 0:MPO_info.no_products]
        + u_market[0, MPO_info.no_products:2*MPO_info.no_products]
```

Step 4

```
for i in range(1, MPO_info.no_periods):
    I[i, :] = I[i-1, :] + MPO_info.periods.duration[i]*prod_plant[i, :]
                - u_market[i, 0:MPO_info.no_products]
                + u_market[i, MPO_info.no_products:2*MPO_info.no_products]
```

Step 5

```
grad = f(grad_prod_plant, grad_constr_plant, MPO_info.no_constraints)
      =  $\begin{pmatrix} \text{plant constraints from plant decisions} & 0 \\ \text{inventory constraints from plant decisions} & \text{inventory from market decisions} \end{pmatrix}$ 
```

Outputs I
 Grad

The process can be divided into five steps. As for the objective function, the inputs of the process are the single period inputs and the xml data, and the first step is identical.

During the second step the variables are reassigned in different vectors.

The calculation of the inventory starts during the third step, when the inventory at the end of the first period is calculated considering the initial inventory levels, the sales and the purchases.

The calculation of the inventory levels during the following periods is calculated during the fourth step, using Equation (2.9).

Finally, during the fifth step the gradients are collected in a matrix.

The outputs of the process are the inventory levels for each products at the end of each period with the respective gradient. These values are passed to the solver in order to perform the optimisation.

Some examples of multiperiod problem with inventories were solved using both the structure described in Figure 2.1 and the prototype structure. The results obtained are described in §Chapter 3.

2.2 Strategic planning Multiperiod Problems

After solving the multiperiod problem with inventories, it has been decided to extend the procedure to strategic planning.

Unlike the previous case, the topic was new for the company. For this reason, the aim was to set up some examples using only gProms, in order to determine a common structure for the strategic planning problems which could be implemented in the future using the prototype structure.

Since the strategic planning multiperiod problem resembles the multiperiod problem with inventories, the resolution structure used is similar. The next paragraphs explains the differences between the two problems, focusing on the general resolution structure and on the xml file.

2.2.1 Resolution structure

The introduction of the strategic planning changes the structure of the multiperiod problem as shown in Figure 2.8.

The main changes are the addition of binary variables, which require a Mixed Integer Non Linear Programming solver, and the change of the objective function, which is formulated in terms of Net Present Value.

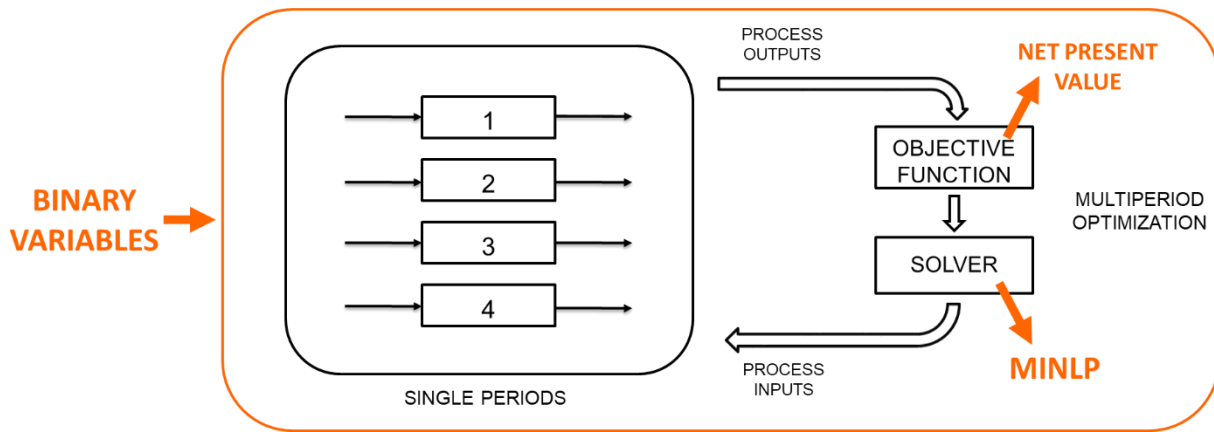


Figure 2.8. Resolution scheme for strategic planning problems.

The scheme differs from the one used for multiperiod problems with inventory levels for three main reasons: there is the introduction of binary variables in the models, the solver changes into a Mixed Integer Non Linear Programming (MINLP) one and the objective function requires the calculation of the Net Present Value.

These new features will be explained in the following paragraphs.

2.2.1.1 Solver

The introduction of the strategic planning into the multiperiod problem transform it into a Mixed Integer Non Linear Programming model. In fact, since this resolution structure is general, the original single period model can be non-linear, while the connections between the single periods are given by the binary variables.

For this reason it is necessary to change the solver, and to use a techniques able to tackle MINLP problems.

It is possible to formulate the model as

$$\min_{x,y} f(x,y) \quad \text{with } x \in X, y \in 0,1. \quad (2.29)$$

In this case x represents the continuous variables and y the binary ones.

The problem is subject to equality and inequality constraints, as shown below.

$$c(x,y) = 0 \quad (2.30)$$

$$d(x,y) \leq 0 \quad (2.31)$$

As seen in the Literature Review section, one of the most common method to solve this type of problems is the Branch and Bound Method (BB).

This resolution method assumes that an algorithm able to solve the Non Linear Problem exists and generalizes its application to the MINLP problem.

The first step of the BB Method is to find a solution for the continuous problem. If the solution is integral, it is a solution to the complete problem. If it is non-integral, one of the integer

variables has to be non-integral. This variable, which is denoted with b , is divided into an integral and a fractional part, as shown below.

$$b = [b] + b^* \tag{2.32}$$

where $[b]$ is an integer and $b^* \in]0,1[$.

In a step called “branching”, the problem is then divided into two subproblems, which are formed adding the following constraints.

$$b \leq [b] \tag{2.33}$$

$$b \geq [b] + 1 \tag{2.34}$$

Each of the two subproblems are solved as a continuous problem, and the branching procedure is applied again. The logical structure of this method is that of a tree, where the optimal solution for each subproblem is stored into a node, as shown in the picture.

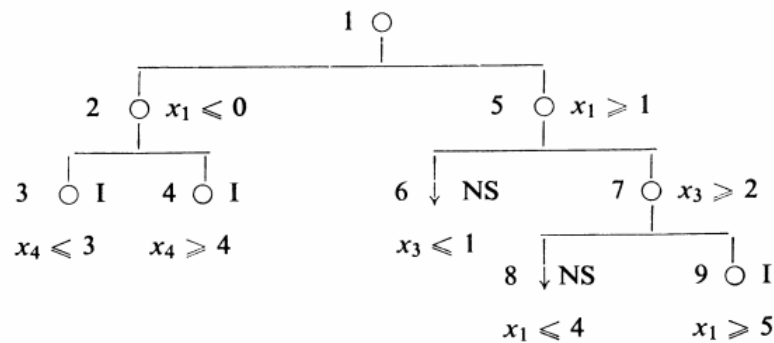


Figure 2.9. Logical structure of the BB method.
Image form Dakin (1965).

The tree may terminate if an integer solution I is found or if the set of constraints has no solution (NS). In this last case, the branch is not followed anymore.

It is possible to eliminate nodes if a feasible solution is found. Every time that the objective function value is lower than a previous one, it is used as an upper bound to restrict the search.

The search stops when all the nodes are examined and the solution to the complete problem is the lower integer solution which was reached.

2.2.1.2 Net Present Value

Strategic planning problems usually cover a time horizon wider than the one used for the multiperiod problems with inventory levels. For this reason it is necessary to take into account the variation is the value of money.

In order to do so, the Net Present Value, an index that calculates the value of money in the future taking into account uncertainty, is used. The objective function of the optimisation is reformulated as

$$\max \sum_{t=1}^T \frac{P_t}{(1+r)^{t-1}} \quad (2.35)$$

where r is the discount rate and $t \in [1, T]$ is the index of the period.

Using this index means that money has more value in the present moment, so the optimisation will try to postpone the payments and anticipate the selling of the products.

2.2.1.3 Binary variables

In order to implement the strategic planning decisions into the problem, it is necessary to include binary variables in the process. These variables can tell if a part of the plant or of the supply chain exists in a certain period or if a contract is valid.

In this work it was decided to take into account three types of strategic planning decisions: the signing of a contract, the revamping of a plant and the building of a new plant.

A general model for each one of this problems was formulated, and it is discussed in the following paragraphs. These formulations were then applied to some plants, as described in §Chapter 4, in order to test them.

2.2.1.3.1 Contracts

As seen in the literature review, there are many types of contracts which can be considered in strategic planning. For this work, only a very simple case had been modelled.

It is assumed that a contract is signed to provide or purchase a minimum amount of product S at a price w . The optimisation has to decide if and when to sign a contract. Once the contract is signed, it lasts for a determined number of years n .

To model this situation, it is necessary to introduce two binary variables: the decision variable y_t , which defines if the contract is signed in period t , and the variable z_t , which define if the contract is valid in period t .

$$y_t = \begin{cases} 1 & \text{if in year } t \text{ the contract is signed} \\ 0 & \text{otherwise} \end{cases} \quad (2.36)$$

$$z_t = \begin{cases} 1 & \text{if in year } t \text{ contract is valid} \\ 0 & \text{otherwise} \end{cases} \quad (2.37)$$

The contract is signed only in one period, but then it is valid for a certain number of years. For this reason the equation which links the two binary variables is the following one.

$$z_t = \sum_{i=0}^{n-1} y_{t-i} \quad (2.38)$$

It is assumed that it is possible to negotiate the value of S within certain boundaries, which are expressed by the following constraint.

$$S_{min} \leq S \leq S_{max} \quad (2.39)$$

The signing of the contract may influence other parts of the model, such as the mass balance and the profit calculation. In particular, if the amount to be provided by contract is produced as an addition to the normal production, the overall mass balance of a single period assumes the following form.

$$in = out + S z_t \quad (2.40)$$

With this formulation the additional production is added only in the periods when the contract is valid.

The profit P calculation is changed in a similar way, as shown in the following equation.

$$P_t = \dots + (Sw)z_t \quad (2.41)$$

If the contract is signed during period p , there is an additional source of income derived by the contract, which has to be added to the profit.

2.2.1.3.2 Revamping

This class includes all the possible modifications that it is possible to apply on a plant or on a piece of equipment. For example, it is possible to increase the overall capacity of a plant during its life, or just to change a faulty heat exchanger, or to modify a distillation column.

All of these possible changes are represented in the model as a variable d , which can be the area of the heat exchanger, the diameter of a pipe, the volume of a reactor etc.

As in the previous case, it is necessary to introduce a binary variable to express if the revamping happens in the period of time t . In particular, the variable is defined as below.

$$y_t = \begin{cases} 1 & \text{if in year } t \text{ the revamping is performed} \\ 0 & \text{otherwise} \end{cases} \quad (2.42)$$

where y_t is a decision variable controlled by the solver.

The decision influences the plant operation through the following equation.

$$d_t = d_{t-1} + y_t \Delta d \quad (2.43)$$

The meaning of this equation is that during period t the variable d will change only if the revamping is performed.

It is reasonable to assume that the revamping of a particular piece of equipment or plant will happen only one time during the time horizon. For this reason the following constraint is used.

$$\sum_{t=t_{min}}^{t_{max}} y_t \leq 1 \quad (2.44)$$

where t_{min} and t_{max} delimitate the time periods when the revamping can be performed.

The revamping will improve the performance of the plant, but it required additional costs to be paid. The cost C of the revamping is subtracted to the profit of the period when it is performed.

$$P_t = \dots - y_t C, \quad (2.45)$$

The cost calculation is assumed to be modelled through the following equation.

$$C = \text{fixed cost} + \text{variable cost} * \text{variation} \quad (2.46)$$

The cost of the revamping can be divided into a fixed part and a variable part. The variable cost is linearly dependent from the magnitude of the change, which has an upper and a lower limit. For example, a heat exchanger with a big exchange area would be more expensive than one with a small area.

2.2.1.3.3 New plant

A common decision which has to be taken in supply chain problems is the expansion of the network of plants through the building of a new one.

To add this feature to the model, two new variables are defined.

$$y_t = \begin{cases} 1 & \text{if in year } t \text{ the plant is built} \\ 0 & \text{otherwise} \end{cases} \quad (2.47)$$

$$z_t = \begin{cases} 1 & \text{if in year } t \text{ the plant exists} \\ 0 & \text{otherwise} \end{cases} \quad (2.48)$$

The two variables are linked through the following equation.

$$z_t = z_{t-1} + y_t \quad (2.49)$$

This equation assures the continuity between the periods, stating that a plant exists for all the periods after its construction.

Usually, the construction of a plant takes some years, and this is reflected in the model. To simplify the notation, a specific example has been taken into account.

If the plant requires three years to be built, the equation should be modified, so that the plant will be active after some periods.

$$z_t = z_{t-1} + y_{t-3} \quad (2.50)$$

Since the construction takes more than one period, the costs should be distributed in the three periods that are required to complete the plant. Assuming that 10% of the costs will be paid during the first year, 40% during the second and 50% during the third year, the profit during period k is calculated as following.

$$P_t = \dots - (0.1y_t + 0.4y_{t-1} + 0.5y_{t-2}) C \quad (2.51)$$

As seen for the revamping section, the cost calculation is performed using the following equation.

$$\text{cost} = \text{fixed cost} + \sum_i \text{variable cost}_i * \text{variation}_i \quad (2.52)$$

It is assumed that the cost is divided into a fixed and a variable part. The variable part is proportional to the magnitude of the key variables. For example, a plant with a big capacity will be more expensive than one with a smaller capacity.

2.2.1.4 XML file

The strategic planning problems are solved using exclusively gProms, since the MINLP solver is not available yet as an external C++ code. Nevertheless, some considerations were done about a possible future implementation, with the purpose of finding a simple common structure.

The easiest way to describe this structure is to prepare an xml file. In fact this format gives a good understanding of the type of problems that would be tackled by the optimisation and is the most user-friendly part.

In order to pass the new data to the solver, the code is modified as shown below.

```
<?xml version="1.0" encoding="UTF-8"?>
<test:MPOProblem name="Simple template example">
  <Units...>
  <Periods...>
  <ExternalMaterials...>
  <Operation...>
  <Contracts...>
  <Revamping...>
  <NewPlants...>
  <Availability...>
  <Model...>
</test:MPOProblem>
```

Four new sections are added:

- Contract
- Revamping
- New Plants
- Availability

This new sections are explained in the following paragraphs, using some fictitious data as examples.

2.2.1.4.1 Contracts

In this section all the variables related to the possibility to sign a contract are listed.

```
<Contracts>
  <Contract Name = "First contract">
    <TimeHorizon>
      <Beginning EarliestStart = "1" LatestStart = "3"/>
      <Duration MinLength = "1" MaxLength = "2"/>
      <Ending EarliestEnd = "2" LatestEnd = "5" />
    </TimeHorizon>
    <Sales ProductName="Zone 1 product" Price="0.0004" MinAmount="50" MaxAmount="500"
InitialGuess="100"/>
  </Contract>
</Contracts>
```

It is assumed that multiple contracts could be signed, each one valid for a different time period and for different products. The different contract are distinguished through their names.

The first section of this xml is related to the time horizon which can be considered for the contract. It is assumed that it is possible to negotiate the beginning, the ending and the length of the period when the contract will be valid.

The second section is related to the sales which are ruled by the contract. It is possible to sign the contract for some of the products or for all of them. The products are defined by their name, by the price and by the amount to be sold. It is assumed that the customer would fix the price and that the amount to be sold can be negotiated between an upper and a lower bound.

2.2.1.4.2 Revamping

This section contains the data related to the possible revamping of a plant. It is assumed that the revamping can be performed to change any characteristic of a plant or of an unit, for example the maximum capacity of a plant, the diameter of a column, the area of a heat exchanger etc.

```
<Revamping>
  <Expansion Name = "Plant capacity" PathName = "example" FixedCost="0.15" MinVariation =
"90" MaxVariation = "110" VariableCost="0.001" >
    <TimeHorizon>
      <Beginning EarliestStart = "1" LatestStart = "2"/>
      <Duration Length = "2" />
    </TimeHorizon>
  </Expansion>
</Revamping>
```

The first section defines the variable which should be changed by a name, a gProms reference and the cost of the revamping. The cost calculation is assumed to be modelled through Equation 2.46. The cost can be divided into a fixed part and a variable part. The variable cost is linearly dependent from the magnitude of the change, which has an upper and a lower limit. For example, a heat exchanger with a big exchange area would be more expensive than one with a small area.

The last data inserted in this section are related to the time horizon. It is assumed that the time required to perform the revamping is fixed and that it is possible to decide the beginning of the operation within a certain time frame.

2.2.1.4.3 New plants

This section is related to the possibility of building a new plant. It is assumed that any number of investments can be taken into account, each characterized by a cost, a time horizon and some key variables.

```
<NewPlants>
  <NewPlant Name="GP3" PathName="example" FixedCost="0.15" >
    <TimeHorizon>
      <Beginning EarliestStart = "1" LatestStart = "2" ConstructionTime = "3"/>
    </TimeHorizon>
    <DecisionVariable name="Capacity" PathName="example" MinValue="1000" MaxValue="1200"
VariableCost="0.002"/>
  </NewPlant>
</NewPlants>
```

The first section defines the new plant through a name, a gProms reference and the fixed cost of the investment.

The second section is related to the time horizon of the construction. The time needed to build the plant in this case is fixed, but it is possible to decide when to start to build it within certain bounds.

The last section gives the information about the decision variables and the cost. It is assumed that it is possible to define some characteristic of the plant, for example the capacity, within certain bounds. This decisions are then reflected in the cost calculation, as seen in Equation 2.52. It is assumed that the cost is divided into a fixed and a variable part. The variable part is proportional to the magnitude of the decision variables. For example, a plant with a big capacity will be more expensive than one with a smaller capacity.

It is assumed that in the new plant it is possible to decide the magnitude of any number of decision variables within determined bounds.

2.2.1.4.4 Availability

This section contains the information related to the availability of certain units during the time horizon taken into account by the optimisation. For example, it is possible that a plant is already in construction, but that it will be available only after some years since the beginning of the optimisation. It is also possible that one of the units is meant to be dismantled after a certain period of time.

```
<Availability>  
  <Unit name="Splitter 8" PathName = "example" />  
  <AvailabilityTime StartTime = "2" FinishTime = "4" />  
</Availability>
```

These type of considerations have an impact on the optimisation, so it is possible to insert here the data related to the availability of any unit or plant during the time horizon.

As written previously, it was only possible to solve the strategic planning problems using gProms, as in Figure 2.1. The examples had the purpose of test the models and to define a general structure for the problem, which was explained in the xml file. The examples used are reported in §Chapter 3.

Chapter 3

Multiperiod problem with inventories

This chapter reports all the examples related to the multiperiod problem with inventories. The purpose is to apply the general problem structure to specific examples to test the prototype structure.

First, the optimisation is applied to a simple case of blending, which is later expanded. The second example is a network of interconnected plants. These problems are solved using gProms and the python prototype structure.

Finally, the multiperiod optimisation is performed for a plant for Ethylene production and solved using gProms.

3.1 Blending problem

The first example of multiperiod optimisation was performed on a very simple problem, in order to find easily any mistakes in the prototype structure. It was necessary to check if the results reached were reasonable and if the prototype structure reacted in a reasonable way. This problem was also used to prove the economic advantage of using a multiperiod optimisation. In addition, it was necessary to check if the results reached with the prototype structure were the same as the ones reached using only gProms.

The next paragraphs show how the problem was formulated, the results obtained for single periods and multiple periods, the comparison between a normal optimisation and a multiperiod one and finally an extension of the problem.

All the examples were solved assuming that during the single periods the plant operates in steady state. This assumption is not mandatory for the solution of a multiperiod problem, but it allows to simplify the problem.

3.1.1 Problem formulation

A single blending process is considered. It is required to produce a stream of product of a determined composition by blending some streams of raw materials. It is possible to purchase three different raw materials, with different compositions and prices.



Figure 3.1. Schematic description of the blending problem

The data relative to the raw materials composition are written in Table 3.1. It is assumed that the streams contain three different components, indicated with the letters A, B and C.

Table 3.1. Inlet streams composition

| Stream | Composition in mass fractions | | |
|--------|-------------------------------|------|-----|
| | A | B | C |
| S1 | 0.1 | 0.6 | 0.3 |
| S2 | 0.99 | 0.01 | 0 |
| S3 | 0 | 0 | 1 |

The product composition requirements are the following

- $w_A \geq 90\%$ weight
- $w_B \leq 5\%$ weight

where w_j indicates the mass fraction of the component j in the final product.

It is worth noticing that in order to satisfy the first constraint, it would be necessary to use a large amount of S2.

It is assumed that the capacity of the mixer allows a maximum flowrate of 100 kg/s.

The optimisation has to calculate the optimal inlet flowrates, which have to respect the constraints and to give the maximum possible profit. The problem is solved first for a single period of time, then extended to a 4 period optimisation.

3.1.2 Single period of time

In order to perform the optimisation, it is necessary to associate a price to each streams, so to give a selection criterion to the solver. The prices of the streams are shown Table 3.2.

Table 3.2. Inlet and outlet stream prices.

| Stream | | S1 | S2 | S3 | S4 |
|-------------|-------|----|----|----|----|
| Price/Value | \$/kg | 5 | 65 | 8 | 70 |

In particular the table shows how S2 is the most expensive.

The flowrates and compositions of the streams are calculated using the following mass balance equations.

$$\dot{m}_{S4} = \dot{m}_{S1} + \dot{m}_{S2} + \dot{m}_{S3} \quad (3.1)$$

$$\dot{m}_{S4}w_{S4,j} = \dot{m}_{S1}w_{S1,j} + \dot{m}_{S2}w_{S2,j} + \dot{m}_{S3}w_{S3,j} \quad \text{with } j = A, B, C \quad (3.2)$$

where \dot{m}_i is the mass flowrate in kg/s of the stream i and $w_{i,j}$ is the mass fraction of the component j in the stream i .

The objective function is the profit, which is calculated using the following equations.

$$\text{total cost} = \dot{m}_{S1}p_{S1} + \dot{m}_{S2}p_{S2} + \dot{m}_{S3}p_{S3} \quad (3.3)$$

$$\text{revenue} = \dot{m}_{S4}p_{S4} \quad (3.4)$$

$$\text{profit} = \text{revenue} - \text{total cost} \quad (3.5)$$

where p_i is the price in \$/kg of the stream i and the profit, the cost and the revenue are expressed in \$/s.

The profit is maximised respecting the constraints to find the optimal values of the flowrates.

$$\max(\text{profit}) \quad (3.6)$$

The results of the optimisation are shown in Table 3.3.

Table 3.3. Optimisation results in terms of flowrates and compositions.

| Flowrate | | | | |
|-------------|---------------|-------|------|------|
| | S1 | S2 | S3 | S4 |
| kg/s | 6.83 | 90.22 | 2.95 | 100 |
| Composition | | | | |
| | | A | B | C |
| S4 | mass fraction | 0.90 | 0.05 | 0.05 |

The optimal outlet flowrate is the one that allows the plant to work at maximum capacity, with an outlet flowrate of 100 kg/s. Since the stream S2 is the more expensive, the optimal flowrate of S2 is the minimum allowed by the composition constraint, while the other two cheaper streams are used to reach the maximum total flowrate. It is not possible to use only S1, the cheapest stream, because otherwise the concentration of B would surpass the upper bound. These results are reasonable, so the single periods were linked to form the multiperiod problem.

3.1.3 Multiperiod optimisation

The problem is extended to include multiple periods, in order to take into account different costs and prices of the streams.

Four periods of different lengths are modelled, each one with different prices. The data are collected in Table 3.4.

Table 3.4. Multiperiod problem data.
Prices and length of the periods.

| Period | | | 1 | 2 | 3 | 4 |
|--------|-------|----|----|----|----|----|
| Cost | \$/kg | S1 | 3 | 6 | 5 | 4 |
| | \$/kg | S2 | 60 | 65 | 63 | 62 |
| | \$/kg | S3 | 8 | 7 | 10 | 70 |
| Value | \$/kg | S4 | 65 | 72 | 72 | 70 |
| Length | day | | 1 | 2 | 1 | 3 |

The prices are chosen so that stream S2 is the most expensive during the first three periods, while during the fourth period S3 is the most expensive one. It is expected that the solver takes into account this difference.

The length of the periods is different. This characteristic should not affect the optimisation, but it is assumed that the product can be stored and sold in successive periods. The amount of product stored at the end of the period t is indicated by the symbol $INV_{S4,t}$ and is expressed in kilograms. The only additional constraint is $INV_{S4,t} \geq 0$, meaning that it is not possible to sell more than the production.

The different periods are linked together through the equation for the inventory level.

$$INV_{S4,t} = INV_{S4,t-1} + production_{S4,t} - sales_{S4,t} \quad (3.7)$$

The meaning is that the amount of product stored is equal to the amount stored at the beginning of the period increased of the quantity produced and decreased of the amount that is sold.

It is assumed that nothing is stored at the beginning of the first period.

The equations used to calculate the costs and the revenues for the single periods are modified to take the period length into account. A difference from the single period optimisation is that not all the product is sold, so the revenues are calculated only considering the sales.

$$cost_{i,t} = \dot{m}_{i,t} p_{i,t} d_t \quad (3.8)$$

$$total\ cost_t = \sum_i cost_{i,t} \quad (3.9)$$

$$production_t = \dot{m}_{S_4,t} d_t \quad (3.10)$$

$$revenues_t = sales_t p_{i,t} \quad (3.11)$$

$$profit_t = revenues_t - total\ cost_t \quad (3.12)$$

Where d_t indicates the length of the period t in seconds. All the variables are relative to the period t .

The objective function is calculated as the sum of the single period profits.

$$total\ profit = profit_1 + profit_2 + profit_3 + profit_4 \quad (3.13)$$

$$\max(total\ profit) \quad (3.14)$$

The aim of the optimization is to find the optimal flowrates and to establish the amount of product to sell for each single period, taking into account the price variations of Table 3.4. The results are shown in Table 3.5 and Table 3.6.

Table 3.5. Results of the multiperiod optimisation.
Composition of the outlet stream.

| Mass fraction of S4 | | | |
|---------------------|------|------|------|
| Period | A | B | C |
| 1 | 0.90 | 0.05 | 0.05 |
| 2 | 0.90 | 0.05 | 0.05 |
| 3 | 0.90 | 0.05 | 0.05 |
| 4 | 0.93 | 0.05 | 0.02 |

Table 3.5 shows that there is a difference between the product obtained during the first three periods and the product obtained during the last period. The product respects the quality constraints, so the result is reasonable.

Table 3.6. Results of the multiperiod optimisation.
Flowrates, sales, inventory and profit.

| Results | | | | | | |
|--------------------|----|---------------------|-------|-------|-------|-------|
| Period | | | 1 | 2 | 3 | 4 |
| Flowrate | S1 | kg/s | 6.83 | 6.83 | 6.83 | 6.78 |
| | S2 | kg/s | 90.22 | 90.22 | 90.22 | 93.22 |
| | S3 | kg/s | 2.95 | 2.95 | 2.95 | 0 |
| sold _{s4} | | kg*10 ⁻³ | 0 | 3.47 | 1.16 | 3.47 |
| INV _{s4} | | kg*10 ⁻³ | 1.16 | 0 | 0 | 0 |
| Profit | | \$ | -5457 | 9748 | 1453 | 3580 |
| Total profit | | \$ | 9323 | | | |

In Table 3.6 it is possible to read the different flowrates chosen by the solver during the different periods. Since during the first three periods the prices of the raw materials are not changing significantly, the optimal mass flowrates are the same for each period. During the last period, the S3 price is very high, so the optimisation results suggest not to use it, and a higher amount of stream S1 and S2 is purchased in order to keep the production at the maximum capacity. These results explain the change in compositions which was seen in Table 3.5.

The price of the product is the highest during the second and the third period, so the production of the first period is stored to be sold later. There are not any constraints to keep a minimum inventory at the end of the time span considered, so in the end everything is sold to obtain the highest possible profit.

The profit calculation and the sales are both affected by the length of the periods, as expected. All the results obtained are reasonable, which means that the prototype structure is working.

3.1.4 Comparison between single period and multiperiod optimisation

A multiperiod optimisation has a higher computational cost than a single period one. In order to show its advantages, an additional optimisation has been performed on the blending problem. The data of the problem are the same used for the multiperiod optimisation and are shown in Table 3.4. The difference is that the single periods are solved independently.

The results are shown in Table 3.7 and Table 3.8.

Table 3.7. Results of a single period optimisation.
Composition of the outlet stream.

| Mass fraction of S4 | | | |
|---------------------|------|------|------|
| Period | A | B | C |
| 1 | 0.90 | 0.05 | 0.05 |
| 2 | 0.90 | 0.05 | 0.05 |
| 3 | 0.90 | 0.05 | 0.05 |
| 4 | 0.93 | 0.05 | 0.02 |

Table 3.8 shows the composition of the final product, which is identical to the result obtained by the multiperiod optimisation (Table 3.5). The increase of the computational cost is not justified by this data.

Table 3.8. Results of the single period optimisation.
Flowrates, sales, inventory and profit.

| Results | | | | | | |
|--------------------|----|---------------------|-------|-------|-------|-------|
| Period | | | 1 | 2 | 3 | 4 |
| Flowrate | S1 | kg/s | 6.83 | 6.83 | 6.83 | 6.78 |
| | S2 | kg/s | 90.22 | 90.22 | 90.22 | 93.22 |
| | S3 | kg/s | 2.95 | 2.95 | 2.95 | 0 |
| sold _{s4} | | kg*10 ⁻³ | 1.16 | 2.31 | 1.16 | 3.47 |
| INV _{s4} | | kg*10 ⁻³ | 0 | 0 | 0 | 0 |
| Profit | | \$ | 1043 | 2548 | 1453 | 3580 |
| Total profit | | \$ | 8623 | | | |

Table 3.8 shows that the selling schedule obtained solving the period independently is different (the multiperiod problem results are reported in Table 3.6). In Table 3.8 the inventory level at the end of the period is always zero. In fact, even if it is possible to store the product, this operation results in a loss in profit for the single period because there are less revenues. Instead if the global profit is considered, storing the products in a period when the prices are lower and selling it when the prices are higher results in higher revenues. Performing a multiperiod optimisation it is possible to take into account fluctuation in the price of the product and of the raw materials, and consequently to obtain better results. For this reason the profit

obtained solving the four periods of time independently is 8623 \$, against the 9323 \$ obtained performing a multiperiod optimisation.

These results confirms that a multiperiod optimisation can be more performing than a single period one.

3.1.5 Extension of the problem



Figure 3.2. Schematic representation of the extended blending problem

In order to make the blending problem more realistic, it was extended to multiple products and the possible inlet streams were increased to four. The constraints for the mass composition of the products are the following.

- $w_{A,P1} \geq 90\%$ weight
- $w_{B,P1} \leq 5\%$ weight
- $w_{B,P2} \geq 70\%$ weight

The maximum capacity of the plant is 100 kg/s for P1 and 25 kg/s for P2.

In addition, lower and upper constraints for the inventory were considered.

$$5 \leq INV_{P1,t}, INV_{P2,t} \leq 100 \quad \forall t \quad (3.15)$$

The lower constraint assures that it is possible to compensate for accidental events such as a delay in the production, a shortage a raw materials or an increase in the demand. The upper constraints represents the maximum capacity of the warehouse. It is important to check if the solver reacts properly to these new constraints, since they are common in these types of problem.

The multiperiod optimisation is performed considering four periods of time, as in the previous case. The data related to prices, duration and composition of the inlet streams are shown in Table 3.9 and Table 3.10.

Table 3.9. Multiperiod problem data.
Stream compositions.

| Stream | Composition in mass fractions | | |
|--------|-------------------------------|------|-----|
| | A | B | C |
| S1 | 0.1 | 0.6 | 0.3 |
| S2 | 0.99 | 0.01 | 0 |
| S3 | 0 | 0 | 1 |
| S4 | 0.1 | 0.8 | 0.1 |

It is added an additional stream S4, which is rich in component B. It is expected that this stream will be used to produce P2.

Table 3.10. Multiperiod problem data.
Prices and periods length.

| Period | | | 1 | 2 | 3 | 4 |
|--------|-------|----|----|----|----|----|
| Cost | \$/kg | S1 | 3 | 6 | 5 | 4 |
| | \$/kg | S2 | 60 | 65 | 63 | 62 |
| | \$/kg | S3 | 8 | 7 | 10 | 8 |
| | \$/kg | S4 | 20 | 22 | 25 | 18 |
| Value | \$/kg | P1 | 65 | 73 | 72 | 70 |
| | \$/kg | P2 | 22 | 30 | 20 | 35 |
| Length | day | | 1 | 2 | 1 | 3 |

Table 3.10 shows that S3 is still the most expensive raw material, and that S4 is more expensive than both S1 and S3. For this reason it is expected that the solver would use S4 only if it is not possible to use S1 and S3. The value of products P2 is lower than the price of product P1. It is assumed that at the beginning of the first period an inventory is already present, as shown in Table 3.11.

Table 3.11. *Multiperiod problem data.*
Initial inventory.

| | | Initial inventory |
|----|---------------------|-------------------|
| P1 | kg*10 ⁻³ | 0.17 |
| P2 | kg*10 ⁻³ | 0.06 |

It is assumed that the initial amount of P2 is lower than the amount of P1.

The results of the optimisation are shown in Table 3.12, 3.13, 3.14, 3.15 and 3.16.

Table 3.12. *Multiperiod problem results.*
Product 1 composition.

| Mass fraction of P1 | | | |
|---------------------|------|------|------|
| Period | A | B | C |
| 1 | 0.90 | 0.05 | 0.05 |
| 2 | 0.90 | 0.05 | 0.05 |
| 3 | 0.90 | 0.05 | 0.05 |
| 4 | 0.90 | 0.05 | 0.05 |

Table 3.12 shows the final composition of P1. It can be noticed that the results are very similar to the ones obtained for the simple blending problem. The difference is that the composition is constant during all the periods, which is reasonable since the prices of the raw materials does not fluctuate much.

Table 3.13. *Multiperiod problem results.*
Raw materials for Product 1, selling schedule and inventory.

| P1 | | | | | | |
|----------|----|---------------------|-------|-------|-------|-------|
| Period | | | 1 | 2 | 3 | 4 |
| Flowrate | S1 | kg/s | 6.83 | 6.83 | 6.83 | 6.83 |
| | S2 | kg/s | 90.22 | 90.22 | 90.22 | 90.22 |
| | S3 | kg/s | 2.95 | 2.95 | 2.95 | 2.95 |
| | S4 | kg/s | 0 | 0 | 0 | 0 |
| Sold | | kg*10 ⁻³ | 0.17 | 3.41 | 1.16 | 3.47 |
| INV | | kg*10 ⁻³ | 1.16 | 0.06 | 0.06 | 0.06 |

Table 3.13 confirms that the same inlet flowrates are used during all the period, since it is the configuration more profitable. As expected, the stream S4 is not used to produce P1 because of the high cost.

Since the highest price for the product is reached in the second period, the product is stored until the maximum capacity is reached and the remaining is sold. During the second period all the product is sold, except for the minimum inventory required.

As in the previous case, the maximum capacity of the plant, 100 kg/s, is reached during every period.

Table 3.14. *Multiperiod problem results.
Product 2 composition.*

| Mass fraction of P2 | | | |
|---------------------|------|------|------|
| Period | A | B | C |
| 1 | 0.10 | 0.70 | 0.20 |
| 2 | 0.10 | 0.70 | 0.20 |
| 3 | 0.10 | 0.70 | 0.20 |
| 4 | 0.10 | 0.70 | 0.20 |

Table 3.14 shows that the composition of P2 is the same during all the periods, and that the constraints are respected.

Table 3.15. *Multiperiod problem results.
Raw materials for Product 2 selling schedule and inventory.*

| P2 | | | | | | |
|----------|----|---------------------|------|------|------|------|
| period | | | 1 | 2 | 3 | 4 |
| flowrate | S1 | kg/s | 12.5 | 0 | 0 | 12.5 |
| | S2 | kg/s | 12.5 | 0 | 0 | 12.5 |
| | S3 | kg/s | 12.5 | 0 | 0 | 12.5 |
| | S4 | kg/s | 12.5 | 0 | 0 | 12.5 |
| sold | | kg*10 ⁻³ | 0 | 0.06 | 0 | 1.97 |
| INV | | kg*10 ⁻³ | 0.35 | 0.87 | 1.16 | 0.06 |

Table 3.15 shows that since the prices fluctuations are low, the optimal flowrates are the same during all the periods. To produce P2 it is necessary to use S4, which contains a high percentage of the component B. S1 is used instead because of the low price.

The highest price for P2 is reached in the fourth period, so the maximum amount of product is stored during the previous periods. The warehouse capacity is not enough to store all the product, so part of it has to be sold previously. The product is sold during the second period because the prices is higher than during the first of the third period.

The plant works at the maximum capacity, 25 kg/s, for each period.

Table 3.16 shows the profit made during the single periods and the total profit.

Table 3.16. *Optimisation results in terms of profit.*

| Results | | | | | |
|--------------|----|-------|------|------|------|
| Period | | 1 | 2 | 3 | 4 |
| Profit | \$ | -4770 | 9133 | 1078 | 9191 |
| Total profit | \$ | 14632 | | | |

It is worth noticing that in order to maximise the total profit, there is a loss during the first period. This situation is typical of multiperiod optimisation.

The examples presented in this chapter were all solved both using gProms and the prototype resolution structure, and the same results were obtained.

The examples show that the results change as expected when there are inventory constraints and prices fluctuation. In addition, it was shown how using a multiperiod optimisation in place of multiple optimisations of the single periods allows to reach more profitable results.

3.2 Network of plants

After that the simple blending problem was solved using the prototype function, the method needed to be tested for a more complex model. For this reason it has been decided to solve the multiperiod problem for a network of interconnected plant.

As in the previous case, it is assumed that the plant works in steady state during each period.

3.2.1 Plant description

The flowsheet represents a network of interconnected plant. There are four different inlet flowrates that are distributed to four stabilizer plants and then fed to six plants which produce the final three products.

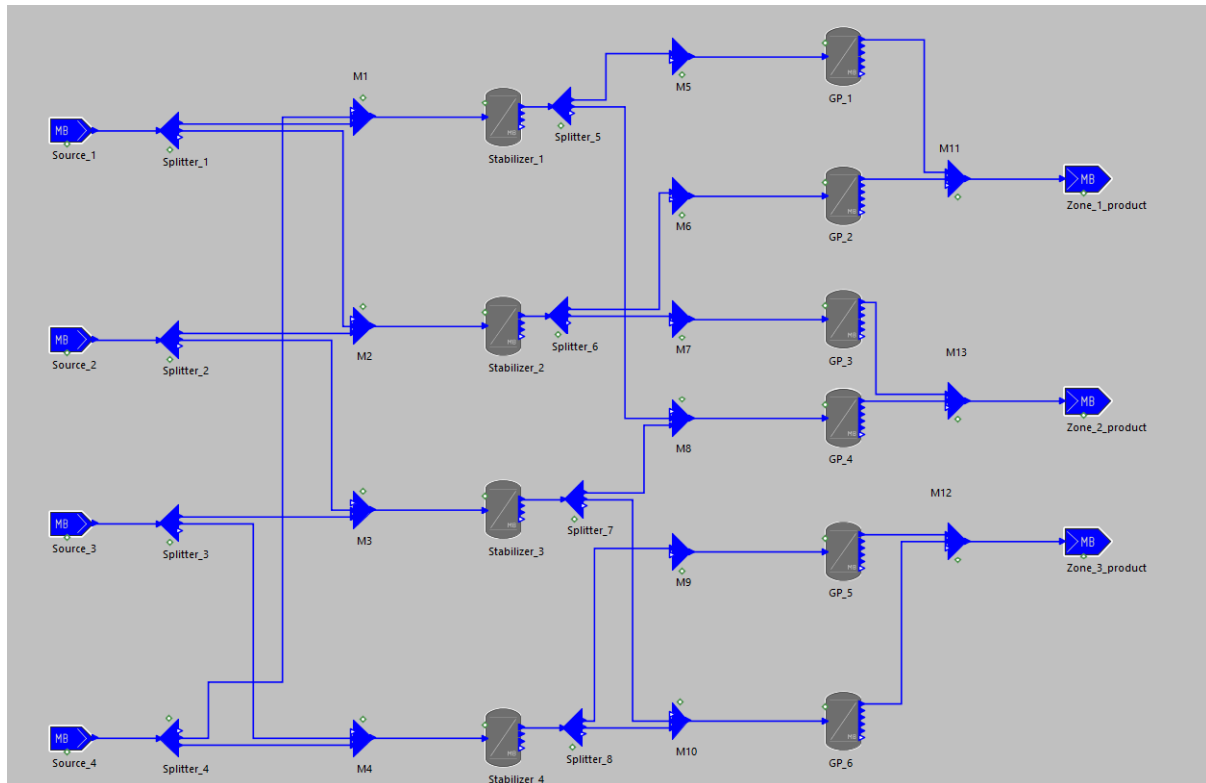


Figure 3.3. Network of plants flowsheet.

The network includes ten refineries, which can be divided into two different types of plants. The first treatment to the raw materials is given by the four stabilizers, which have a bigger capacity. The intermediate products are then sent towards the six gas plants, which are smaller refineries that produce the final products.

It is possible to decide the inlet flowrates to each refinery splitting the raw materials flowrates. The outlet of the superstructure are three products with different compositions.

The refineries are defined through a model to calculate the outlet flowrates and the operating costs. The composition of the products exiting a refinery is fixed, and is different for each plant. The three final products have different compositions.

The operating cost is calculated through the following equation.

$$\text{operating cost} = \alpha * \frac{\text{inlet flowrate}}{\text{maximum capacity}} \quad (3.16)$$

where α is a constant. The operating costs increases if the inlet flowrates increases. According to economies of scale, the intensive cost decreases if the capacity of the plant is bigger.

The flowrates passing through the plants are constrained by the plant maximum capacity, which is different for each refinery.

3.2.2 Single period problem

The first operation was to check the correct functioning of the model of the network of plants performing an optimisation on the single period.

The aim of the optimisation is to maximise the profit of the single period. This objective is reached changing the position of the splitters, so that the initial flowrates will be directed to the plants with less operating cost in order to produce the most profitable product. The final amount of each product is also controlled by the split position.

In particular, two cases with different products prices were solved.

It is assumed that the operating costs and the raw materials prices are unvaried.

3.2.2.1 Case 1

In the first case it is assumed that Product 1 is the less valuable, while Product 3 is the more profitable, as in Table 3.17.

Table 3.17. Prices of the products for Case 1.

| Product | Prices |
|---------|--------------------------|
| | \$/kg * 10 ⁻⁵ |
| 1 | 15 |
| 2 | 20 |
| 3 | 17 |

The optimisation finds the splitter positions, which defines the final product flowrates, as in Table 3.18.

Table 3.18. Optimisation results for Case 1.

| | |
|---------------------------|-------|
| Split 1 | 1 |
| Split 2 | 0 |
| Split 3 | 1 |
| Split 4 | 0.920 |
| Split 5 | 0 |
| Split 6 | 0.001 |
| Split 7 | 0.317 |
| Split 8 | 1 |
| Flowrate product 1 [kg/s] | 0 |
| Flowrate product 2 [kg/s] | 10.21 |
| Flowrate product 3 [kg/s] | 17.73 |

When the splitter assumes the value 0 or 1, it means that all the flowrates is sent to a determined part of plant. The values were reported in order to confront them with Table 3.19.

The most important data are the flowrates. Since the value of Product 2 and Product 3 are higher than the value of Product 1, Product 1 is not produced.

This decisions allows to have lower costs, since the operative costs of the plants are proportional to the flowrates passing through them.

3.2.2.2 Case 2

Since in Case 1 Product 1 was not produced, its value is now raised, and Product 1 results to be the most profitable product. It is expected that the solver would pick another splitter configurations as the most profitable one.

The prices are shown in Table 3.19.

Table 3.19. Prices of the products for Case 2.

| Product | Prices |
|---------|--------------------------|
| | $\$/\text{kg} * 10^{-5}$ |
| 1 | 20 |
| 2 | 15 |
| 3 | 17 |

The results of the optimisation are shown in Table 3.20.

Table 3.20. *Optimisation results for Case 2.*

| | |
|---------------------------|-------|
| Split 1 | 0.220 |
| Split 2 | 0.452 |
| Split 3 | 0.797 |
| Split 4 | 0.745 |
| Split 5 | 1 |
| Split 6 | 1 |
| Split 7 | 0 |
| Split 8 | 1 |
| Flowrate product 1 [kg/s] | 10.21 |
| Flowrate product 2 [kg/s] | 0 |
| Flowrate product 3 [kg/s] | 17.73 |

As expected, the splitter positions changes, and the part of the network producing Product 2 is deactivate. The raw materials that in Case 1 are used to produce Product 2 are in this case directed to produce Product 2.

These two simple cases show that the optimisation is able to change the position of the splitters in order to find the most profitable configurations. It is possible to procede to solve the multiperiod problem.

3.2.3 Multiperiod problem

In order to solve the multiperiod problem, some assumptions were needed.

It is assumed that the prices of the products are different during the different periods, while the operating costs of each plant and the raw material costs are constant. It is possible to deactivate parts of the network, and in that case the operating costs of the deactivated plants is zero. Deterministic prices are assumed.

The periods are linked together through the inventory levels, since it is possible to store the products. It is not possible to store the raw materials.

The inventory for the product j in the period t is defined as in the equation below.

$$Inventory_{t,j} = Inventory_{t-1,j} + Production_{t,j} - Sale_{t,j} \quad (3.17)$$

As in the blending problem, to calculate the inventory level at the end of a period of time it is necessary to consider the initial stored amount, the production and the sales.

The profit for the period t is calculated as in the expression below.

$$Profit_t = Revenues_t - Operating\ cost_t * Time_t - Raw\ material\ cost_t \quad (3.18)$$

The profit is calculated taking into account the revenues which derives from the product selling, the cost of the raw materials and the operating costs, which depends on which plant is used.

The objective function to be maximised is the total profit, calculated as the sum of the profits of the single periods.

$$Total\ Profit = \sum_t Profit_t \quad (3.19)$$

This model was applied to three cases, which are described in the next paragraphs. The aim was to check if the results obtained with different input data were reasonable, and if gProms and the prototype structure reached the same solution.

3.2.3.1 Case 1

As a first example, a three period simulation is taken into account. It is assumed that it is not necessary to buy the raw materials.

The prices of the products are written in Table 3.21.

Table 3.21. Prices of the products.

| Period | | 1 | 2 | 3 |
|-------------|--------------------------|----|----|----|
| Product 1 | \$/kg * 10 ⁻⁵ | 15 | 10 | 17 |
| Product 2 | \$/kg * 10 ⁻⁵ | 20 | 30 | 20 |
| Product 3 | \$/kg * 10 ⁻⁵ | 17 | 18 | 16 |
| Time length | h | 1 | 1 | 1 |

The table shows how the most profitable product is always Product 2.

It is also assumed that the operative costs change during the time horizon, as shown in table 3.22. In particular, the operative costs of each plant are calculated as a percentage of the costs of the first period.

In general, it is cheaper to operate the plant during the second period, while the third period is the most expensive.

Table 3.22. *Operative costs of the plants.*

| Period | 1 | 2 | 3 |
|--------------|--------|------|------|
| | % cost | | |
| Stabilizer 1 | 1 | 0.8 | 0.75 |
| Stabilizer 2 | 1 | 1.2 | 0.95 |
| Stabilizer 3 | 1 | 0.9 | 1.15 |
| Stabilizer 4 | 1 | 0.85 | 1.1 |
| Plant 1 | 1 | 0.8 | 1.1 |
| Plant 2 | 1 | 0.8 | 1.2 |
| Plant 3 | 1 | 0.9 | 1.05 |
| Plant 4 | 1 | 0.95 | 1.15 |
| Plant 5 | 1 | 0.85 | 1 |
| Plant 6 | 1 | 0.9 | 1.15 |

It is also assumed that there is an initial inventory level for each product, as in Table 3.23.

Table 3.23. *Initial inventory level.*

| | | Initial Inventory |
|-----------|----|-------------------|
| Product 1 | kg | 5 |
| Product 2 | kg | 5 |
| Product 3 | kg | 5 |

The results of the optimisation are written in Table 3.24.

Table 3.24. *Optimisation results.*

| Period | | 1 | 2 | 3 |
|----------------------|------|-------|---------|---------|
| Outlet Product 1 | kg/h | 0 | 0 | 0 |
| Outlet Product 2 | kg/h | 36759 | 36759 | 36759 |
| Outlet Product 3 | kg/h | 63817 | 63817 | 63817 |
| Inventory Product 1 | kg | 5 | 5 | 5 |
| Inventory Product 2 | kg | 200 | 5 | 5 |
| Inventory Product 3 | kg | 200 | 5 | 5 |
| Sales Product 1 | kg | 0 | 0 | 0 |
| Sales Product 2 | kg | 36564 | 36953.5 | 36758.5 |
| Sales Product 3 | kg | 63622 | 64012 | 63817 |
| Single period profit | \$ | 6.53 | 12.39 | 5.28 |
| Total profit | \$ | 24.21 | | |

The result shows that it is not profitable to produce Product 1, since the price is the lowest of the three. The flowrates are directed to the plant with the less operating costs and which produce the most profitable product. It is not possible to change the inlet flowrates.

Since the price of the products is higher during the second period, the maximum capacity of the warehouse is used during the first period and the products are sold during the first period.

In addition to the high price of the products, during the second period the operating costs of the plants are lower, so the resulting single period profit is the highest.

3.2.3.2 Case 2

After testing the model on three periods, another case were solved considering a 10 periods time horizon, which is more complex to solve. Differently from Case 1, the cost of the purchase of the raw materials are taken into account for the calculation.

The data for the multiperiod optimisation are written in Table 3.25, 3.26 and 3.27.

Table 3.25. Prices of the products and of the raw materials for Case 2.

| | Price | | | | | | | | | |
|----------------|--------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | \$/kg * 10 ⁻⁵ | | | | | | | | | |
| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| Product 1 | 15 | 10 | 16 | 20 | 18 | 19 | 20 | 15 | 19 | 20 |
| Product 2 | 20 | 30 | 25 | 25 | 21 | 26 | 27 | 22 | 25 | 27 |
| Product 3 | 17 | 20 | 18 | 19 | 17 | 17 | 18 | 19 | 18 | 19 |
| Raw material 1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| Raw material 2 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| Raw material 3 | 0.7 | 0.7 | 0.7 | 0.7 | 0.7 | 0.7 | 0.7 | 0.7 | 0.7 | 0.7 |
| Raw material 4 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 | 0.9 |
| Time length | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

Table 3.25 shows the prices of products and raw materials during the time horizon. Product 2 is the most profitable, while the cheaper raw material is Raw Material 1. The prices of the raw materials do not vary during the periods.

Table 3.26 shows how the operative costs of the plant change during the periods. In general, the second period is the cheapest and the third period is the most expensive, but it is assumed that the price fluctuation of each plant are different.

Table 3.26. Operative costs of the plants.

| Period | % cost | | | | | | | | | |
|--------------|--------|------|------|------|------|------|------|------|------|------|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| Stabilizer 1 | 1 | 0.8 | 0.75 | 0.6 | 0.9 | 0.6 | 0.7 | 0.8 | 0.75 | 0.8 |
| Stabilizer 2 | 1 | 1.2 | 0.95 | 1 | 1.3 | 1.15 | 0.85 | 0.95 | 1 | 1.2 |
| Stabilizer 3 | 1 | 0.9 | 1.15 | 0.95 | 0.95 | 1.1 | 1 | 0.95 | 1.2 | 0.8 |
| Stabilizer 4 | 1 | 0.85 | 1.1 | 0.95 | 1.2 | 1 | 0.9 | 1.1 | 0.8 | 1 |
| Gas plant 1 | 1 | 0.8 | 1.1 | 1.05 | 0.9 | 0.95 | 1 | 1.1 | 0.8 | 0.95 |
| Gas plant 2 | 1 | 0.8 | 1.2 | 1 | 1.2 | 1.1 | 1 | 0.9 | 0.8 | 0.85 |
| Gas plant 3 | 1 | 0.9 | 1.05 | 1.1 | 1.05 | 1 | 0.95 | 0.9 | 0.85 | 1 |
| Gas plant 4 | 1 | 0.95 | 1.15 | 1.1 | 0.95 | 0.8 | 1.2 | 0.85 | 1.1 | 0.9 |
| Gas plant 5 | 1 | 0.85 | 1 | 0.95 | 0 | 0.95 | 1.05 | 1 | 1.05 | 0.95 |
| Gas plant 6 | 1 | 0.9 | 1.15 | 0.75 | 0.8 | 0.9 | 1.2 | 0.8 | 0.75 | 1.2 |

As in the previous case, there is an initial inventory, which is written in Table 3.27.

Table 3.27. Initial inventory level.

| | | Initial Inventory |
|-----------|----|-------------------|
| Product 1 | kg | 5 |
| Product 2 | kg | 5 |
| Product 3 | kg | 5 |

The results of the optimisation are written in Table 3.28.

Table 3.28. Optimisation results.

| Period | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Sale Product 1 | kg | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Sale Product 2 | kg | 36564 | 36954 | 36759 | 36759 | 36564 | 36759 | 36954 | 36564 | 36759 | 36954 |
| Sale Product 3 | kg | 63622 | 64012 | 63622 | 64012 | 63719 | 63719 | 63817 | 64012 | 63622 | 64012 |
| Inventory Product 1 | kg | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| Inventory Product 2 | kg | 200 | 5 | 5 | 5 | 200 | 200 | 5 | 200 | 200 | 5 |
| Inventory Product 3 | kg | 200 | 5 | 200 | 5 | 102.5 | 200 | 200 | 5 | 200 | 5 |
| Flowrate Product 1 | kmol/h | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Flowrate Product 2 | kmol/h | 36759 | 36759 | 36759 | 36759 | 36759 | 36759 | 36759 | 36759 | 36759 | 36759 |
| Flowrate Product 3 | kmol/h | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 |
| Single Period Profit | \$ | 6.51 | 13.66 | 8,34 | 11.07 | 9.77 | 9.98 | 9.50 | 9.50 | 9.78 | 11.00 |
| Total Profit | \$ | 99.08 | | | | | | | | | |

As in the previous case, Product 1 is not produced, since it is the less valuable. The price fluctuations of the operative conditions and of the raw materials are not intense enough to change the optimal product flowrates, which is constant during the periods.

The products are correctly stored and sold when the price is higher. For example, the price of Product 3 is higher during the second period than during the first one. For this reason the product is stored at the maximum inventory capacity during the first period and sold as to reach the minimum inventory level during the second period.

This solutions are the ones which were expected.

3.2.3.2.1 Python and gProms results comparison

Case 2 was solved using both the prototype function and gProms.

The main difference between the two resolution structures is that the prototype function would allow to solve the single periods independently, which is an advantage. The gProms results are obtained using a resolution method which has been already tested, so if the two solutions are the same, it means that the python prototype structure is working correctly.

The average difference between the solutions is reported in Table 3.35.

Table 3.29. *Comparison between python and gProms results.*

| Max difference % | Min difference % | Average difference |
|------------------|------------------|--------------------|
| 0.00001 | -0.00008 | -0.00001 |

The order of the magnitude of the percentage differences between the results obtained from the two simulations is 10^{-5} , which can be attributed to the number of digits printed. For this reason the results obtained with the prototype model are considered equivalent to the gProms results.

The examples developed for the network of plant models shows that the prototype structure is able to solve problems of a moderate dimension and to reach reasonable results.

The confrontation between gProms and the prototype structure shows that the final solution is equivalent.

3.3 Ethylene plant

The final plant where the multiperiod optimisation has been applied is a cracking plant for ethylene production. The model is more complex than the ones described so far.

The purpose of the examples is to check if the prototype structure can handle problems of very big size and reach reasonable results.

The model provides a good example of a typical application of a multiperiod problem.

As in the previous case, it is assumed that the model works in steady state, but the operating conditions change during the periods.

3.3.1 Plant description

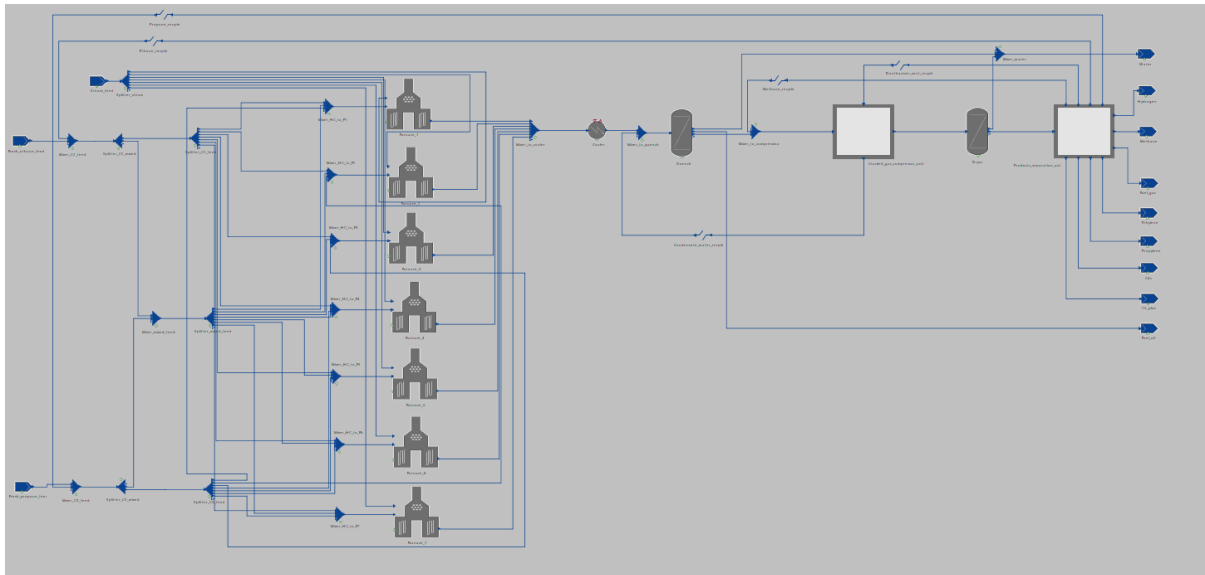


Figure 3.4. *Ethylene Plant Flowsheet.*

The plant is composed by a reaction section, a compression section and a separation section. The cracking process takes place in seven furnaces running in parallel. The raw materials are ethane and propane, which are fed to the furnaces with steam. The kinetic model used for the reaction is the one by Sundaram and Froment (1977). It is possible to perform a steady state of a dynamic simulation and to take into account the coking process with its consequences. The furnace model comprehends also the TLE model. In the following cases it is assumed that the plant is working in steady state.

The products exiting the furnaces are cooled and quenched, then they are sent to a five stage compression, which is shown in the following picture.

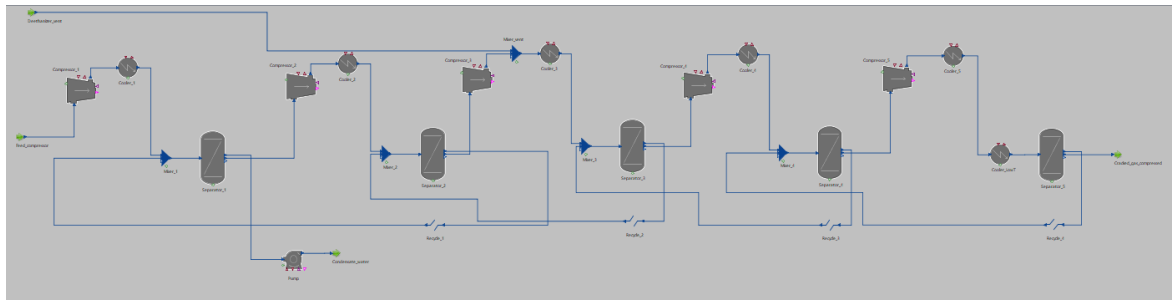


Figure 3.5. Compression Section Flowsheet.

After that, the gas are dried and sent to a separation section, which is simulated in the flowsheet using splitters, as shown in the flowsheet.

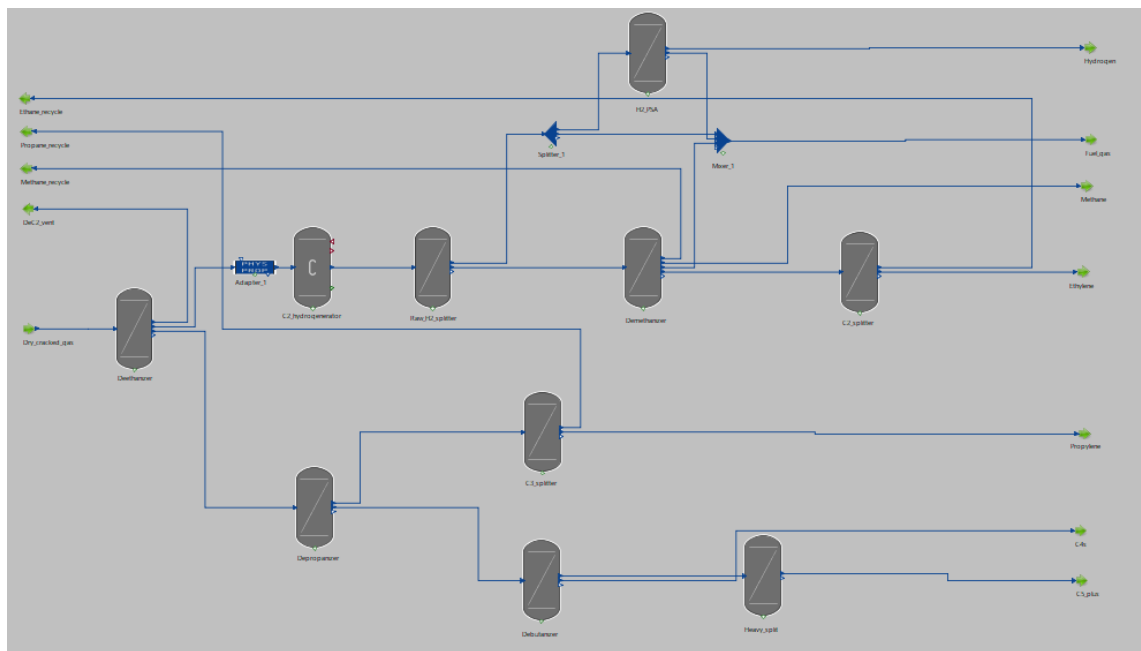


Figure 3.6. Separation Section Flowsheet.

In this last section the unreacted ethane and propane are separated and recycled to the furnaces. The final products are: Hydrogen, Methane, Ethylene, Propylene, the C4 fraction and the C5+ fraction. A mixture of Hydrogen and Methane is separated and used in the furnaces as fuel. A stream of Fuel Oil is also obtained from the quench.

3.3.2 Single period problem

In order to test the flowsheet, a single period optimisation was performed, with the aim of finding the optimal values of the conversion for each furnace. The objective function to be maximised is the profit, but since the model does not include any cost calculation, a simple equation is introduced.

$$\begin{aligned} \text{profit} = & \text{products value} - \text{raw materials cost} - \text{fuel cost} \\ & - \text{recycle cost} - \text{compression cost} \end{aligned} \quad (3.20)$$

The recycle cost depends directly on the recycled flowrates, while the compression cost depends on the volume of gas that exit the furnace and that have to be send to the separation section.

The profit depends on the final flowrates of the main products, ethylene and propylene, which are influenced by many factors. With a high conversion at the furnaces there is a high flowrate of products, but the selectivity is lower so the more valuable products are present in lower concentration. On the contrary, with a low conversion the selectivity is higher, but the costs for the recycle are also higher. The fuel cost is high both if the conversion is high, because higher temperatures are required, and if the conversion is low, because the volume of gas to heat up is larger. For this reason the optimal value is a trade-off between the need to obtain high selectivity and the cost of the recycle.

The prices assumed for raw materials and products are reported in Table 3.30.

Table 3.30. Prices of raw materials and products.

| Raw materials | Prices | Products | Prices |
|---------------|--------|----------------|--------|
| | \$/ton | | \$/ton |
| Propane | 500 | Hydrogen | 3510 |
| Ethane | 190 | Ethylene | 1382 |
| Fuel gas | 194 | Propylene | 1340 |
| | | C4 (Butadiene) | 1960 |
| | | C5+ (Benzene) | 1400 |
| | | Fuel gas | 194 |

The most profitable products are hydrogen and ethylene, which requires higher selectivity to be produced.

Additional data used to calculate the prices of recycle and compression are in Table 3.31.

Table 3.31. Other data related to operation.

| | |
|-----------------------------|------------|
| Electricity cost | 0.12 \$/kW |
| Energy required for recycle | 1 kW/ton |

An important variable for the building of the multiperiod problem is the coke thickness, which is accumulated during the operation of the plant. It is assumed that at the beginning of the operation there is an initial layer of coke deposited on every furnace. The thickness is different

for each one because it is assumed that they started to work at different times. The initial values are written in the Table 3.32.

Table 3.32. *Initial coke thickness in the furnaces.*

| Furnace | Initial thickness |
|---------|-------------------|
| | mm |
| 1 | 1 |
| 2 | 3 |
| 3 | 4 |
| 4 | 7 |
| 5 | 2 |
| 6 | 5 |
| 7 | 6 |

Starting from those data, the optimisation find the conditions to reach a profit of $1,65 \cdot 10^{12}$ \$.

The conversions which allow to reach this result are written in Table 3.33.

Table 3.33. *Conversion in the furnaces.*

| Furnace | Product | Conversion |
|---------|---------|------------|
| | | % |
| 1 | Ethane | 50.05 |
| 2 | Ethane | 49.57 |
| 3 | Ethane | 49.38 |
| 4 | Ethane | 48.98 |
| 5 | Propane | 47.26 |
| 6 | Propane | 47.35 |
| 7 | Propane | 47.38 |

The result show how in general the Propane conversion is lower than the Ethane conversion. As expected, there are differences between each furnace, which depends on the initial layer of coke.

Since the periods would be linked through the coke thickness, it is important to check if there are variations in the layer of coke deposited in the furnaces at the end of the period. The values obtained are shown in Table 3.34.

Table 3.34. *Final coke thickness.*

| Furnace | Final thickness | Difference in Thickness |
|---------|-----------------|-------------------------|
| | mm | mm |
| 1 | 2.71 | 1.71 |
| 2 | 4.64 | 1.64 |
| 3 | 5.61 | 1.61 |
| 4 | 8.55 | 1.55 |
| 5 | 3.01 | 1.01 |
| 6 | 6.03 | 1.03 |
| 7 | 7.03 | 1.03 |

As expected, the layer of coke changes during the period. The amount of accumulated coke is largest if the conversion at the furnace is higher, as expected. It is possible to notice that the coke layer accumulated is thicker in the Ethane furnaces.

The results show that the conversion is different for each furnace, that there is a difference between the ethane and the propane furnaces, and that there is an accumulation of coke during the operations. The model behaves as expected, so it is possible to proceed to the multiperiod optimisation.

3.3.3 Multiperiod problem

The formulation of the multiperiod problem is slightly different from the one used for the blending problem and the network of plant, since it is assumed that neither the products nor the raw materials could be stored. This assumption makes an inventory unnecessary.

However during the cracking process there is an accumulation of a coke layer on the internal surface of the reactor. For this reason the periods are linked together considering how the thickness of the layer of coke grows at the end of each period, as in the following equation.

$$\begin{aligned} coke\ thickness_{t,n} = & coke\ thickness_{t-1,n} + \\ & + period\ length_t * \max(coking\ rate_{t,n}) \end{aligned} \quad (3.21)$$

All the variables are relative to a period of time t and to a furnace n . The coke thickness represents the value assumed at the end of the period. The coking rate assumes different values in different positions of the furnace, so the maximum value is considered.

During the normal operation of a cracking plant it is necessary to stop the furnaces to remove the coke layer every time that the thickness exceed a given value. For this reason an upper bound for the thickness is introduced.

$$\text{coke thickness} \leq 8 \text{ mm} \quad (3.22)$$

Introducing this condition without further specifications, the results would be to have conversions low enough not to deposit much coke, but this is not realistic. In real plant the furnaces are periodically switched off and a decoking is performed, pumping steam and air into the furnace. It is assumed that in the plant there are eight furnaces, and that one is constantly being decoked.

To simulate this situation, an additional binary variable y to take the decoking process into account is introduced. The coke thickness is calculated using the following equation, where n marks the furnace and t the period. The thickness is expressed in meters.

$$\begin{aligned} \text{Thickness}_{t,n} = & (\text{Thickness}_{t-1,n} + \text{period length}_t \\ & * \text{maximum coking rate}_{t,n}) * (1 - y_{t,n}) + 0.0001 \\ & * y_{t,n} \end{aligned} \quad (3.23)$$

If the decoking is performed, the coke thickness will be set at 0.1 mm at the beginning of the period, while if the decoking is not performed the thickness is calculated using the equation previously described. It is not possible to set the thickness to zero because of the boundaries of the variable, but the set thickness is small enough not to interfere with the simulation.

It is assumed that it is possible to decoke one furnace every week, so a constraint is set according to the time length of each period.

As for the single period problem, the objective function to be maximized is the profit, which is calculated using the following equations.

$$\text{profit}_t = \text{single period profit}_t - \sum_i y_{t,n} * \text{decoking cost} \quad (3.24)$$

$$\text{total profit} = \sum_t \text{profit}_t \quad (3.25)$$

The single period profit contains the decoking cost, which is assumed to be $2.1 * 10^4$ \$.

The aim of the optimisation is to find the optimal conversions for each furnace and for each period, taking into account prices variation. It is expected that the optimisation finds the best period to perform the decoking for every furnace.

The model is tested both assuming the prices are constant and assuming that the prices change during the time horizon.

3.3.3.1 Case 1

In this first example the prices of products and raw materials, the electricity cost and the energy requirement for the recycle are constant, and can be found in Table 3.30 and 3.31. The plant operates for three periods, and each period covers two weeks. It is assumed that the initial values of the thickness are the ones written in Table 3.32.

The optimisation reached a total profit at the end of the period of $4.95 \cdot 10^{13}$ \$. The conversions and final thickness found for each furnace are shown in Figure 3.7, 3.8, 3.9 and 3.10.

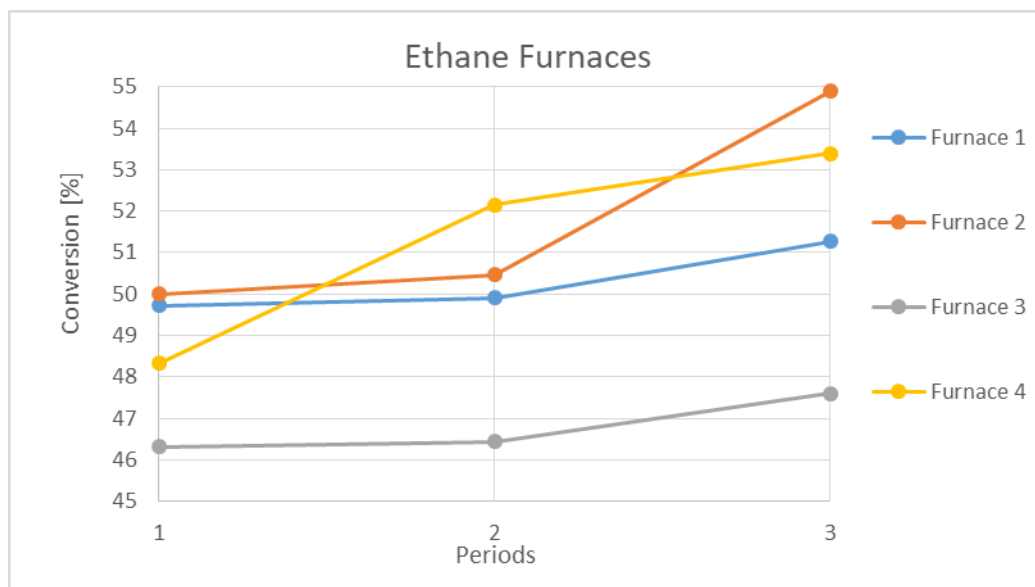


Figure 3.7. Conversion of ethane furnaces.

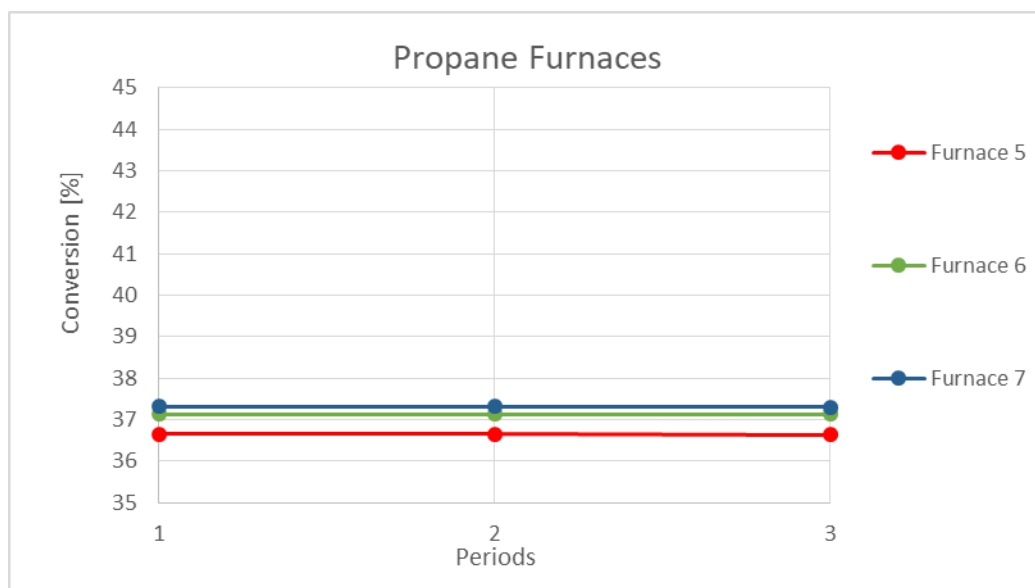


Figure 3.8. Conversion of propane furnaces.

Comparing Figure 3.7 and 3.8, it is possible to see a difference between the conversion of the Ethane and Propane furnaces. In general, the Propane furnaces conversions are lower and very similar to each other. By contrast the conversions of the Ethane furnaces cover a wider range. This fact can be explained by the decoking schedule.

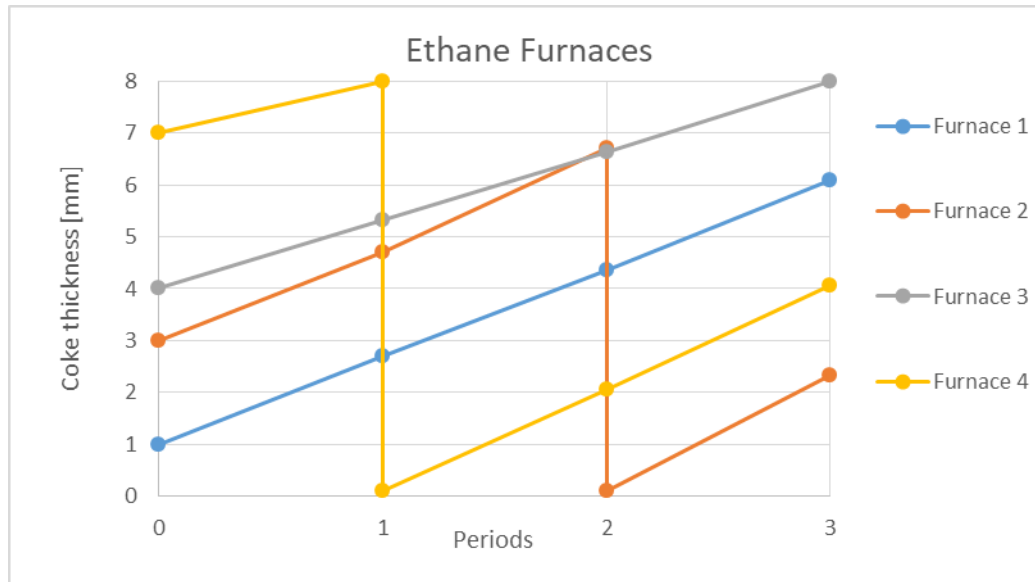


Figure 3.9. Coke thickness in the ethane furnaces at the beginning and at the end of each period of operation.

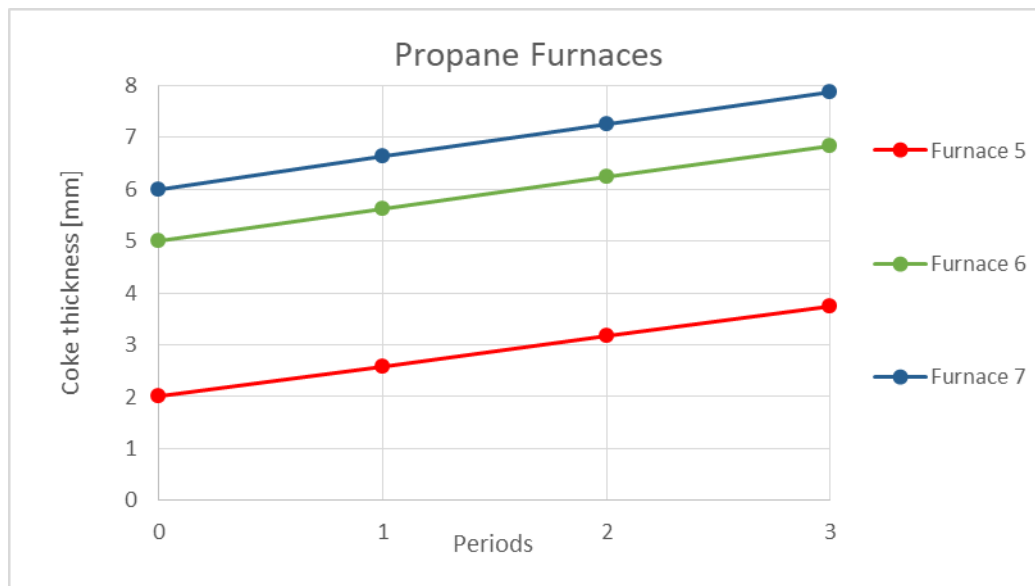


Figure 3.10. Coke thickness in the propane furnaces at the beginning and at the end of each period of operation.

In Figure 3.9 and 3.10 it is possible to identify when the decoking happens because the coke layer on the furnaces drops. A decoking is performed on furnace 1 at the end of the first period and on furnace 2 at the end of the second period. No decokings are performed at the end of the third period, since the constraint on coke thickness is respected.

It is not necessary to perform decoking on the propane furnaces, since there are lower conversions and the accumulation of coke is lower and stays within the boundaries.

It can be noticed that after the decoking on furnaces 2 and 4 the conversions are higher. The conversion of furnace 3 is the lowest, since the initial layer of coke was high and the furnace is not decoked. As a consequence, it is necessary to limit the coke deposition and lower the conversion.

3.3.3.2 Case 2

After solving Case 1, another case is performed to gauge the effect of a change in the prices in the optimisation results. The data used are the same as for Case 1, except for the prices of raw materials, products and electricity. These prices change accordingly to Table 3.35.

Table 3.35. Prices during the periods.

| | | Periods | | |
|------------------|--------|---------|------|------|
| Period | | 1 | 2 | 3 |
| Propane | \$/ton | 500 | 600 | 450 |
| Ethane | \$/ton | 200 | 180 | 190 |
| Fuel gas | \$/ton | 194 | 200 | 194 |
| Hydrogen | \$/ton | 3530 | 3510 | 3550 |
| Ethylene | \$/ton | 1382 | 1382 | 1382 |
| Propylene | \$/ton | 1340 | 1300 | 1380 |
| C4 (Butadiene) | \$/ton | 1900 | 1900 | 1960 |
| C5+ (Benzene) | \$/ton | 1350 | 1400 | 1450 |
| Electricity cost | \$/kW | 0.12 | 0.13 | 0.11 |

The optimisation finds a result which allows to reach a total profit of $4.86 \cdot 10^{13}$ \$, which is reasonable because the prices do not change much.

The conversions and the coke thickness found by the optimisation are shown in Figure.3.11, 3.12, 3.13 and 3.14.

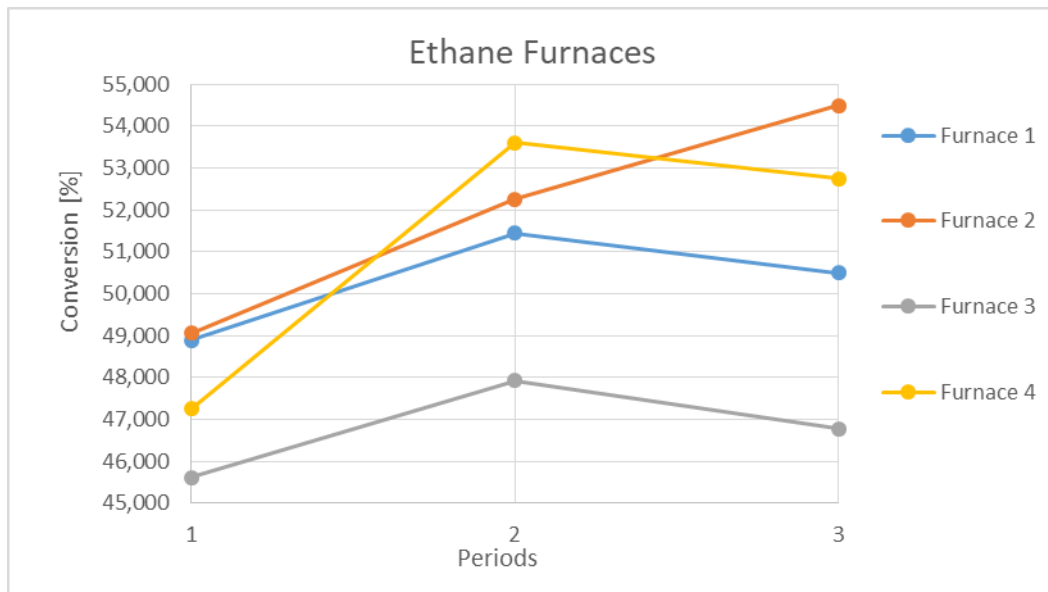


Figure 3.11. Conversion of ethane furnaces.

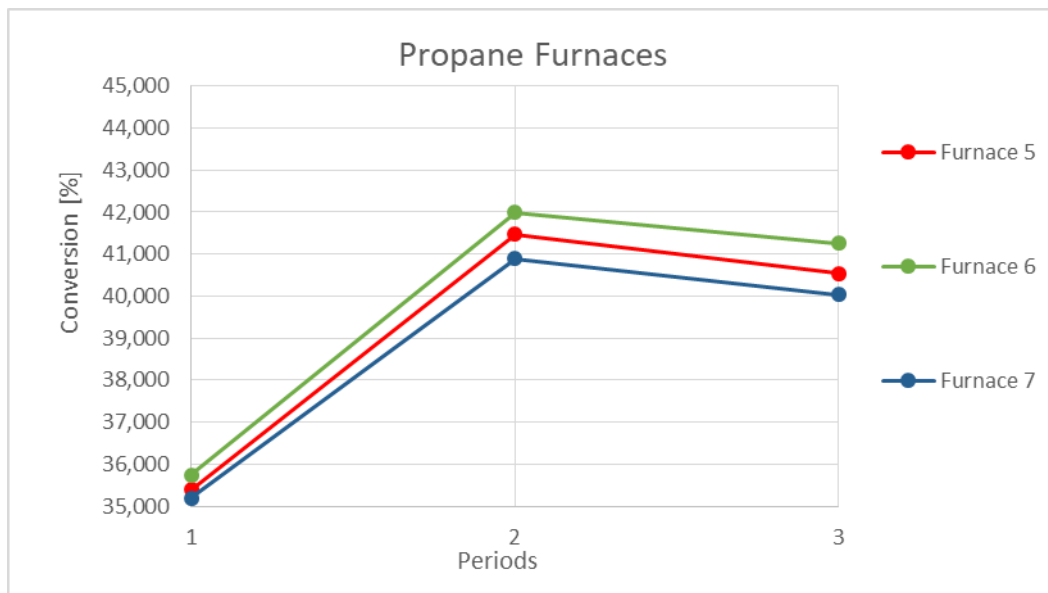


Figure 3.12. Conversion of propane furnaces.

The conversions are very similar to the previous case, but they are slightly adjusted to adapt to the change of prices of the raw materials. In particular, the conversions are lower during the first period, and higher during the second because the price of the Ethane is low. During the third period, the conversions of the furnaces processing Ethane are lower, while the conversions of the furnaces processing Propane are higher because the cost of Propane is the lowest.

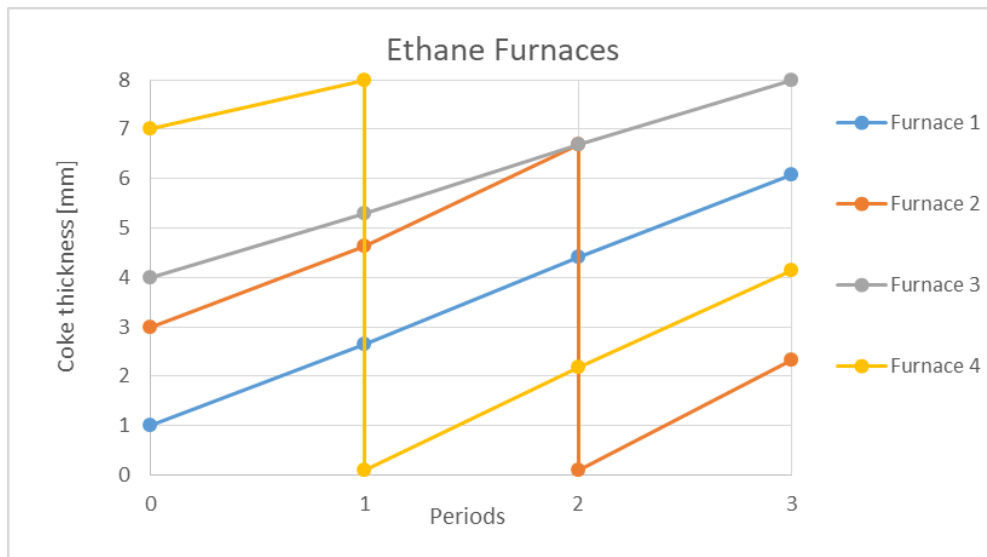


Figure 3.14. Coke thickness in the ethane furnaces at the beginning and at the end of each period of operation.

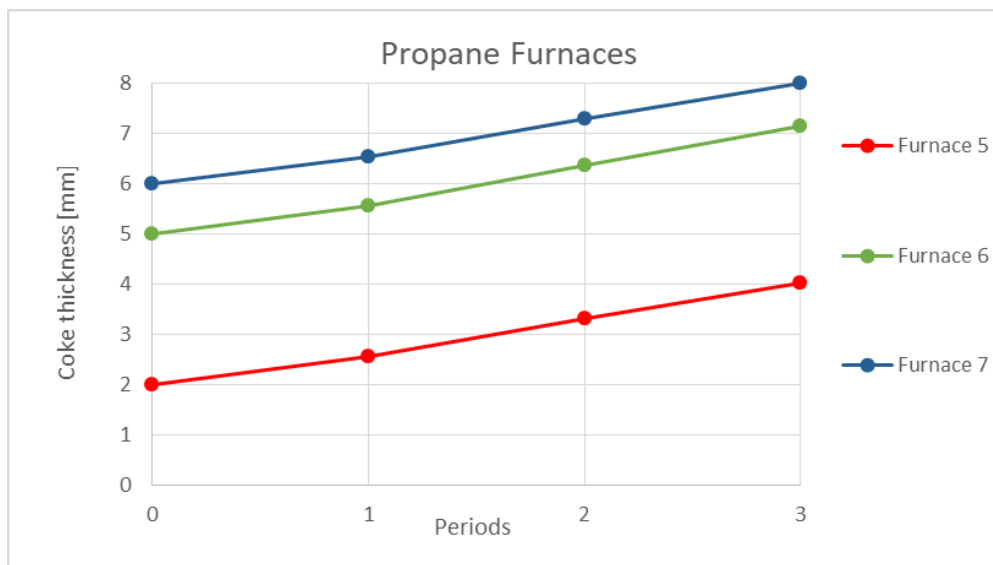


Figure 3.13. Coke thickness in the propane furnaces at the beginning and at the end of each period of operation.

The decoking schedule remains the same as the previous case. The coke thickness is very similar. This result was expected because the thickness constraint, which is the one influencing the decoking schedule most, was not changed.

The results of the two cases are reasonable and show that the model works. However, these cases were solved only using gProms, since the prototype structure could not handle them.

The problem was in the gradient calculations, which are not accurate when the model is highly non linear. In conclusion, the prototype structure can handle models of average size as the blending problem and the network of plants, but more work will be required to tackle bigger non linear models

Chapter 4

Strategic planning multiperiod problem

This chapter contains all the strategic planning problems. The purpose is to add the strategic planning decisions, in particular contract stipulations, revamping and the construction of new plants, to the specific model of a plant, and to solve a multiperiod optimisation.

The strategic planning for solved for the blending problem and the network of plants. The calculation of the Net present value is added to the blending problem, and the problem is solved including contract stipulations. The network of plant is solved including contract stipulation, revamping and constructions of new plants.

4.1 Blending Problem

First, some features of the strategic planning had been added to the blending problem, since the model is very simple, and the multiperiod problem had been solved. In particular, the Net Present Value calculation and the decisions related to contracts had been implemented.

4.1.1 Net Present Value

Since the strategic planning problems cover a longer time horizon than a multiperiod problem with inventories, it becomes important to calculate the value of the money. The NPV value has been implemented to see the effect of the discounted cash flow on the sales schedule.

The economic evaluation has been added to the model using the following equation.

$$NPV = \sum_{t=1}^T \frac{profit_t}{(1+r)^t} \quad (4.1)$$

where r is the discount rate, T is the number of periods and $profit_t$ is the profit obtained during period t .

Since the periods are measured in days, while the discount rates are usually annual, j has to be recalculated. In order to refer r to the correct length of the period, the equation below is used.

$$1 + i = (1 + l)^{\frac{365}{x}} \quad (4.2)$$

where r is the annual discount rate and l is the discount rate for a period of x days.

The discount rate l is calculated for each single period of time, so it is possible to use periods of time of different length.

The simplest way to see the effect of the NPV is to solve a multiperiod problem with inventories, using the model described in §3.1.3. The results of the optimisation is the optimal schedule of the sales. The results are affected by the discount rate, because if it is high, it is more convenient to sell the products soon.

The data used for the optimisation are the same used in §3.1.3, with some exceptions that are listed below.

- Constraints. The inventory constraints are changed as in the equation.

$$5 \leq \text{product stored} \leq 50 \quad (4.3)$$

where the unit of measure is $\text{kg} \cdot 10^6$.

- Period length. It is assumed that the period of time had a fixed length, 15 days.
- Annual discount rate. A discount of 0.15 is added.

4.1.1.1 Case 1

As a first example, the optimisation is performed using two different discount rates: 0.15 and 500. The values are not realistic, but they are chosen because they have different order of magnitude. The results are shown in Table 4.1.

Table 4.1. *Optimisation results. Inventory and sales.*

| | | Discount rate | | 0.15 | | Discount rate | | 500 | |
|-----------|--------------------|---------------|--------|----------------------|--------|---------------|--------|----------------------|--------|
| | | NPV (\$) | | 6.51*10 ⁹ | | NPV (\$) | | 3.29*10 ⁹ | |
| Period | | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 4 |
| Price | \$/kg | 65 | 72 | 72 | 70 | 65 | 72 | 72 | 70 |
| Inventory | kg*10 ⁶ | 50 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| Sales | kg*10 ⁶ | 79.60 | 174.60 | 129.60 | 129.60 | 124.60 | 129.60 | 129.60 | 129.60 |

The results show that if the discount rate is very high, the resulting NPV is low and the solver schedule the sales as soon as possible, even if the price of the product is at the lowest. For this reason if the discount rate is 0.15 during the first period the maximum inventory capacity is reached, while if the discount rate is 500 only the minimum required inventory is stored.

4.1.1.2 Case 2

As a second example, the results found using a 0.15 discount rate are compared with the results found without considering the Net Present Value calculation. The results are shown in Table 4.2.

Table 4.2. Optimisation results. Inventory and sales.

| | | Discount rate | | 0.15 | | Discount rate | | 0 | |
|-----------|--------------------|---------------|--------|----------------------|--------|---------------|--------|----------------------|--------|
| | | NPV (\$) | | 6.51*10 ⁹ | | NPV (\$) | | 6.63*10 ⁹ | |
| Period | | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 4 |
| Price | \$/kg | 65 | 72 | 72.00003 | 70 | 65 | 72 | 72.00003 | 70 |
| Inventory | kg*10 ⁶ | 50 | 5 | 5 | 5 | 50 | 50 | 5 | 5 |
| Sales | kg*10 ⁶ | 79.60 | 174.60 | 129.60 | 129.60 | 79.60 | 129.60 | 174.60 | 129.60 |

The results shown the meaning of the NPV. In the examples the period in which the value of the product is higher is the third one. For this reason if the discount rate is not considered, the product is stored and sold during the third period. By contrast, if the present value of money is taken into account the product is stored during the second period in order to obtain the money sooner.

Those two simple example shows how the NPV affects the optimisation results. The sales schedule is a trade-off between the necessity to sell the products as soon as possible and the prices fluctuations. The products are sold sooner if the NPV is higher.

4.1.2 Contracts

After implementing the NPV calculation in the blending problem, the model was modified to include strategic planning decisions. The flowsheet of the blending problem does not allow to plan an expansion or a revamping, so it is possible to solve only the signing of a contract.

The contract which is implemented offer a fixed price for the purchase of the product, and cover two periods. The aim of the optimisation is to decide if the contract should be signed and the best moment to sign it. It is also possible to negotiate the amount of product to provide, within certain boundaries.

The inlet flowrates are decided by the optimisation, but the maximum capacity of the plant is fixed. For this reason the amount of product sold by contract is subtracted from the total amount produced during the period. The following equation is used to calculate the revenues.

$$revenue_t = [(sales_t - S) * price_{j,t} + S * w] * z_t + sales_t * price_t * (1 - z_t) \quad (4.4)$$

In this equation S is the amount of product to be supplied at the price w_i as signed in the contract. z_t is the variable that indicates if the contract is effective in the period t , so that the sales due to the contract will be added only in the periods when the contract is effective.

To close the mass balance, the following equations are applied.

$$Inventory_t = Inventory_{t-1} + produced_t - sales_t \geq 0 \quad (4.5)$$

$$sales_t - S \geq 0 \quad (4.6)$$

The two conditions assure that both the sales to the public and the sales due to the contract do not exceed the production.

The decision to sign the contract is represented by the variable y_t , which is linked to z_t through the equation below.

$$z_t = y_t + y_{t-1} \quad (4.7)$$

The following constraint is settled to assure that just one contract is signed during the period of time.

$$\sum_t y_t \leq 1 \quad (4.8)$$

The amount of product to be sold can be negotiated within the following boundaries.

$$15 \leq contract\ sales_t \leq 25 \quad (4.9)$$

The unit of measure is $kg * 10^{-6}$.

The multiperiod problem is solved for three different cases, which differ for the prices fluctuation during the time horizon.

4.1.2.1 Case 1

As a first example, it is assumed that the price offered by the contract is 70 \$/kg, while the prices for the public which are expected for each periods are in Table 4.3.

Table 4.3. Prices of the product.

| | | | | | |
|---------------|-------|----|----|----|----|
| Period | | 1 | 2 | 3 | 4 |
| Price | \$/kg | 65 | 72 | 72 | 70 |
| Period length | days | 15 | 15 | 15 | 15 |

It is expected that the solver compares the prices, taking into account the NPV, and decides if it is profitable or not to sign the contract. In addition, it is required to identify the best period to sign the contract and the amount to provide.

The total profit obtained by the optimisation is $6.59 \cdot 10^9$ \$. The other results are in table 4.4.

Table 4.4. Results of the optimisation.

| | |
|------------------------------------|-----|
| Should the contract be signed? | Yes |
| Period to sign the contract | 1 |
| Amount to provide [millions of kg] | 25 |

It is more profitable to sign the contract during the first period, when the price of the product for the public is at its lowest. The revenues obtained during the first period are enough to compensate the loss that occurs during the second period, when the price for the public is higher than the one offered by the contract. The Net Present Value is taken into account in this decision, because it is better to receive money during the first period.

4.1.2.2 Cases 2 and 3

For the following examples it is assumed that the price offered by the contract is the same as previously, 70 \$/kg. The prices expected for the public are expressed in Table 4.5.

Table 4.5. Prices of the product.

| | | Case 2 | | | | Case 3 | | | |
|---------------|-------|--------|----|----|----|--------|----|----|----|
| Period | | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 4 |
| Price | \$/kg | 70 | 72 | 68 | 72 | 70 | 72 | 72 | 68 |
| Period length | days | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 |

As in Case 1, the aim of the optimisation is to decide if the contract should be signed or not. The results are written in Table 4.6.

Table 4.6. Results of the optimisation.

| | Case 2 | Case 3 |
|------------------------------------|--------|--------|
| Should the contract be signed? | Yes | No |
| Period to sign the contract | 3 | |
| Amount to provide [millions of kg] | 25 | |

The total profit obtained is $6.81 \cdot 10^9$ \$ for Case 2 and $6.66 \cdot 10^9$ \$ for Case 3.

The NPV has a strong effect in these decisions. In fact, the two cases are very similar, but while in Case 2 the third period has a lower price than the fourth, in Case 3 the values are inverted. Without taking into account the NPV, there would not be any difference between signing the contract or not because the total profit would be the same in the two cases.

The NPV calculation gives more value to revenues that are cashed sooner. For this reason it is profitable to sign a contract in Case 2 because the profit would be anticipated, while it is not profitable to sign it in case 3 because the profit would be delayed.

The multiperiod optimisations were successfully solved for the blending problem, and the results show that the NPV is correctly taken into account. It is possible to proceed to apply the strategic planning multiperiod problem to the network of plants.

4.2 Network of plants

Strategic planning is usually applied to superstructures incorporating more than one plant. For this reason its optimal application is to the network of plants described in §Chapter 2.

A particularity that makes this plant particularly suitable for a strategic planning optimisation is the way in which the operating cost of the single plant is calculated, as seen in Equation 3.16. This equation takes into account the fact that if the capacity of the plant is increased, the operating cost decreases. This difference is important in the choice of the plant to use to produce one product, especially when revamping and construction of new plants are considered. Furthermore, in this type of flowsheet the costs are calculated only on the plants that are active during the period.

As in the multiperiod problems solved in §Chapter 3, it is assumed that the prices of the products are different during the different periods. The costs related to the operation, such as utilities and raw material costs, are constant. Deterministic prices are assumed.

A feature of strategic planning is the long period of time that is covered by the optimisation. For this reason, the length of the period is of the order of magnitude of the years and it is assumed that everything is sold at the end of the period. The inventory levels are not taken into account in this optimisation.

The objective function is calculated considering the Net Present Value. The annual discount ratio is adapted to calculate the interest over time periods of different length.

The model is modified to include the three types of strategic planning which are considered in this thesis: contract stipulation, revamping and building of a new plant. The three types of strategic planning decisions are solved separately in the next paragraphs.

4.2.1 Contract

To introduce the strategic decisions related to the contract, it is necessary to change the revenues calculation. Since the raw materials flowrates are fixed, there are not any changes in the global mass balance. The revenues are calculated using the following equation.

$$\begin{aligned} revenue_{j,t} = & [(flowrate_{j,t} * time_t - S) * price_{j,t} + S * w] * z_t \\ & + flowrate_{j,t} * time_t * price_{j,t} * (1 - z_t), \end{aligned} \quad (4.10)$$

where t is the period of time considered and j is used to indicate both the product j and the zone of the plant where that product is processed. S and w are respectively the minimum amount of product to be provided and the price defined by the contract.

In this formulation it is assumed that S is the same for all the products and that S and w are fixed for the length of the contract. This means that if the contract is signed all the three products have to be produced. The variable z_t is a Boolean variable which define if the contract is valid during the period t .

If the contract had been signed, $z_t = 1$, so the second part of the equation becomes equal to zero. In this situation the revenues are calculated as a sum of the products sold at the market price and of the sales bound to the contract. If $z_t = 0$, the contract has not been signed and the revenues are calculated normally using the second part of the equation.

To close the mass balance, the following constraint is added.

$$flowrate_{j,t} * time_t - S > 0 \quad (4.11)$$

This condition is necessary to avoid to sell more of the production, and is used only during the periods when the contract is signed. It is possible to use this equation only because an inventory is not taken into account.

The decision to sign the contract is marked using the variable y_t , which is controlled by the optimisation and used to calculate z_t using the following equation.

$$z_t = \sum_{k=0}^3 y_{t-k} \quad (4.12)$$

Since the contract will last for four years, the variable z_t is calculated as a sum that consider the current period and the decisions made in the previous three periods.

y_t is defined for all the periods, but it is assumed that is not possible to sign the contract during the last three periods, because it will exceed the time horizon considered.

To avoid that more than one contract is signed during the time horizon, the following condition is used.

$$\sum_{t=1}^8 y_t \leq 1 \quad (4.13)$$

Three different cases are taken into account for the optimisation. In each one of them it is assumed that if the contract is signed, the amount to be provided could be negotiated within the following boundaries.

$$20 \leq S \leq 500 \quad (4.14)$$

The aim of the optimisation is to determine if signing the contract is profitable and which is the best moment to sign it.

The model has been solved for three different cases, each one with different prices. A time horizon of 10 years, divided into 10 periods, is taken into account.

4.2.1.1 Case 1

As a first case, it is assumed that the prices of the products for the public during the 10 periods change as shown in Figure 4.1.

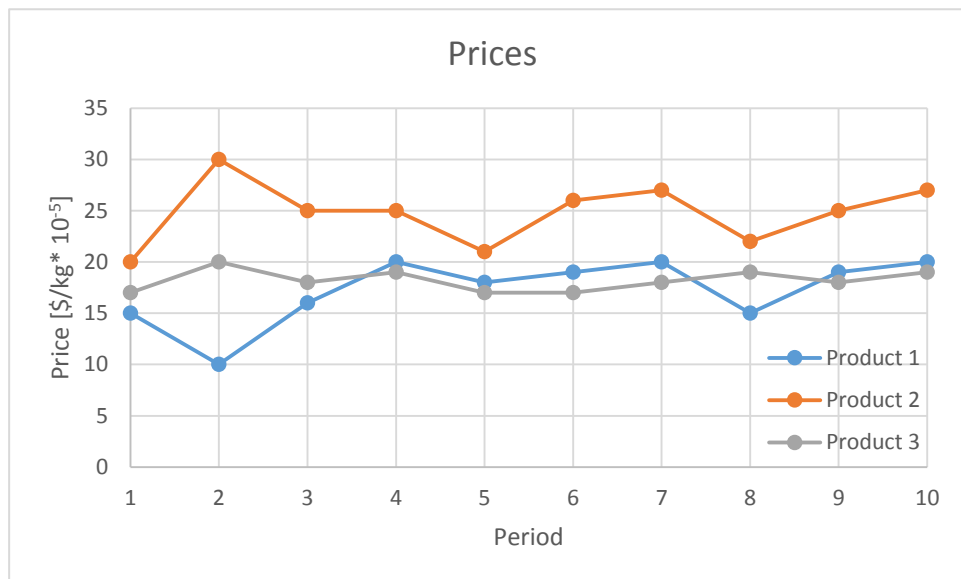


Figure 4.1. Expected prices of the three products.

The graph shows how the prices fluctuates during the time horizon. In general, Product 2 is the most valuable. The solver should compare these prices with the ones granted by the contract, which are in Table 4.7.

Table 4.7. Prices offered by the contract.

| Product 1 | Product 2 | Product 3 |
|-------------------------|-----------|-----------|
| \$/kg* 10 ⁻⁵ | | |
| 40 | 40 | 10 |

The situation can be summarized in Figure 4.2.



Figure 4.2. Comparison between the expected prices of the products, represented by the continuous lines, and the prices offered by the contract, represented by the dotted lines.

The straight lines represent the prices offered by the contract, which are constant during the time horizon, while the broken lines shows the prices fluctuations which are expected during the periods. The optimisation is expected to compare the prices offered and expected, considering the whole time horizon, and decide if the contract should be signed or not.

It is not possible to sign the contract only for one product. Even if it is clear that the prices offered by the contract are more convenient for Product 1 and 2, it is unclear if the profit obtained for them would compensate for the loss in profit for Product 3.

The optimisation obtains a total profit of $1.63 \cdot 10^9$ \$.

The results of the optimisation are written in Table 4.8 and 4.9.

Table 4.8. *Optimisation results. Contract.*

| | |
|--------------------------------|----------------------------------|
| Should the contract be signed? | Yes |
| Period to sign the contract | 1 |
| Amount to provide | 500 kmol * h ⁻¹ *year |

Table 4.8 shows the long term decisions. It is profitable to sign the contract because globally the prices offered are higher than the expected ones. It is better to sign the contract during the first period, when the expected prices are lower.

The amount to be provided is the maximum which is allowed by the boundaries.

Table 4.9. *Optimisation results. Production.*

| | Production | | | | | | | | | |
|-----------|----------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| | kmol h ⁻¹ | | | | | | | | | |
| Product 1 | 500 | 500 | 500 | 500 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 2 | 36259 | 36259 | 36259 | 36259 | 36759 | 36759 | 36759 | 36759 | 36759 | 36759 |
| Product 3 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 | 63817 |

The details about the production are shown in Table 4.9. It is not profitable to sell Product 1 to the public, so just the amount necessary to fulfil the contract is produced, and only during the periods covered by it.

4.2.1.2 Case 2

As for Case 1, the prices fluctuations expected are represented in Figure 4.1. The difference between this case and the previous one is in the prices offered by the contract, which are written in Table 4.10.

Table 4.10. *Prices offered by the contract.*

| Product 1 | Product 2 | Product 3 |
|-------------------------|-----------|-----------|
| \$/kg* 10 ⁻⁵ | | |
| 10 | 10 | 25 |

The prices offered for Product 1 and 2 are lower, while the price offered for Product 3 increases. The optimisation is expected to decide if the increase of the price offered for Product 3 is high enough to compensate the decrease of the prices of the other products.

The prices are compared in Figure 4.3.

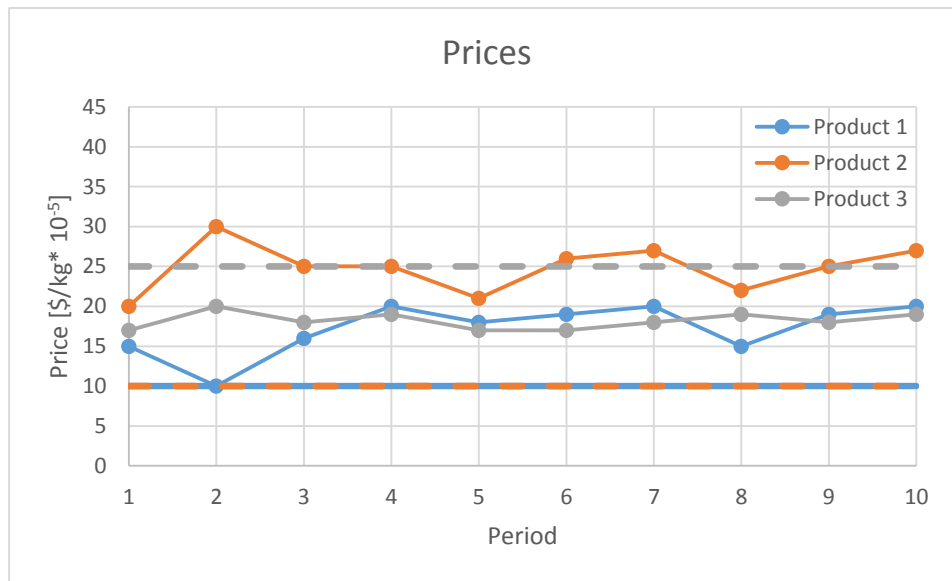


Figure 4.3. Comparison between the expected prices of the products, represented by the continuous lines, and the prices offered by the contract, represented by the dotted lines.

The graph shows how the price offered by the contract for Product 3 is higher than the one expected, while the prices offered for Product 1 and 2 are lower.

The optimisation result is that the contract should not be signed, because the prices offered for the products are on average lower than the one expected. It obtains a total profit of $1,60 \cdot 10^9$ \$.

4.2.1.3 Case 3

For Case 3 it is assumed that there is change both in the prices offered by contract and expected for the sales to the public. The prices offered by the contract are written in Table 4.11.

Table 4.11. Prices offered by the contract.

| Product 1 | Product 2 | Product 3 |
|------------------------------|-----------|-----------|
| $\$/\text{kg} \cdot 10^{-5}$ | | |
| 40 | 40 | 20 |

It is expected that the prices for the public would drop from the fourth to the eighth periods, as in Figure 4.4.

Table 4.13 shows that during the years when the prices of the product are lower, just the amount of Product 1 agreed by contract is produced.

The three cases shows that the strategic planning multiperiod optimisation for the signing of the contracts is working as expected.

4.2.2 Revamping

The second type of strategic planning decisions considered is the revamping of an existing plant or of a piece of equipment.

It is decided that for the network of plants the revamping would be applied to the capacity of the single plants, which has an effect both on the operating cost and on the total production capacity of the network. The increase of the capacity would allow for the splits to direct a higher flowrate of raw material towards that plant, and so to produce more of one of the products. The operative costs of the different plants are then calculated according to the maximum capacity. The aim of the optimisation is to decide if it would be profitable to increase the capacity of the plants and when would be the optimal period.

In the superstructure there are two different type of plants: the stabilizers (Stab) and the gas plants (GP) to obtain the final product. It is assumed that it is possible to increase the capacity of both the types and that the prices of the revamping are known.

The decision to increase the capacity is linked to the variable y . $y_{k,j,t}$ indicates that during period t the type of plant k number j has been revamped. The decision is connected to the plant operation through the following equation.

$$\begin{aligned} \text{maximum capacity}_{k,j,t} \\ = \text{maximum capacity}_{k,j,t-1} + y_{k,j,t} * \Delta\text{capacity}_k \end{aligned} \quad (4.15)$$

The capacity of a plant in a certain period is calculated as the capacity in the previous period eventually raised of a fixed capacity ($\Delta\text{capacity}_k$), which is different for each type of plant k .

The cost of the extension is taken into account in the revenues calculation following the same equation.

$$\begin{aligned} \text{profit}_t = \text{revenues}_t - \text{operating costs}_t - \text{cost}_{GP} \\ * \sum_j y_{GP,j,t} - \text{cost}_{Stab} * \sum_j y_{Stab,j,t} \end{aligned} \quad (4.16)$$

In the equation cost_{k1} and cost_{k2} are related to the different types of plant *Stab* and *GP*. The costs are multiplied for the number of plants that are revamped during the period t .

To limit the number of extensions planned by the optimisation, the following constraints are used.

$$\sum_t \sum_j y_{GP,t,j} \leq 3 \quad (4.17)$$

$$\sum_t \sum_j y_{stab,t,j} \leq 2 \quad (4.18)$$

The constraints limits the extensions that can happen during the time horizon.

An additional constraint is added to assure that each plant is revamped just one time.

$$\sum_t y_{k,t,j} \leq 1 \quad (4.19)$$

It is sensible to use this constraint because usually the plants are revamped when one of the units is not behaving in a good way, and the operation is performed just one time.

Three cases are solved using this model, each one with different prices to the public and for the revamping. The optimisation covers 10 years. It is assumed that the cost of the raw products is constant and it is the same as in Table 3.25.

4.2.2.1 Case 1

The prices of the products used for this case are the same as in §4.2.1.1 and are shown in Figure 4.1. The plants to be revamped are chosen considering the initial capacity of the plants, which are the same for all the revamping cases, are shown in Table 4.14.

Table 4.14. *Initial capacity of the plants.*

| GP | Initial capacity | Stabilizer | Initial capacity |
|---------|---|------------|---|
| | $\text{kg} \cdot \text{h}^{-1} \cdot \$^{-1} \cdot 10^{-5}$ | | $\text{kg} \cdot \text{h}^{-1} \cdot \$^{-1} \cdot 10^{-5}$ |
| Plant 1 | 600 | Plant 1 | 1000 |
| Plant 2 | 500 | Plant 2 | 1500 |
| Plant 3 | 400 | Plant 3 | 1200 |
| Plant 4 | 1000 | Plant 4 | 900 |
| Plant 5 | 600 | | |
| Plant 6 | 700 | | |

If a revamping is performed, the capacity is changed and the cost of the revamping is paid. These data are added in Table 4.15.

Table 4.15. Possible expansions and costs.

| Type of plant | | GP | Stabilizer |
|------------------------|---|-----|------------|
| Difference in capacity | $\text{kg} \cdot \text{h}^{-1} \cdot \$^{-1} \cdot 10^{-5}$ | 100 | 200 |
| Cost of expansion | $\$ \cdot 10^9$ | 0.7 | 0.5 |

It is assumed that the cost and the capacity expansion are different for the two types of plants which constitute the network.

The optimisation obtains a total profit of $5.85 \cdot 10^9$ \$. The results are shown in Table 4.16, Figure 4.6 and Table 4.17.

Table 4.16. Revamping schedule.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------|----------------------------|---|---|---|---|---|---|---|---|----|
| | Is the capacity increased? | | | | | | | | | |
| y _{GP,1} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,2} | yes | - | - | - | - | - | - | - | - | - |
| y _{GP,3} | yes | - | - | - | - | - | - | - | - | - |
| y _{GP,4} | yes | - | - | - | - | - | - | - | - | - |
| y _{GP,5} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,6} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,1} | yes | - | - | - | - | - | - | - | - | - |
| y _{stab,2} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,3} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,4} | yes | - | - | - | - | - | - | - | - | - |

It is shown that if the fluctuations of the prices are small, as in this case, it is more profitable to perform all the revamping during the first period, so that the operative costs would be decreased and the capacity would be increased as soon as possible.

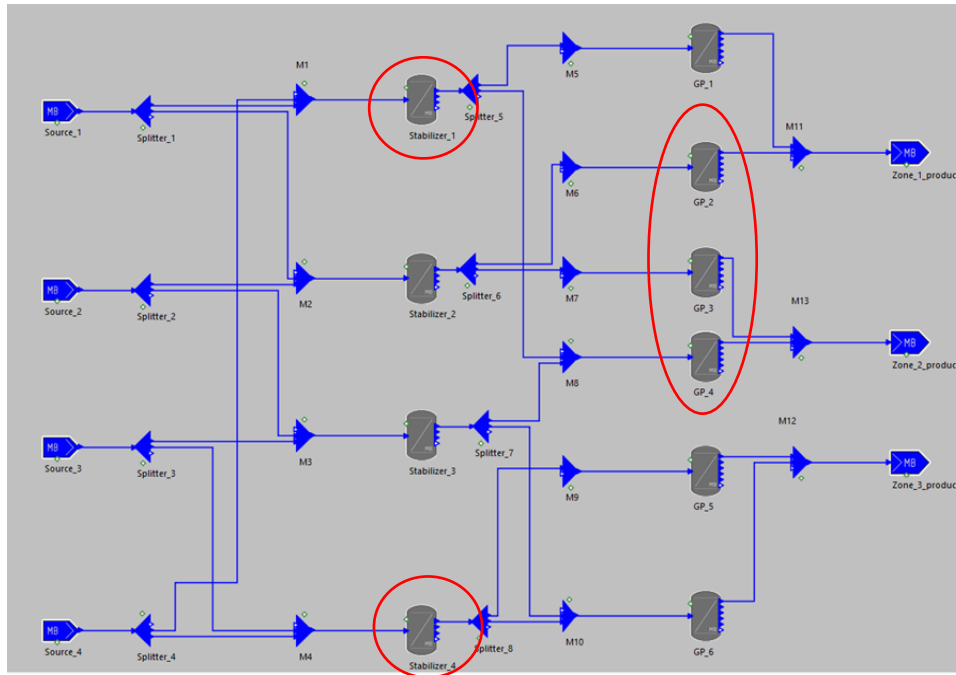


Figure 4.5. Revamped plants.

Figure 4.5 shows which plants are revamped. Those plants were the ones which initially had the lower capacity, which means that they had also the higher operative costs.

Table 4.17. Inlet and outlet flowrates.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|---------|---------|---------|--------|---------|---------|---------|---------|---------|--------|
| | kmol/h | | | | | | | | | |
| Raw Material 1 | 118682 | 85698 | 118682 | 118682 | 118682 | 118682 | 118682 | 118682 | 118682 | 118682 |
| Raw Material 2 | 37493 | 37493 | 37493 | 59764 | 59764 | 59764 | 59764 | 37493 | 59764 | 59764 |
| Raw Material 3 | 32083.3 | 32136.9 | 32083.3 | 41102 | 32083.3 | 32083.3 | 41048.5 | 32083.3 | 32083.3 | 41102 |
| Raw Material 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 1 | 30277 | 0 | 30277 | 58998 | 50720 | 50769 | 58998 | 30277 | 50720 | 58998 |
| Product 2 | 78665 | 78665 | 78665 | 78665 | 78665 | 78665 | 78665 | 78665 | 78665 | 78665 |
| Product 3 | 63866 | 63866 | 63866 | 63866 | 63866 | 63866 | 63866 | 63866 | 63866 | 63866 |

The flowrates of raw material and products are reported in Table 4.17. The revamping increases the final amount of Product 1 and 2, which are the most profitable. The Raw Product 4, the most expensive, is not purchased.

4.2.2.2 Case 2

This case is performed to see what happens is the prices of all the products are very low during period 1 and 2, as shown in Figure 4.6.



Figure 4.6. Expected prices of the three products.

The optimisation is solved, and a total profit of $6.24 \cdot 10^9$ \$ is reached. The results are shown in Table 4.17 and a.18 and in Figure 4.7.

Table 4.18. Revamping schedule.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------|----------------------------|---|-----|---|---|---|---|---|---|----|
| | Is the capacity increased? | | | | | | | | | |
| YGP,1 | - | - | - | - | - | - | - | - | - | - |
| YGP,2 | - | - | - | - | - | - | - | - | - | - |
| YGP,3 | - | - | yes | - | - | - | - | - | - | - |
| YGP,4 | - | - | - | - | - | - | - | - | - | - |
| YGP,5 | - | - | yes | - | - | - | - | - | - | - |
| YGP,6 | - | - | yes | - | - | - | - | - | - | - |
| Ystab,1 | - | - | yes | - | - | - | - | - | - | - |
| Ystab,2 | - | - | - | - | - | - | - | - | - | - |
| Ystab,3 | yes | - | - | - | - | - | - | - | - | - |
| Ystab,4 | - | - | - | - | - | - | - | - | - | - |

In contrast with the previous case, the revamping of four plants is postponed to the third period.

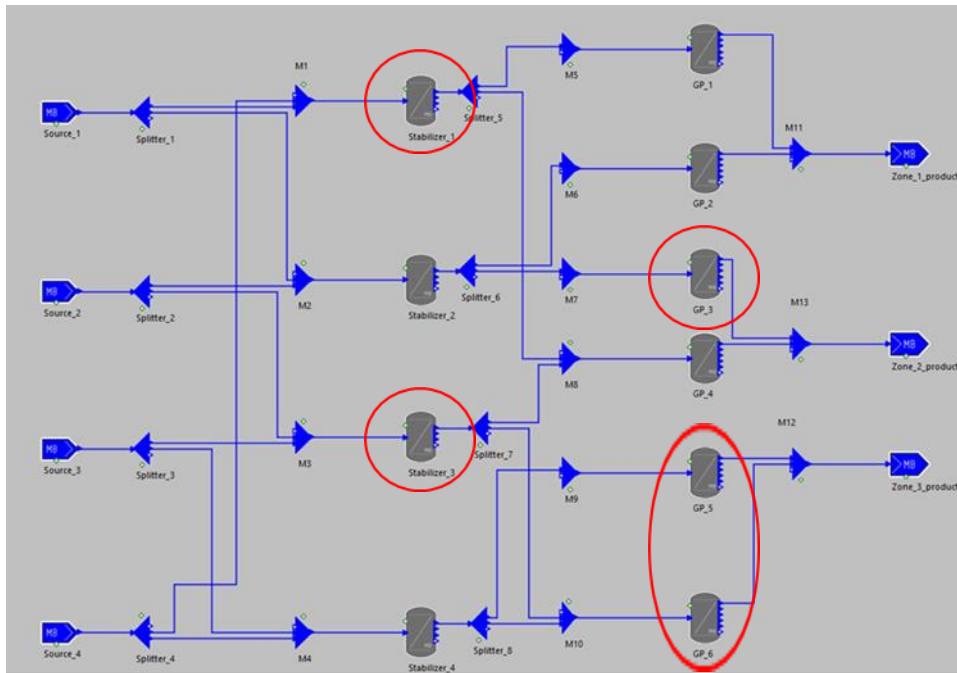


Figure 4.7. Revamped plants.

Figure 4.7 shows the plants which are revamped. Since Product 3 is the most profitable, the two Gas Plants related to its production are revamped. For this reason also the capacity of Stabilizer 3 is increased, even if it is not the lowest one.

Table 4.19. Inlet and outlet flowrates.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|---------|---------|--------|--------|--------|--------|--------|--------|--------|--------|
| | kmol/h | | | | | | | | | |
| Raw Material 1 | 0 | 0 | 113326 | 113326 | 113326 | 113326 | 113326 | 113326 | 113326 | 113326 |
| Raw Material 2 | 37439 | 0 | 68783 | 68783 | 68783 | 68783 | 68783 | 68783 | 68783 | 68783 |
| Raw Material 3 | 32083.3 | 69522.7 | 37493 | 37493 | 37493 | 37493 | 37493 | 37493 | 37493 | 37493 |
| Raw Material 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 1 | 0 | 0 | 54082 | 54082 | 54082 | 54082 | 54082 | 54082 | 54082 | 54082 |
| Product 2 | 0 | 0 | 73748 | 73748 | 73748 | 73748 | 73748 | 73748 | 73748 | 73748 |
| Product 3 | 63817 | 63817 | 73748 | 73748 | 73748 | 73748 | 73748 | 73748 | 73748 | 73748 |

During the first two periods it is profitable to produce only Product 3 because the prices are low. For this reason only Stabilizer 3, which is related to the production of Product 3, is revamped during the first period. The other plants are revamped during period 3, when the increase of capacity is exploited by the production. The NPV is responsible for the delay of the decision to revamp the plant.

As in the previous case, Raw Material 4 is not purchased. During the first two periods the decision of the raw material to purchase is a trade off between the price of the products and the operating costs of the plants involved in their treatment.

4.2.2.3 Case 3

The purpose of this case is to see how the optimisation reacts if the price of product 2 drops after the second period. The prices during the time horizon are shown in Figure 4.8.

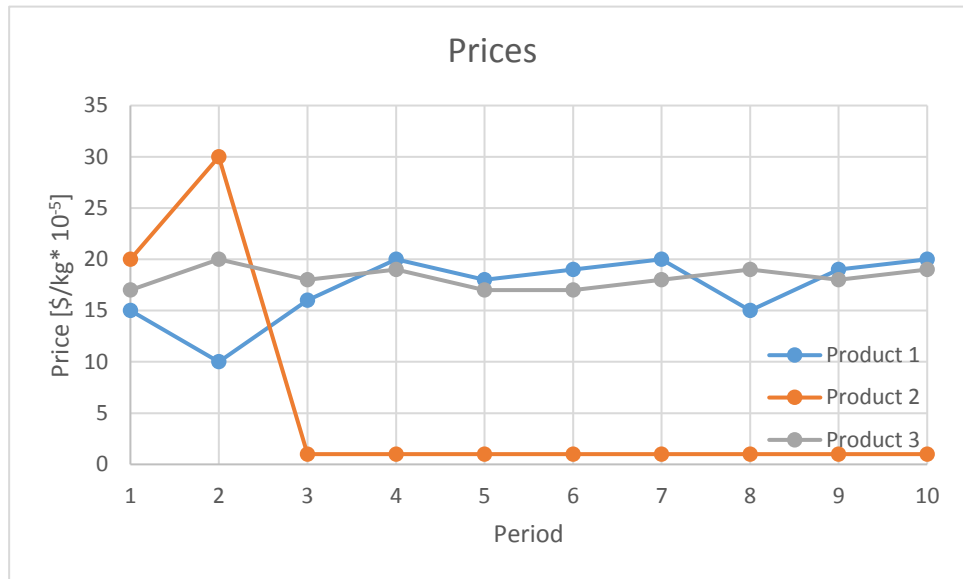


Figure 4.8. Expected prices of the three products.

Product 3 is the most profitable to produce during the first and second period, but then its price drops and its almost close to zero. The optimisation has to decide if it is still profitable to invest some money in its production, or if it is better to increase the production of the other products. The optimisation obtains a total profit of $2.83 \cdot 10^9$ \$, which is much lower than the profits obtained for Case 1 and Case 2. This results is expected, since the price of the most profitable product is very low. The other results are shown in Table 4.20 and 4.21 and in Figure 4.9. Table 4.20 shows how four of the plants are revamped during the first period, while the first Gas Plant is revamped during the third period.

Table 4.20. Revamping schedule.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------|----------------------------|---|-----|---|---|---|---|---|---|----|
| | Is the capacity increased? | | | | | | | | | |
| YGP,1 | - | - | yes | - | - | - | - | - | - | - |
| YGP,2 | yes | - | - | - | - | - | - | - | - | - |
| YGP,3 | - | - | - | - | - | - | - | - | - | - |
| YGP,4 | - | - | - | - | - | - | - | - | - | - |
| YGP,5 | - | - | - | - | - | - | - | - | - | - |
| YGP,6 | yes | - | - | - | - | - | - | - | - | - |
| Ystab,1 | yes | - | - | - | - | - | - | - | - | - |
| Ystab,2 | - | - | - | - | - | - | - | - | - | - |
| Ystab,3 | - | - | - | - | - | - | - | - | - | - |
| Ystab,4 | yes | - | - | - | - | - | - | - | - | - |

Figure 4.9 shows the revamped plants. As in Case 1, Stabilizer 1 and 4 are revamped, since they are the ones with the lower capacity and consequently higher operative cost. The gas plants related to the production of Product 1 and 3 are revamped, while the gas plants related to Product 2 are not revamped.

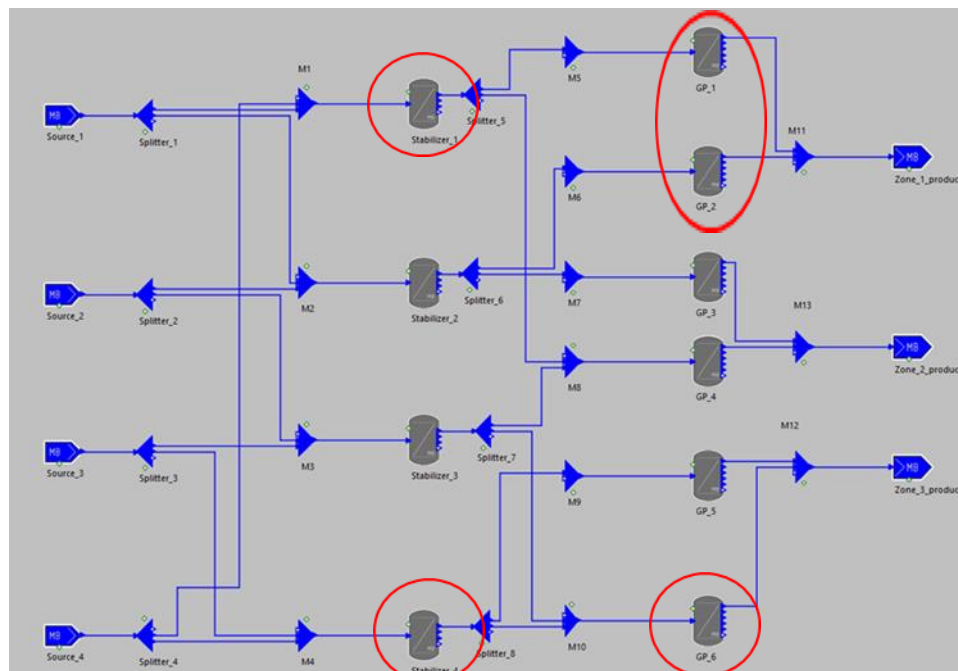
**Figure 4.9.** Revamped plants.

Table 4.21. Inlet and outlet flowrates.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| | kmol/h | | | | | | | | | |
| Raw Material 1 | 113326 | 74986 | 69629.9 | 69629.9 | 69629.9 | 69629.9 | 69629.9 | 69629.9 | 69629.9 | 69629.9 |
| Raw Material 2 | 42849 | 42849 | 42849 | 42849 | 0 | 0 | 42849 | 42849 | 0 | 42849 |
| Raw Material 3 | 32083 | 32137 | 32083 | 32083 | 74879 | 74879 | 32083 | 32083 | 74879 | 32083 |
| Raw Material 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 1 | 35193 | 0 | 63915 | 63915 | 63915 | 63915 | 63915 | 63915 | 63915 | 63915 |
| Product 2 | 68831.5 | 68831.5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 3 | 68782 | 68832 | 68782 | 68782 | 68733 | 68733 | 68782 | 68782 | 68782 | 68782 |

Table 4.21 shows how Product 2 is produced only during the first and the second periods. After that the price drops, the production of Product 1 is increased, which is the reason for the revamping which happens during the third period.

No revamping is performed on the plants responsible for the production of Product 2.

The three cases show how the multiperiod optimisation for strategic planning problems related to the revamping works with different input data. The results are the ones which were expected.

4.2.3 New Plant

The last type of strategic planning decision which is applied to the network of plants is the possibility of building a new plant. In this case the aim of the optimisation is to decide if and when it is profitable to build it. The initial network is shown in Figure 4.10.

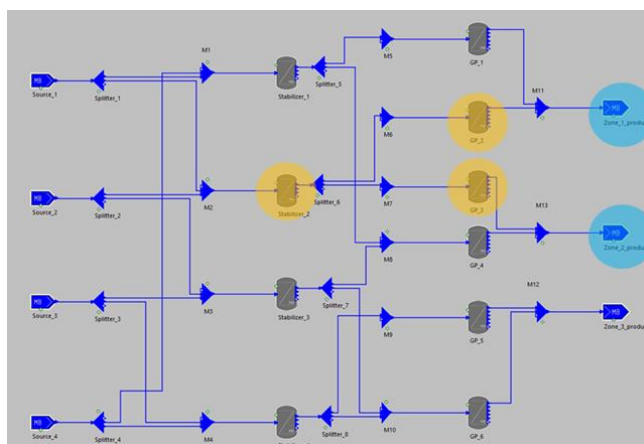


Figure 4.10. Initial network of plants

It is assumed that at the beginning of the time horizon Gas Plant 2 and 3 and Stabilizer 2 have already been built. These plants produce Product 1 and 2, while Product 3 is not originally produced.

All the possible plants that can be built are already modelled in the flowsheet, and they can be enabled by the optimisation solver. The construction of the plant has an impact on the economic balance through the following equation.

$$\begin{aligned} profit_t = revenues_t - operating\ costs_t - cost_{GP} \\ * \sum_j y_{GP,j,t} - cost_{Stab} * \sum_j y_{Stab,j,t} \end{aligned} \quad (4.20)$$

where $y_{k,j,t}$ represent the decision to build the plant of type k number j in the period t .

The continuity from a period to the following one is assured by the equation below, which tracks the plants that were built during the previous periods.

$$plant\ in\ operation_t = plant\ in\ operation_{t-1} + y_{k,j,t} \quad (4.21)$$

Plant in operation is a variable that defined if a plant exists in period t .

The constraints of the problem are the following ones.

$$\sum_t y_{k,j,t} \leq 1 \quad (4.22)$$

$$\sum_j y_{k,j,t} \leq a_k \quad (4.23)$$

The first constraint assures that the variable y just assumes the values 0 and 1, while the second one defines the total number of plants a_k of type k that can be built during period t .

Four cases are solved using this model. Each case differs for the prices, or for the number of new plants which is possible to build.

4.2.3.1 Case 1.

As a first approximation, this case is solved assuming that the new plant is completely operative in the same period in which it is built. The prices of the products during the time horizon are the same as in §4.2.1.1.

The number of possible plants which can be built is explicitly bound by the following constraints.

$$\sum_t \sum_j y_{GP,t,j} \leq 2 \quad (4.24)$$

$$\sum_t \sum_j y_{stab,t,j} \leq 1 \tag{4.25}$$

The data related to the construction costs are shown in Table 4.22, and are used for all the cases of this section.

Table 4.22. Costs of constructions.

| | | |
|----------------------|--------------------|------------|
| Type of plant | GP | stabilizer |
| | \$*10 ⁹ | |
| Cost of construction | 0.5 | 2 |

The optimisation has to decide if and when a new plant should be built, and to find the operative conditions for each period.

The solution found has a total profit of 3.97 10⁹ \$. The other results are reported in Table 4.23 and 4.24 and Figure 4.11.

Table 4.23. Plant building schedule.

| | | | | | | | | | | |
|---------------------|---------------------|---|---|---|---|---|---|---|---|----|
| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| | Is the plant built? | | | | | | | | | |
| y _{GP,1} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,4} | yes | - | - | - | - | - | - | - | - | - |
| y _{GP,5} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,6} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,1} | yes | - | - | - | - | - | - | - | - | - |
| y _{stab,3} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,4} | - | - | - | - | - | - | - | - | - | - |

Table 4.23 shows that only two plants are built, even if the boundaries allow the construction of three. All the plants are built during the first period, so that the production would be increased as soon as possible.

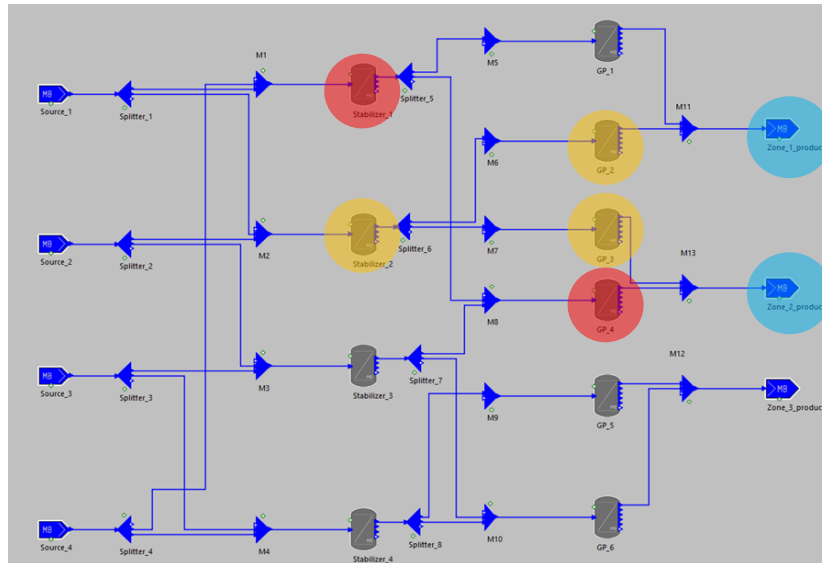


Figure 4.11. Final network of plants

Figure 4.11 shows the final network which is built. The plants necessary for the production of Product 3, the less valuable, are not built. In particular, it is profitable to build another gas plant and stabilizer to produce Product 2. It is better to feed it through stabilizer 1 (not stabilizer 3) because the feed material is cheaper, even if the operative costs are higher.

Table 4.24. Inlet and outlet flowrates.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| | kmol/h | | | | | | | | | |
| Raw Material 1 | 98009 | 71228 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 |
| Raw Material 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Raw Material 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Raw Material 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 1 | 24583 | 0 | 24583 | 24583 | 24583 | 24583 | 24583 | 24583 | 24583 | 24583 |
| Product 2 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 |
| Product 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Table 4.24 shows that the outlet flowrate of Product 2 is the highest. Only Raw Material 1, the cheapest, is purchased.

4.2.3.2 Case 2

For this case and for the next ones, it is assumed that the plant construction lasts one year. The costs are paid during the construction.

The total number of new plants that is possible to build is modified, as show in the following equations.

$$\sum_t \sum_j y_{GP,t,j} \leq 3 \tag{4.26}$$

$$\sum_t \sum_j y_{stab,t,j} \leq 2 \tag{4.27}$$

The prices used for this case are the same one used in 0.

The optimisation obtains a total profit of $3.84 \cdot 10^9$ \$. The other results are reported in Table 4.25 and 4.26 and in Figure 4.12.

Table 4.25. Plant building schedule.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------|---------------------|----|-------|----|----|----|----|----|----|----|
| | Is the plant built? | | | | | | | | | |
| y _{GP,1} | - | - | Built | On | On | On | On | On | On | On |
| y _{GP,4} | Built | On | On | On | On | On | On | On | On | On |
| y _{GP,5} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,6} | Built | On | On | On | On | On | On | On | On | On |
| y _{stab,1} | Built | On | On | On | On | On | On | On | On | On |
| y _{stab,3} | Built | On | On | On | On | On | On | On | On | On |
| y _{stab,4} | - | - | - | - | - | - | - | - | - | - |

Table 4.25 shows that all the plants allowed by the boundaries are built. Four plants are built during the first period, so that the production would increase as soon as possible, while Gas Plant 1 is built during the third period for effect of the NPV.

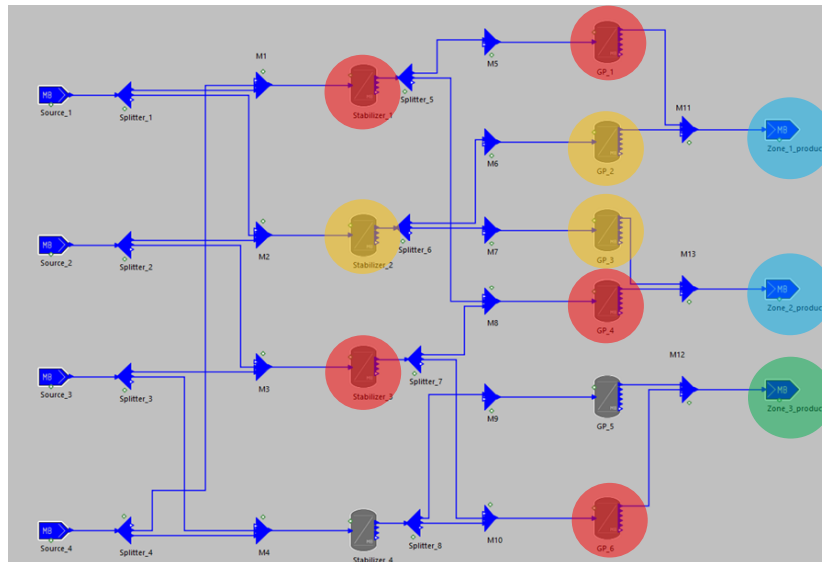


Figure 4.12. Final network of plants.

In fact, Figure 4.12 show the final network which is obtained. The building of new plants allows the production of Product 3 and an increase of the production of Product 1 and 2. Between Gas Plant 5 and Gas Plant 6, the optimisation decides to build Gas Plant 6 because it has a larger capacity, and consequent lower operative cost.

Table 4.26. Inlet and outlet flowrates.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| | kmol/h | | | | | | | | | |
| Raw Material 1 | 48205 | 71228 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 |
| Raw Material 2 | 0 | 41251 | 41251 | 59764 | 59764 | 59764 | 59764 | 41251 | 59764 | 59764 |
| Raw Material 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Raw Material 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 1 | 24583 | 0 | 24583 | 41577 | 41577 | 41577 | 41577 | 24583 | 41577 | 41577 |
| Product 2 | 19666 | 68832 | 68832 | 68832 | 68832 | 68832 | 68832 | 68832 | 68832 | 68832 |
| Product 3 | 0 | 34416 | 34416 | 34416 | 34416 | 34416 | 34416 | 34416 | 34416 | 34416 |

Table 4.26 shows the increases in the flowrates when the plants have been built. In particular, during the second period it is possible both to start to produce Product 3 and to increase the production of Product 2. The production of Product 1 increases after the third period, since it is the moment when its price increases.

At the beginning only Raw Material 1, the cheapest, is purchased, but starting from the second period it is necessary to purchase also Raw Material 2.

4.2.3.3 Case 3

This case differs from the previous one because the constraints are stricter, in order to see which plant is more profitable to build.

$$\sum_t \sum_j y_{GP,t,j} \leq 2$$

$$\sum_t \sum_j y_{stab,t,j} \leq 1$$

It is still assumed that the plant is paid during the construction, which lasts one year. The prices are the same one used in §4.2.1.1.

The optimisation obtains a total profit of $3.56 \cdot 10^9$ \$. The other results are reported in Table 4.27 and 4.28 and Figure 4.13.

Table 4.27. Plant building schedule.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------|---------------------|----|----|----|----|----|----|----|----|----|
| | Is the plant built? | | | | | | | | | |
| y _{GP,1} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,4} | Built | On | On | On | On | On | On | On | On | On |
| y _{GP,5} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,6} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,1} | Built | On | On | On | On | On | On | On | On | On |
| y _{stab,3} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,4} | - | - | - | - | - | - | - | - | - | - |

Table 4.27 shows that only two plants are built, even if it would be possible to build three. Both the plants are built during the first period, so that the production is increased as soon as possible.

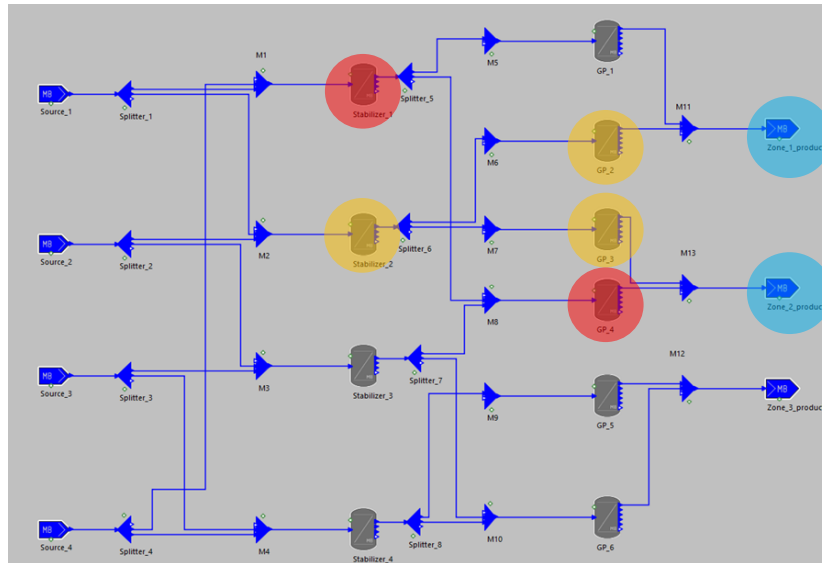


Figure 4.13. Final network of plants.

Figure 4.13 shows the final network which is obtained. With this configuration, it is possible to produce only Product 1 and 2. The plants for the production of Product 3 are not built because of the constraints,

Table 4.28. Inlet and outlet flowrates.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| | kmol/h | | | | | | | | | |
| Raw Material 1 | 48205 | 71228 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 | 98009 |
| Raw Material 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Raw Material 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Raw Material 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 1 | 24583 | 0 | 24583 | 24583 | 24583 | 24583 | 24583 | 24583 | 24583 | 24583 |
| Product 2 | 19666 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 | 65382 |
| Product 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Table 4.28 shows that the production of Product 2 is increased. Only Raw Material 1, the cheapest, is purchased.

4.2.3.4 Case 4

This cases uses the same constraints on the number of new plants as the previous case, but the products prices are different. The purpose is to see how the optimisation deal with a drop in the price of product 2. The prices are shown in figure 4.14.

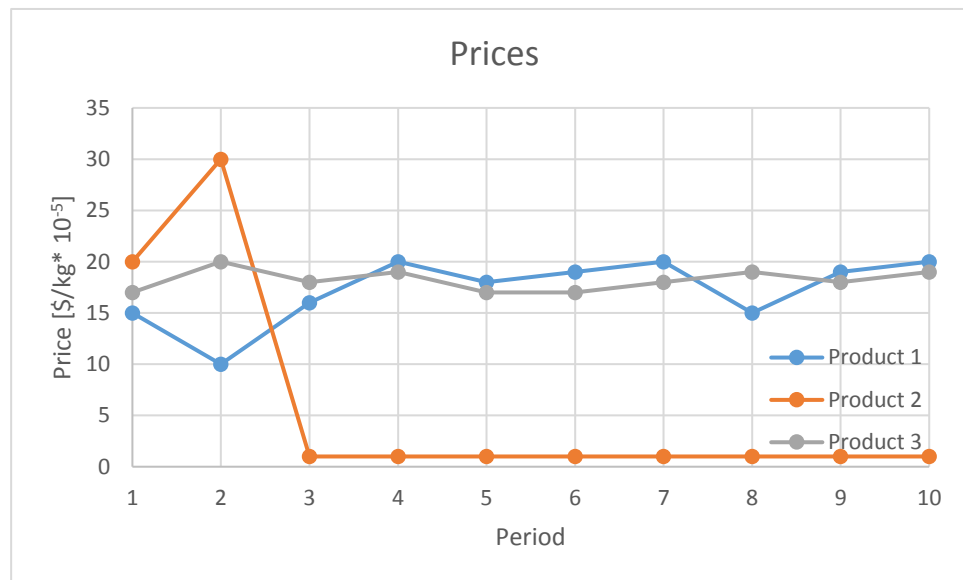


Figure 4.14. Expected prices of the three products.

It is expected that the optimisation decide if the production of Product 2 has to be increased even if the price is expected to drop.

The optimisation obtains a total profit of $1.34 \cdot 10^9$ \$. The other results are reported in Table 4.29 and 4.30 and in Figure 4.15.

Table 4.29. Plant building schedule.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------|---------------------|----|-------|----|----|----|----|----|----|----|
| | Is the plant built? | | | | | | | | | |
| y _{GP,1} | - | - | Built | On | On | On | On | On | On | On |
| y _{GP,4} | Built | On | On | On | On | On | On | On | On | On |
| y _{GP,5} | - | - | - | - | - | - | - | - | - | - |
| y _{GP,6} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,1} | Built | On | On | On | On | On | On | On | On | On |
| y _{stab,3} | - | - | - | - | - | - | - | - | - | - |
| y _{stab,4} | - | - | - | - | - | - | - | - | - | - |

Table 4.29 shows that all the plants which are allowed by the constraints are built

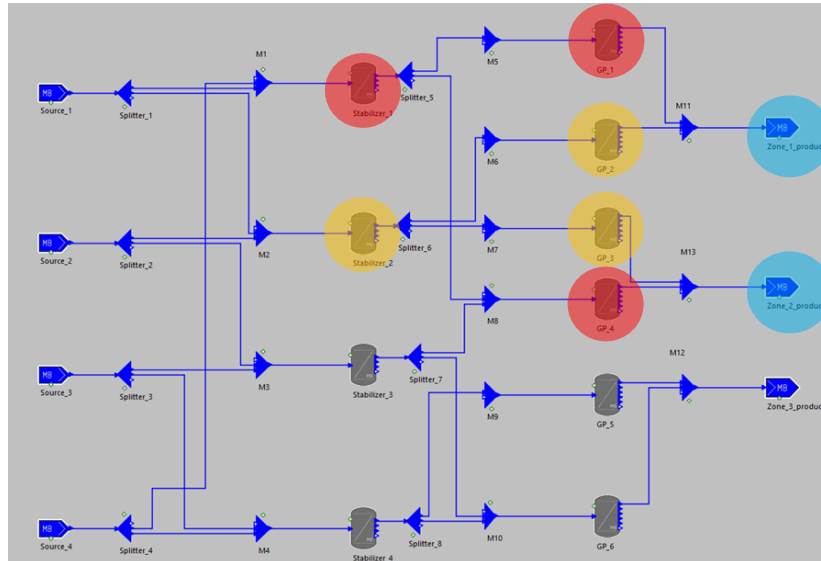


Figure 4.15. Final network of plants.

Figure 4.15 shows the final network of plants. It is not possible to produce product 3 with the final network.

Table 4.30. Inlet and outlet flowrates.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|--------|-------|---|-------|-------|-------|-------|---|-------|-------|
| | kmol/h | | | | | | | | | |
| Raw Material 1 | 48205 | 71228 | 0 | 58918 | 58918 | 58918 | 58918 | 0 | 58918 | 58918 |
| Raw Material 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Raw Material 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Raw Material 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 1 | 24583 | 0 | 0 | 54082 | 54082 | 54082 | 54082 | 0 | 54082 | 54082 |
| Product 2 | 19666 | 65382 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Product 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

It is still profitable to increase the production of Product 2 during the second period, even if then the value drops and Product 2 is not produced anymore. For this reason Gas Plant 4 is built during the first period. The production of Product 1 is increased during the third period, when its price increases, because the construction costs are delayed for effect of the NPV. From the fourth period on Product 1 is the only outlet flowrate.

As in the previous case, only Raw Material 1 is purchased.

The cases show that the optimisation reaches the expected results for the three cases of strategic planning considered, even if the flowsheet is relatively complex.

The chapter shows some simple applications of strategic planning multiperiod problem. Three general situations, the signing of a contract, the revamping of an old plant or the building of a new plant, were applied to two different problems, the blending problem and the network of plants. The optimisations reach the expected results both with the simple blending problem and with the more complex network of plants.

The problems were solved using gProms, which was only the first step. The next phase would be to solve the same problems with the prototype structure, and to check if the same results are reached. After that, it would be possible to implement the new feature in gProms, allowing for the periods to be solved independently.

Conclusions

This thesis tackles the topic of multiperiod optimisation. In particular, the work can be divided into two sections: multiperiod problem with inventory levels and with strategic planning.

For the multiperiod problem with inventories, the purpose was to apply the general multiperiod problem to some specific examples, and to solve them using the python prototype structure. The code was adapted to solve the specific problems.

For the blending problem and the network of plants, the same results were reached using both the prototype structure and gProms, which means that the prototype structure is able to solve successfully problems of small and average size. It was not possible to reach a result for the ethylene problem using the prototype structure because of a problem in the solver, even if the solution could be obtained using gProms.

The second part of the thesis is related to the strategic planning multiperiod problem. The purpose was to apply the multiperiod optimisation to the model of a plant, and to obtain a set of working examples in gProms. In particular, the optimisation was solved for the blending problem and for the network of plants. After reaching the solution, a general structure for the problem was defined, and expressed through an xml file. It was not possible to solve the strategic planning problems using the prototype structure, since a solver able to tackle binary variables was not available.

In conclusion, further work is required for both types of multiperiod problems so as to have the prototype structure suitable for real-world case studies.

First, the part of the code related to the solver for the multiperiod problem with inventories has to be modified until it is possible to solve the multiperiod optimisation of large models (e.g. the ethylene plant example). Afterwards, it will be necessary to compare the results with the ones that can be obtained using gProms.

Another step will be to build the prototype structure for the strategic planning multiperiod problems. In particular, it will be necessary to adapt the codes to work with the new xml file and with a different solver. It will be then necessary to solve several case studies using the prototype structure and to check if the results reached are the same obtained using only gProms. The examples should include complex models.

After these results will be reached, it will be possible to pass to the following step: implementing the structure into gProms, so that the platform will be able to solve the periods independently.

Nomenclature

Indices

| | |
|-----|--|
| i | input variable index |
| m | always present input variable index, $m \in i$ |
| n | unexpected events variable index, $n \in i$ |
| k | raw material specie index, $k \in i$ |
| j | output variable index |
| p | storable outputs (materials) variable index, $p \in j$ |
| q | not storable outputs (utilities) variable index, $q \in j$ |
| f | constraint index |
| t | time period index |

Variables

| | |
|----------------|--|
| $u_{i,t}$ | input i at time period t |
| $\mu_{m,t}$ | inputs always present |
| $\Theta_{n,t}$ | unexpected events |
| $y_{j,t}$ | output j at time period t |
| $M_{p,t}$ | outputs that can be stored (raw materials) |
| $U_{q,t}$ | outputs that cannot be stored (utilities) |
| $c_{f,t}$ | constraints f at time period t |
| $CR_{k,t}$ | raw material consumption at time period t , $CR_{k,t} \in u_{i,t}$ |
| $PR_{p,t}$ | raw material consumption at time period t , $PR_{l,t} \in y_{j,t}$ |
| $A_{k,t}$ | fresh feed flowrate of raw material k at time period t |
| $IR_{k,t}$ | inventory of raw material k at the end of time period t |
| $S_{p,t}$ | sale of product l at time period t |
| $IP_{p,t}$ | inventory of product l at the end of time period t |
| P_t | profit at time period t |
| ν, λ | KKT multipliers |
| S | product amount specified by contract |
| b | BB variable |

| | |
|-------|--|
| $[b]$ | integer part of b |
| b^* | fractional part of b |
| y_t | binary variable |
| | contract: define if contract is signed in t |
| | revamping: define if plant is revamped in t |
| | new plant: define if new plant is built in t |
| z_t | binary variable |
| | contract: define if contract is valid in t |
| | new plant: define if the new plant exists in t |
| d | generic variable modified during the revamping |

Parameters

| | |
|----------------------------------|---|
| $\alpha_{i,t}^u$ | cost associated with variable $u_{i,t}$ |
| $\alpha_{q,t}^U$ | price associated with variable $U_{q,t}$ |
| $\beta_{k,t}^A$ | purchase cost of raw material k at time period t |
| $\beta_{p,t}^S$ | sale price of product p at time period t |
| $\gamma_{k,t}^{IR}$ | inventory cost of raw material k at time period t |
| $\gamma_{p,t}^{IP}$ | inventory cost of product p at time period t |
| $u_{i,t}^{min}, u_{i,t}^{max}$ | lower and upper bounds of process model input variable i at time t |
| $y_{j,t}^{min}, y_{j,t}^{max}$ | lower and upper bounds of process model output variable j at time t |
| $A_{k,t}^{min}, A_{k,t}^{max}$ | lower and upper bounds of raw material feedstock $A_{k,t}$ |
| $IR_{k,t}^{min}, IR_{k,t}^{max}$ | lower and upper bounds of raw material inventory $IR_{k,t}$ |
| $S_{p,t}^{min}, S_{p,t}^{max}$ | lower and upper bounds of product sale $S_{l,t}$ |
| $IP_{p,t}^{min}, IP_{p,t}^{max}$ | lower and upper bounds of product inventory $IP_{l,t}$ |
| $IR_{k,0}, IP_{p,0}$ | initial inventory levels |
| I | total number of input u_i |
| M | total number of inputs that are always present |
| N | total number of inputs that are not always present |
| K | total number of raw materials |
| J | total number of output y_i |
| P | total number of storable inputs (materials) |
| Q | total number of not storable inputs (utilities) |

| | |
|--------------------|---|
| F | total number of constraints |
| T | total number of periods |
| D_t | duration of the time period t |
| δ | trust region radius |
| r | annual discount rate |
| w | product price specified by contract |
| S_{min}, S_{max} | lower and upper bound for product amount specified by contract |
| n | length of a contract |
| t_{min}, t_{max} | lower and upper bound for the time periods when the revamping can be performed. |
| C | cost of revamping or of building a new plant |

Functions

| | |
|-----------|-----------------------------------|
| $f_{r,t}$ | mathematical model of the process |
| $g_{f,t}$ | constraint |
| c | equality constraints |
| f | inequality constraints |
| m | quadratic approximation of f |

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