THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

OPTIMISATION OF LONG-TERM INDUSTRIAL PLANNING

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Optimisation of Long-Term Industrial Planning

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Abstract

In this thesis, long-term optimisation methods for industrial transition processes have been developed, taking monetary and environmental considerations into account. Two different methods for investment optimisation have been developed. First, an optimisation method comprising simultaneous calculation of the long-term investment strategy and the short-term utilisation scheme for a deterministic demand was developed. The method has been applied to the case of finding an investment strategy for minimising the production cost for a single hydrogen refuelling station. The problem was shown to be convex; thus the resulting solution is the global optimum. Second, an investment optimisation method using stochastic demand scenarios and multi-objective optimal control to produce the Pareto front of the two conflicting objectives *expected production cost* and *expected unsatisfied demand* was developed. This method was applied to the case of finding the optimal investment strategy for a combined hydrogen and hythane refuelling station. Depending on the preferences of the decision-maker, many different feasible solutions can be found. However, it was also found that, due to the uncertainty of the stochastic demand function, satisfying all the estimated demands would require a production capacity well above the mean demand, which would be very costly to maintain.

In addition to the two methods for investment optimisation, a modelling approach for systems combining economic and environmental aspects has been developed as well. This approach has been used for modelling cement production facilities, taking both economic and environmental issues into consideration.

In order to deal with prediction uncertainties, time series prediction using genetic algorithms was investigated as well. Discrete-time prediction networks, a novel type of recurrent neural networks, were introduced, and were shown to provide one-step macro-economic time series prediction with greater accuracy than several other methods.

Keywords: Transition strategy optimisation, Investment strategies, Multi-objective decision making, Optimisation under uncertainty.

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APPENDED PAPERS

List of publications

The work presented is based on the following publications, which are included in the thesis.

I. Karin Gäbel, Peter Forsberg and Ann-Marie Tillman, The design and building of a lifecycle-based process model for simulating environmental performance, product performance and cost in cement manufacturing, *Journal of Cleaner Production*, Volume 12, Issue 1, February 2004, pp. 77-93.

II. Peter Forsberg and Magnus Karlström, On optimal investment strategies for a hydrogen refueling station, *International Journal of Hydrogen Energy*, In press, corrected proof available online 25 July 2006.

III. Peter Forsberg and Mattias Wahde, Macroeconomic and financial time series prediction using networks and evolutionary algorithms, Proceedings of Computational Finance 2006, London, 27-29 June 2006, pp. 403-411.

IV. Peter Forsberg and Magnus Karlström, Optimization of the investment strategy for a combined hydrogen and hythane refueling station, submitted to *International Journal of Hydrogen Energy*.

The author has also contributed to research in the following related subjects.

V. Peter Forsberg, Modelling and Simulation in LCA, CPM Technical Report 2000:1, 2000.

VI. Wim Dewulf, Raul Carlson, Åsa Ander, Peter Forsberg and Joust Duflou, Integrating Pro-Active Support in Ecodesign of Railway Vehicles, *Proceedings of 7th CIRP Seminar on Life Cycle Engineering*, Tokyo, 27-29 Nov. 2000, pp 111-118.

VII. Raul Carlson, Peter Forsberg, Wim Dewulf and Lennart Karlsson, A full design for environment (DfE) data model, *Proceedings of Product Data Technology*, Brussels, 25-26 April 2001, pp 129-135.

VIII. Raul Carlson, Maria Erixon, Peter Forsberg and Ann-Christin Pålsson, System for Integrated Business Environmental Information Management, *Advances in Environmental Research*, 5 2001, pp 369-375.

IX. Wim Dewulf, Joost Duflou, Raul Carlson, Peter Forsberg, Lennart Karlsson., Dag Ravemark, Åsa Ander and Gerold Spykman, Information Management of Rail Vehicle Design for Environment for the entire Product Life Cycle, *Proceedings of 1st International Conference on Life Cycle Management*, LCM 2001, Copenhagen, 27-29 August 2001, pp 69-72.

Nomenclature

Allele 19
In a GA, the possible settings for a gene.

Auto-regression, AR 28
In time series prediction, using a linear combination of past values to calculate the predicted future value.

Chromosome 18
In a GA, a string of genes representing a potential solution to a problem.

Convex curve 13
A curve that is bulging outward over its total extension.

Crossover 19
In a GA, exchange of genetic material between two individuals.

Crowding distance 21
The mean distance to the neighbouring solution for a multi-objective optimisation problem.

Dynamic programming 22
A dynamic optimisation method that makes use of Bellman's principle of optimality to solve the problem by backward induction.

Dynamical optimisation 21
An optimisation problem defined over a time period.

Dynamical problem 13
A problem defined over time and containing time-continuous or discrete dynamic parts.

Feasible point 17
A point satisfying all constraints for an optimisation problem.

Flow semantics 38
The connection between, and use of, the general variables intensity and flow..

Functional unit 9
In LCA, a reference to which the inputs and outputs of a product system are related as parts of the normalisation.

Gene 19
In a GA, the smallest part of a chromosome.

Generation 19
In a GA, the procedure of evaluating the individuals in a population and replacing the population by its offspring.

Genetic algorithm (GA) 18
Genetic algorithm. A stochastic optimisation method inspired by natural evolution.

Hydrogen reformer 41
A device to produce hydrogen from hydrocarbons, e.g. methane gas.

Hythane 44
Natural gas with a small ratio of hydrogen.

Individual 18
In a GA, a member of a population, carrying one chromosome.

LCA 9
Life cycle assessment. A systematic method to assess the environmental impact of a product or function produced. Also called Life cycle analysis.

LCI 9
Life cycle inventory analysis. Quantifying the relevant products, resources used and emissions released for the entire life cycle of a product.

Markov decision process (MDP) 33
A process where the decisions taken at a certain point only depend on the state at the previous point in time, and not states further back in time.

Moving average 28
In time series prediction, to calculate the predicted future value by averaging a number of past values.

Multi-objective optimisation problem (MOOP) 18
An optimisation problem having more than one objective function, see also Pareto front.

Mutation 19
In a GA, the operation of probabilistically changing one gene at random.

Normalisation 9
In LCA, relating the flows in a product system to the functional unit.

Objective function 13
The function to be optimised in an optimisation problem.

Optimal control 22
See Dynamical optimisation.

Pareto front 18
A curve of points such that, for points on the curve, no criterion can become better without making another criterion worse.

Reference flow 9
A measure of the needed outputs from processes in a given product system required to fulfill the function expressed by the functional unit.

Sample 24
In stochastic optimisation, one outcome of the disturbance generated from a scenario.

Selection 19
In a GA, selection of individuals for crossover.

Stochastic dynamic optimisation 24
A dynamic optimisation method for systems under the influence of a stochastic disturbance.

Stochastic programming 24
An optimisation method for solving stochastic dynamical optimisation problems.

Time series prediction 28
The process of predicting future values in a time series using past data.

Unit process 9
In LCA, the smallest part of a product system for which data is collected when undertaking an LCA.

Chapter 1

Introduction

This thesis focuses on optimisation of *industrial transition processes*. A transition process can involve change of equipment, re-location of premises or some other structural change in, for example, societal infrastructure. These processes often involve large investments that are implemented over a long time, and in a situation of uncertain future development. Under such circumstances, finding the optimal investment strategy is not an easy task. A common approach in investment planning [1, 2] is to list a number of alternatives, and then to pick the best one by hand or to use a rule-of-thumb technique, a procedure that, in the case of highly complex systems, most often results in a sub-optimal solution being found. A better approach for finding the optimal solution is to make use of mathematical optimisation techniques such as **dynamical optimisation** to search for the optimal investment strategy; Such approaches are considered in this thesis.

The research objective in this thesis is to develop methods for optimisation of industrial transition processes with monetary and environmental considerations. In doing so, three areas are investigated: (1) modelling of production systems, (2) prediction of future behaviour using TSP and (3) optimisation of investment strategies using **optimal control**.

In the field of economics, investment planning is an important topic [3, 4]. Of highest interest is then, of course, to find the optimal investment strategy. This problem, which can be solved using optimal control theory, is in general defined over some period of time. In other, related applications, optimal control theory is used for, e.g. maximising growth in national economics [5], finding optimal investments in funds [6], production planning [7], optimisation of sequential investments [8], and maximising return on capital funds [9]. Under the influence of a stochastic disturbance, here in the form of an uncertain future development, the optimisation problem becomes a **stochastic dynamic optimisation** problem. In economics, this type of problem is referred to as *investment under uncertainty* [10, 11, 12] and in process engineering as *process design under un-*

certainty [13, 14]. In Paper IV, stochastic optimal control theory is used to find the lowest expected production cost for a combined hydrogen and **hythane** refuelling station under the influence of three stochastic demand scenarios. In both the above cases, discussed in Papers II and IV, the developed methods are intended to be used for decision support.

Recent studies have been made regarding the economical feasibility of hydrogen in regard to the infrastructure that must be built [15, 16, 17, 18, 19, 20, 21]. However, none of these studies investigates the implications of investments over time. By contrast, in Paper II optimal control theory is used to find a short-term equipment variable utilization for one-week periods and, at the same time, a long-term investment strategy for the whole investment period covering 20 years with the aim of minimising the production cost for a plant. The method is exemplified by a hydrogen dispensing infrastructure case.

Predicting future values of key variables is, of course, highly relevant in the optimisation of transition processes. Even short-term prediction is important. Such prediction is considered in the field of **time series prediction** (TSP). Due to the often high level of noise present, standard procedures, such as the **auto-regressive** and **moving-average** methods, are sometimes not fully successful [22, 23, 24]. Instead other, more adaptive methods based, for example, on neural networks can be used [25, 26]. In Paper III of this thesis, a novel type of neural network is developed for prediction of noisy time series.

When evaluating transition processes the economic consequences are important. The environmental awareness in today's society is constantly raising the requirements of a cleaner production process. Thus, in this thesis, the environmental effects are considered as well. At the same time the increasing complexity of the production systems makes the environmental analysis more difficult to carry out. In the 1990s more advanced methods were developed to assist environmental analysis of technical systems. One of these methods is life cycle assessment (LCA). Much has been written about LCA. The ISO standards 14040-42 [27] give very general guidelines on how an LCA should be performed. In fact, many standard papers on LCA, e.g. [28, 29, 30, 31, 32, 33], approach the topic in a rather non-mathematical way. Until 1998 only one paper [34] was published regarding guidelines on how to carry out the actual calculation, the so called **normalisation**. After 1998, the subject of normalisation in LCA has been considered in a mathematical point-of-view by Heijungs [35, 36, 37]. All of the mathematical methods presented by Heijungs only consider the standard LCA which includes a linear and static model representation. For other approaches there is only a limited number of texts available. Examples include linear optimisation of LCA systems [38, 39], multi-objective optimisation [40] and dynamic life cycle inventory models [41, 42]. Some cases with integration of economic cost objectives have also emerged [43, 44]. There is still, however, a large potential for improvements concerning, for example, the range of applicability of the models. This thesis investigates a number of approaches, how they can be used, and possible improvements. The findings are exemplified by a cement production case [45] in Paper I and are intended to be used in investment optimisations, such as those presented in Papers II and IV.

1.1 Main contributions

Transition processes taking place in the societal infrastructure and in large industries are in general very complex systems. This is due to the fact that these systems do not only have technical and economic aspects, but also social, environmental, political and geographic aspects. To take all these considerations into account when constructing a model is, of course, impossible. This thesis focuses on economic and environmental aspects and aims at providing some examples of general tools for carrying out structural transition optimisation. It is the aim of the author that, when the tools presented here are used together, the effort of carrying out the above-mentioned type of optimisations should be reduced considerably.

Mathematical models are generally specific to the application at hand. Using the type of models discussed in this thesis, the flexibility with regard to the types of calculations that are possible to carry out can be increased considerably [46, 47, 48]. These models come from the study of physical systems [49], but can be successfully applied to other types of systems, e.g. environmental systems [50]. The aim of the models is to provide the optimisation algorithm with the effects of changes in the future strategy. In doing so, the model has to provide the future behaviour of key parameters. Some of these can be modelled in detail but others, where exact knowledge is lacking, must be predicted. One way of achieving this is by time series prediction [23, 51, 52]. In this way the short-term future behaviour can be estimated, something that is important for fast dynamics. Using the above-mentioned tools, the transition strategy is then optimised using stochastic multi-objective optimisation. To summarise, the main contributions of the presented work are:

- A modelling approach for production systems with environmental measures comprising separation of model and problem formulation, and leading to more flexible models (Paper I).

- Progress in time series prediction (TSP) using genetic algorithms (GAs) resulting in increased accuracy for predictions of noisy time series (Paper III).

- Methods for concurrent optimisation of investment strategies and run patterns for long-term planning of industrial production sites, taking economic and environmental considerations into account. In Paper II the model is of the single-objective deterministic kind and in Paper IV of the multi-objective stochastic kind.

- Specific results regarding optimal investments for hydrogen and hythane refuelling stations (Papers II and IV).

The author was the main contributor to Papers II and IV. In Paper I, the author's contributions were to develop the modelling approach and the model framework, to carry out all calculations needed for solving the problem, and to write a significant part of the paper. In Paper III both authors contributed equally.

Chapter 2

Transition processes

Structural transition processes occur in all industries. Examples include change of machinery, moving of production units and change of production at current sites. For decision support, a number of calculations are carried out regarding the economic consequences and, at times, optimisations are done [53]. However, only rarely are both economic and environmental aspects taken into account. This thesis presents some methods for integrating economic and environmental aspects when assessing industrial transition processes. The results are intended to be used for decision support.

In particular, the problem of optimising investment strategies, i.e. selecting when and to what extent investments are to be made for maximum performance, is explored. In connection with this problem, the topic of predictability of variables has also been considered within the framework of time series prediction. In most cases in this thesis the connections to economy are explicit, i.e. economic measures appear in the model, and the environmental connections are implicit, i.e. they are present through the use of an environmentally favourable technique. It should be kept in mind that this implies a constraint in the sense that only environmentally favourable techniques are considered to be part of the set of acceptable solutions. However, the developed methods, such as the multi-objective optimisation procedure described in Paper IV, have originally been designed for use in cases with explicit connections between environmental and economic aspects.

When considering large industrial structures, the economic consequences are distributed over a number of years. For a complete production line in a factory or for a major societal infrastructure change, the consequences might be distributed over a period exceeding 20 years [54, 55]. To be able to carry out an optimisation of the economic results, the variation in a number of variables, e.g. the rate of interest, the technical development within the field and the yearly production and demand, must be estimated. In order to improve the accuracy of such variables, a study of time series prediction (TSP) has been undertaken in Paper III, aimed at improving short-term (one-step) prediction of macroeconomic time series, where the time step length often equals one year or a quarter of a year. However, long-term predictions are much harder, and it is generally not possible to make optimisations of investment strategies that will be valid for the whole investment period (20 years, say). Instead, a dynamic approach must be taken to the optimisation of transition processes, such that, when the assumed values of a parameter have deviated substantially from the expected path, a new calculation is carried out, based on the new, corrected behaviour of the parameter in question. This makes it possible always to have the best and most up-to-date structural transition strategy at hand.

Life cycle assessment (LCA) [31, 32, 33, 34] is a way to quantify environmental influences of a product (or service) over its entire life. In the study presented in Paper I, similarities and differences between LCA and technical system theory [56][1] were investigated in order to make improvements in combining economic and environmental modelling. Incorporating the new findings, a model of a cement production process was generated and calculations for improving the economic and environmental performance were performed. The variables involved express aspects of quality and economy, as well as resource use and emissions. The model developed was intended for many types of calculations regarding, e.g. economy, product quality and emissions.

Changes toward more environmentally favourable solutions frequently incorporate large investments in infrastructure. The cost and uncertainty of changing these facilities are usually considered to be obstacles for the introduction of new techniques. In Papers II and IV, methods for finding optimal investment strategies for this type of environmentally favourable production facilities are investigated. Based on an assumed future development scenario, optimal investment strategies are calculated. In Paper IV, special emphasis is put on reducing the uncertainties by using several different scenarios and stochastic optimisation. The applicability of the developed method is exemplified in two studies on profitable investment strategies for a hydrogen station and a combined hydrogen and hythane refuelling station.

Finding the optimal solution to the set of problems discussed above is far from trivial. Nevertheless, in reality, many such problems are solved in an intuitive manner based on experience [57, 58], in a large part due to the fact that the mathematical formulation of the problems usually is very hard to find for these *complex systems* [59, 60]. A complex system here signifies a system composed of a number of simpler subsystems with a large, often huge, number of interconnections. Due to the large number of connections, these systems are usually very hard to

[1] The term technical system theory is here used for the science of constructing models of processes etc. as is done in control theory.

understand and model. One example of this is emergence [61, 62, 63]. Emergent properties are properties possessed by a system, which cannot be traced back to any of its parts. A good explanation of emergence is given in [64] as "*A complex system usually involves a large number of components. These components may be simple, both in terms of their internal characteristics and in the way they interact. Still, when the system is observed over longer time and length scales, there may be phenomena that are not easily understood in terms of the simple components and their interactions*".

Optimisation of complex systems can therefore play a very important role, by revealing unforeseen solutions better than those currently available. One should keep in mind though, that accurate optimisation over periods extending 20 years into the future is not easy, even using techniques that reduce the effects of uncertainty such as stochastic optimisation with multiple scenarios. When predictions are generated using models built from time series data, like the DTPNs in Paper III, an implicit assumption is that the future development follows a pattern similar to that of the past data. In this case an unforeseen major event can disrupt all predictions instantaneously. Another option is to make prediction based on a detailed model of the system combined with probable future developments, as is done in Paper IV. However, even in this case, an unforeseen event not covered by the model can disrupt all predictions. Since nothing in nature is discontinuous there are, however, always precursor events to major events. To identify these events is, of course, very important and therefore successful optimisation requires extensive knowledge of the system under study. Ideally all possible future outcomes should be included in the model. In reality this is impossible though, and one therefore has to settle for less-than-perfect models.

2.1 Economic and environmental aspects

The objectives explored in this thesis are mostly related to economy. Therefore this section starts with a discussion of the economic measures used in Papers II and IV, after which some important aspects of one possible quantification of environmental impact is presented, namely LCA. Both economic and environmental measures are considered, since it is desirable to find environmentally viable solutions that are still economically favourable. No company can support non-profitable environmental sustainability.

In the literature, future costs and incomes are usually discounted with regard to the discount rate $D > 0$ using the net present value correction [65]

$$C_p(t) = \frac{1}{(1+D)^t}, \tag{2.1}$$

where t is the time. The above equation reflects investors' preference of immediate return of cash in contrast to future returns. The actual discounting depends on the length of time and the discount rate. Usually, the discount rate is the risk-free interest rate added to an interest rate reflecting the risk involved in the specific venture. As the name implies, the risk-free interest rate is the safe rate earned from a completely risk-free investment. When optimising policies that span a long time, as the calculations in Papers II and IV do, the value of the discount rate can have a significant effect. As is pointed out in Paper IV, for a discount rate of 0.1 and in the case of an evenly distributed cost, the effective discounting is $C(t) = 0.4466$ for a time period of 20 years. $C(t)$ is the mean value of $C_p(t)$ over the time period considered. The high discount rate in Paper IV is motivated by the high risk; the investments are made in a new technique with uncertain potential and acceptance.

In both Paper II and Paper IV, the loan for purchase of equipment is assumed to be of the annuity type. In this case, it is possible to calculate a capital cost per time unit for the refuelling station. The additional costs, e.g. for purchase of raw materials and maintenance, are then added and a total instantaneous production cost at time t per produced unit can be calculated, which is measured in USD per kg $\mathrm{H_2}$.

In order to find the mean production cost for the entire investment period, one must integrate the instantaneous production cost. In Paper II, three ways of integrating this cost are shown: (1) adding the costs at all times without discounting, (2) discounting future costs using Eq. (2.1) above and (3) discounting future costs using Eq. (2.1) and distributing the total cost evenly over the whole investment period. One should keep in mind that the third option does not reflect the sum of the real cost to the production facility. The discussed mean production costs represent different ways of calculating the costs for production, depending of preference. They are all candidates for an objective function that can be used for optimisation. It should be noted that if the total capital cost is discounted to present day value using the same interest rate as for an assumed annuity loan, the result is the absolute investment cost. Since, in Paper II, only one week per investment is explicitly evaluated, the above ways of calculating the costs are used, for simplicity. Details on how production costs have been calculated are given in Paper II.

In Paper IV, the optimisation is carried out over the whole investment period covering 20 years. Since loans are considered to be of the annuity type, the costs for investments are not discounted. Investments in equipment are only subject to a decreased cost due to increased production and technology development. This is due to the fact that the effect of the annuity loan and the discounting will cancel each other out, provided that the discount rate is the same. In Paper IV, the production cost was calculated over the entire investment period, taking the total non-discounted purchase cost into account. This is in contrast to Paper II where the production cost was calculated for one week per investment, taking the non-discounted cost for the annuity loan into account, a procedure that results in a time-varying production cost, as can be seen in Paper II. Apart from investments, all other production costs were discounted, however. The mean production costs were calculated as the sum of costs divided by the sum of sold hydrogen and hythane, respectively.

Environmental effects are often less tangible than are economic ones and therefore harder to measure and quantify. One reason is that in the short perspective many environmental aspects tend to have little or no environmental effect. Instead, at a certain level, there is an abrupt and sometimes unforeseen effect. Another reason is that the causality of environmental effects is not always totally understood. One example is the Greenhouse effect. Obviously the global mean temperature is increasing in the short-term perspective, but is this caused by human activities? Economic aspects, on the other hand, tend to have a more direct and immediate effect.

However, one way environmental influences can be quantified is by LCA. The life cycle usually starts with extraction of raw materials and continues with transportation, manufacturing, use and possibly re-use. It then ends with waste management, recycling and disposal. There exists a vast literature on the concept of LCA, see e.g. [30, 34, 66, 67, 68].

In 1997 the ISO standard 14040 on LCA was approved [27]. In this standard LCA is defined as '*...the environmental aspects and potential impact throughout a product's life (i.e. cradle-to-grave) from raw material acquisition through production, use and disposal.*' Each of these stages consumes resources and produces emissions and waste. In LCA all these aspects are taken into account and are related to the product or function produced. LCA further aims at assessing the impact of the production on nature.

In the life cycle inventory analysis (LCI), which is one part of LCA, the resources, emissions and products related to the production system are measured. Then a model over the production system is created. In order to know the effects of each produced unit (in LCA called **functional unit**), the measured resources etc. are scaled to the functional unit. This is done by aggregating all **unit processes** in the product system and scaling the flows of these processes to match the **reference flow** of the system, a process referred to as **normalisation**. The data used in the inventory is based on time-averaged statistics and is hence independent of time. In addition a linear relation between resource use, emissions and production is assumed. The resulting normalisation step is mathematically equivalent to solving a linear equation system. The equation system is usually well-posed by construction, i.e. having equal number of variables and constraints, and hence possible to solve exactly. Publications on LCA cover handbooks, case studies and theoretical studies on the concept that do not, in general give any

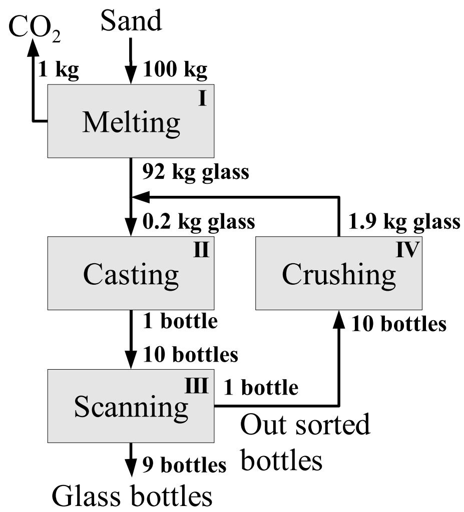

Figure 2.1: Example of a model for a small glass bottle production process. Note that, since the data for the different processes (shown as boxes in the figure) are taken from different sources, e.g. product data sheets, the amounts of flow do not match at this stage. The objective of the normalization is to scale the processes so that the flows do match. The results of the normalization procedure are shown in Figure 2.2 below.

directions on how to represent the flow model and form the resulting equation system [33, 69]. Recently a number of publications on the computational part have appeared [36, 37, 70, 71]. The result of the normalisation to the functional unit presented there is expressed as

$$\mathbf{g} = BA^{-1}\mathbf{f}, \tag{2.2}$$

where A is a matrix describing the internal flows of the technical system (the technology matrix), $\mathbf{f}$ the demand vector, i.e. a vector expressing what is being produced, and B the intervention matrix, i.e. the external flows to and from the technical system.

An example of a model for a small glass bottle production process is shown in Figure 2.1. In this process sand is melted to glass, producing carbon dioxide emissions. The glass is then cast to bottles which are scanned for defects before delivery. Some bottles are discarded in the scanning process due to defects and these bottles are returned to the casting process after crushing. Each of the above processes are unit processes. Using the nomenclature introduced above, the tech-

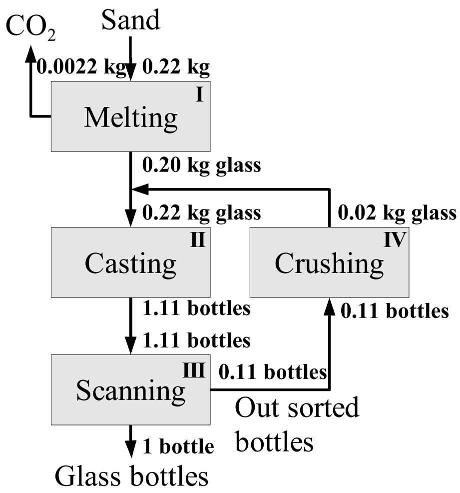

Figure 2.2: The resulting flow model for the small glass bottle production process introduced in Figure 2.1.

nology matrix becomes

$$A = \begin{bmatrix} 92 & -0.2 & 0 & 1.9 \\ 0 & 1 & -10 & 0 \\ 0 & 0 & 1 & -10 \\ 0 & 0 & 9 & 0 \end{bmatrix}, \tag{2.3}$$

where the rows in A represent the flows of glass (row 1, measured in [kg]), bottles ([pcs], row 2), recycled bottles ([pcs], row 3), and delivered bottles ([pcs], row 4), respectively. The columns represent the processes indicated by Roman numerals in Figure 2.1. Note that negative numbers indicate a flow into a process, and positive numbers a flow out from a process. The intervention matrix becomes

$$B = \begin{bmatrix} -100 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \tag{2.4}$$

where the first row represents sand ([kg]) and the second row represents carbon dioxide ([kg]). To calculate the intervention for a reference flow of one produced bottle (after the calculation this flow will become the functional unit), $\mathbf{f}$ is set to $\mathbf{f} = [0\ 0\ 0\ 1]^T$ giving $\mathbf{g} = BA^{-1}\mathbf{f} = [-0.2186\ 0.0022]^T$. The resulting resource use and emissions released are then 0.2186 kg sand and 0.0022 kg carbon dioxide, respectively. The normalised flow model is shown in Figure 2.2.

Chapter 3

Optimisation techniques

The transition processes discussed in Chapter 2 are naturally defined over some time period; they are **dynamical problems**. Industries are, of course, trying to maximize performance, implying the need for optimisation.

In order to optimise a transition process a dynamical optimisation technique must be utilized. In most cases, dynamical optimisation problems are solved by transforming them into static optimisation problems. Therefore, this chapter starts with a short overview of unconstrained and constrained non-linear static optimisation which will lay the foundation for later discussions on dynamical optimisation techniques in Section 3.3 below. In particular, the SQP algorithm used in Paper II and the multi-objective genetic algorithm used in Paper IV will be examined. In Section 3.4 optimisation of systems influenced by stochastic perturbations will be discussed.

The goal of optimisation is to find the optimal point $\mathbf{x}^*$ for a given **objective function** $\mathbf{f}(\mathbf{x})$, where $\mathbf{x} = (x_1, x_2, \ldots, x_N) \in R^N$. For the single-objective case, $f = \mathbf{f}$ is a scalar, taking values in R^1, whereas, for the multi-objective case, $\mathbf{f} \in R^N$. There may also be equality and inequality constraints of the form

$$\mathbf{c}(\mathbf{x}) = 0, \tag{3.1}$$

$$\mathbf{d}(\mathbf{x}) \geq 0, \tag{3.2}$$

as well as limits on the allowed intervals for $\mathbf{x}$, i.e. $\mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$[1]. Despite the modest appearance of this optimisation problem, finding the optimal point is, in general, a difficult task.

A special type of optimisation problem is the **convex** problem. A function $f(\mathbf{x}) : R^N \rightarrow R$ is convex if the domain of the function, denoted $\mathbf{dom}f$, is a

[1]Throughout this thesis relations between vectors such as $\mathbf{x}_l \leq \mathbf{x}$ require equal dimensions and are to be interpreted component-wise.

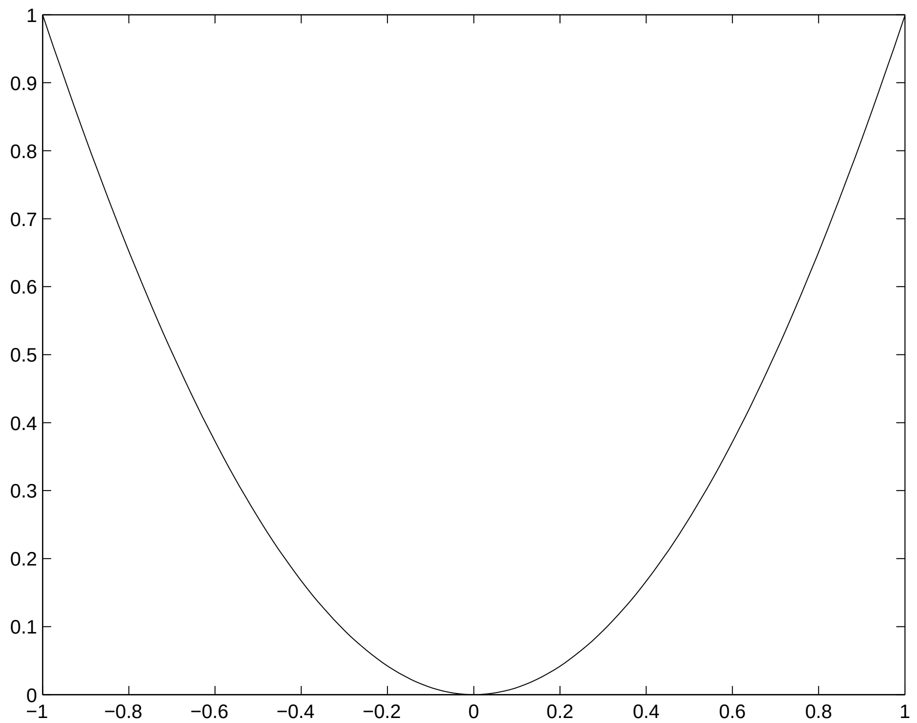

Figure 3.1: Example of a one-dimensional convex function.

convex set and

$$f(\theta\mathbf{x} + (1-\theta)\mathbf{y}) \leq \theta f(\mathbf{x}) + (1-\theta) f(\mathbf{y}) \tag{3.3}$$

$\forall\, \mathbf{x}, \mathbf{y} \in \mathbf{dom} f,\ 0 \leq \theta \leq 1.$ A non-scientific geometrical interpretation is that if f draws a curve that is bulging outward over its total extension, then it is convex. An arbitrary example of a one-dimensional convex function is given in Figure 3.1. A problem is called convex if both the objective function and the constraints are convex. Such functions are important in optimisation since they make it possible to guarantee convergence [72]. Furthermore, many non-convex optimisation problems can be transformed into convex ones [73].

3.1 Deterministic optimisation techniques

The term *deterministic* is here used to indicate that the optimisation algorithms do not contain any stochastic parts. Thus, if such an algorithm is run twice, using the same set of inputs, the results will be identical to each other, i.e. they are perfectly predictable. In deterministic optimisation there exists robust algorithms with guaranteed convergence for the linear case, i.e. the case in which the objective function and all constraints are linear. One such algorithm is the Simplex method [74]. However, in most practical problems the objective functions are non-linear. Such functions will usually have both a global optimal point and many local optimal points. Since it is very difficult to distinguish between a local and a global optimal point, simple gradient-descent algorithms are usually not successful. Such algorithms tend to get stuck on a local optimal point instead of finding the true global optimal point.

Finding the global optimal point is the major task of *non-linear programming* (NLP) [75, 76]. Consider the general NLP problem

$$\begin{aligned} \min_{\mathbf{x}\in R^N} \quad & f(\mathbf{x}) \\ \text{s.t. } \mathbf{c}(\mathbf{x}) \quad &= \quad 0 \\ \mathbf{d}(\mathbf{x}) \quad &\geq \quad 0 \end{aligned} \tag{3.4}$$

where $f(\mathbf{x})$ is the (scalar, i.e. single-objective) criterion function, $\mathbf{c}(\mathbf{x})$ the non-linear equality constraints and $\mathbf{d}(\mathbf{x})$ the non-linear inequality constraints. The functions $f(\mathbf{x})$, $\mathbf{c}(\mathbf{x})$ and $\mathbf{d}(\mathbf{x})$ are assumed to be smooth, i.e. at least twice-continuously differentiable. Let $\mathbf{g}(\mathbf{x}) = \nabla_x f(\mathbf{x})$ denote the gradient vector of the objective function, $\mathbf{C}(\mathbf{x}) = \frac{\partial \mathbf{c}}{\partial \mathbf{x}}$ the Jacobian matrix of the constraint vector $\mathbf{c}(\mathbf{x})$, and $\mathbf{D}(\mathbf{x}) = \frac{\partial \mathbf{d}}{\partial \mathbf{x}}$ the Jacobian matrix of the constraint vector $\mathbf{d}(\mathbf{x})$. Now define the (scalar-valued) Lagrangian function in the classical way [77]

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) - \boldsymbol{\lambda}^T \mathbf{c}(\mathbf{x}) - \boldsymbol{\mu}^T \mathbf{d}(\mathbf{x}), \tag{3.5}$$

where $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ are Lagrange multiplier vectors. In an optimal point the first derivative of the Lagrangian with respect to $\mathbf{x}$ is zero, i.e

$$\nabla_x \mathcal{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) = \mathbf{g}(\mathbf{x}^*) - \boldsymbol{\lambda}^{*T} \mathbf{C}(\mathbf{x}^*) - \boldsymbol{\mu}^{*T} \mathbf{D}(\mathbf{x}^*) \quad = \quad 0 \tag{3.6}$$

where $(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*)$ is the optimal point. In addition, requirements have to be put on the inequality part variables $\boldsymbol{\mu}$ and $\mathbf{d}$. At the optimal point, it is clear that an inequality constraint $d_i(\mathbf{x}^*)$ can either be satisfied as an equality, $d_i(\mathbf{x}^*) = 0$ or strictly satisfied, $d_i(\mathbf{x}^*) > 0$. In the former case the constraint is said to be *active* and hence a part of the *active set* $\mathcal{A}$, i.e. $i \in \mathcal{A}$. In the latter case the constraint is *inactive* and part of the *inactive set* $\mathcal{A}'$, i.e. $i \in \mathcal{A}'$. For the active set the requirements equal those for equality constraints, i.e. $\boldsymbol{\mu} \geq 0$. For the inactive set the multiplier *must* be zero. This can also be formulated $\boldsymbol{\mu}^{*T}\mathbf{d}(\mathbf{x}^*) = 0$, which is sometimes referred to as the *complementary slackness condition*. With these requirements, the Karush-Kuhn-Tucker (KKT) [78] condition for optimality is defined as

$$\begin{aligned} \mathbf{g}(\mathbf{x}^*) - \boldsymbol{\lambda}^{*T} \mathbf{C}(\mathbf{x}^*) - \boldsymbol{\mu}^{*T} \mathbf{D}(\mathbf{x}^*) \quad &= \quad 0 \\ \boldsymbol{\mu}^{*T} \mathbf{d}(\mathbf{x}^*) \quad &= \quad 0 \\ \boldsymbol{\mu}^* \quad &\geq \quad 0 \end{aligned} \tag{3.7}$$

and $\boldsymbol{\mu}$ is sometimes referred to as the KKT multiplier. In addition the original constraints from Eq. (3.4), $\mathbf{c}(\mathbf{x}^*) = 0$ and $\mathbf{d}(\mathbf{x}^*) \geq 0$ must be satisfied at the optimal point. In order to solve the KKT for $\mathbf{x}^*$, the active inequality constraints are treated as equality constraints and the inactive ones are ignored, giving

$$\begin{aligned} \mathbf{g}(\mathbf{x}^*) - \boldsymbol{\eta}^{*T}\mathbf{J}(\mathbf{x}^*) &= 0, \\ \mathbf{r}(\mathbf{x}^*) &= 0, \\ \boldsymbol{\eta} &\geq 0, \end{aligned} \tag{3.8}$$

where $\mathbf{r} \in \left\{\mathbf{x} \in R^N | \mathbf{c}(\mathbf{x}) = 0, d_i(\mathbf{x}) = 0 \,\forall\, i \in \mathcal{A}\right\}$ and $\mathbf{J}(\mathbf{x}) = \partial r/\partial x$. Now these re-defined requirements can be solved with Newton's method by carrying out a Taylor series expansion of Eq. (3.8). Letting $\mathbf{H}_L = \nabla^2_{xx}\mathcal{L}$, the expansion becomes

$$\begin{aligned} \mathbf{g}(\mathbf{x}) - \mathbf{J}^T(\mathbf{x})\boldsymbol{\eta} + \mathbf{H}_L(\mathbf{x})(\bar{\mathbf{x}} - \mathbf{x}) - \mathbf{J}^T(\mathbf{x})(\bar{\boldsymbol{\eta}} - \boldsymbol{\eta}) &= 0 \\ \mathbf{r}(\mathbf{x}) + \mathbf{J}(\mathbf{x})(\bar{\mathbf{x}} - \mathbf{x}) &= 0 \end{aligned} \tag{3.9}$$

which can be written as

$$\begin{bmatrix} \mathbf{H}_L & \mathbf{J}^T \\ \mathbf{J} & 0 \end{bmatrix} \begin{bmatrix} -\mathbf{p} \\ \bar{\boldsymbol{\eta}} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{r} \end{bmatrix}. \tag{3.10}$$

Solving the above equation will yield the step $\mathbf{p}$ and the Lagrange multiplier at the new point, $\bar{\boldsymbol{\eta}}$. The new point is then obtained as $\bar{\mathbf{x}} = \mathbf{x} + \mathbf{p}$. Note that in Eq. (3.10) the new Lagrange multiplier is calculated in an absolute way while, for the new point $\bar{\mathbf{x}}$, the increment $\mathbf{p}$ is calculated. The Newton step is then iterated until convergence.

The Newton method defined above is a local optimisation algorithm. In order to improve the chances of finding the global optimum, one may use a globalization strategy. One example is the line-search method which will adjust the step length $\bar{\mathbf{x}}$ by a factor β to $\bar{\mathbf{x}} = \mathbf{x} + \beta\mathbf{p}$. The value of β is usually determined by the rate of progress measured by a merit function [79, 80]. Another option is to adjust both the magnitude and direction of the search step, so that the search direction $\mathbf{p}$ will lie within a given radius which defines a trusted region [81].

A widely used algorithm to solve the above NLP problem in Eq. (3.10), i.e. to find the global optimum, is *sequential quadratic programming* (SQP), see e.g. [82, 83]. When using SQP, one may observe that Eq. (3.10) represents the first order optimality conditions for the the optimisation problem

$$\begin{aligned} \min_{\mathbf{p}} \; \mathbf{g}^T\mathbf{p} + \frac{1}{2}\mathbf{p}^T\mathbf{H}_L\mathbf{p} \\ \text{s.t. } \mathbf{J}\mathbf{p} = -\mathbf{r}, \end{aligned} \tag{3.11}$$

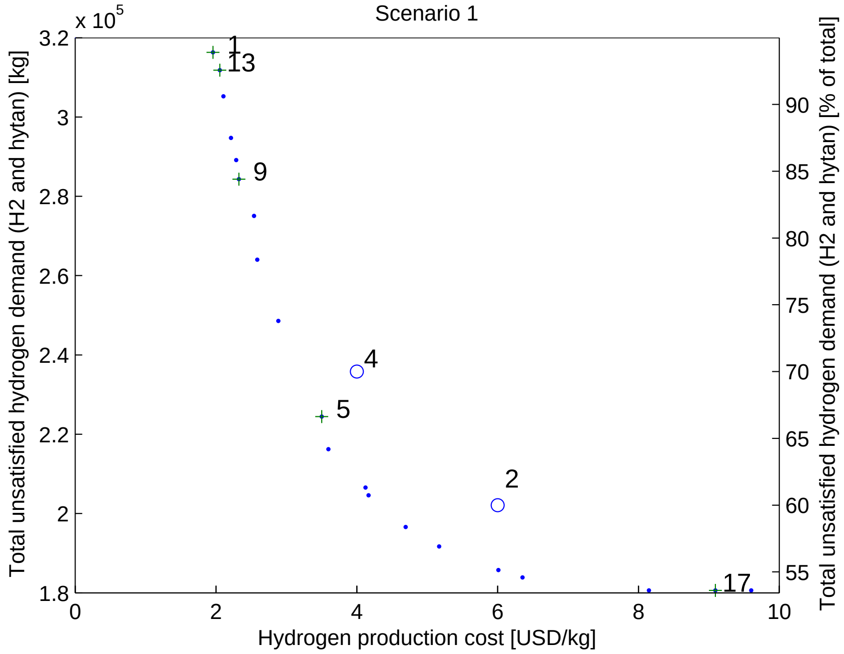

Figure 3.2: Illustration of Pareto optimality. The objective is to minimise both the unsatisfied hydrogen demand and the hydrogen production cost. Solutions marked with small dots and crosses are part of the Pareto front whereas the ones marked with circles are not.

which is a quadratic programming (QP) problem. The SQP is a sequential algorithm that makes use of inner and outer iterations. The objective of the inner iteration is to find a search direction $\mathbf{p}$ which is used in the outer one to fulfill the first order conditions for optimality. The search direction $\mathbf{p}$ is found by solving the optimisation problem in Eq. (3.11). The outer iteration makes use of the new search direction by taking the step $\bar{\mathbf{x}} = \mathbf{x} + \alpha\mathbf{p}$, where the magnitude of the step (α) is determined by a line search method. This makes the SQP a global optimisation algorithm.

In Paper II the resulting NLP optimisation problem was solved using the NPSOL program [84], which is of the above SQP class. First the NPSOL algorithm aims at calculating a point that is **feasible**, starting from a user-initiated point. Then the SQP algorithm described above is used to find the optimal point. Calculating gradients for the investment problem in Paper II is not easy. One reason is the fact that the objective function $f(\mathbf{x})$ is not differentiable in the whole of R^N. Another reason is the complex structure of summations in $f(x)$. Using NPSOL, no algebraic expressions of gradients and Hessians needs to be given. Instead, NPSOL can make use of finite-difference derivatives. The NPSOL algorithm can also deal with minor discontinuities if they are isolated and located away from the solution. The SQL algorithm described above will converge to the global optimum for convex problems [72]. Since the investment problem considered in Paper II is convex, the algorithm will find the global optimal point. The objective function is discussed in Chapter 2 above and the considered optimisation problem will be treated in more detail in Chapter 5.

In the above SQP algorithm, the objective function $f : R^N \rightarrow R$. If $\mathbf{f} : R^N \rightarrow R^M,\ M > 1$, the problem is a **multi-objective optimisation problem** (MOOP). The solution to such a problem does not consist of a single optimal point, but instead a number of points lying on a curve or surface called the **Pareto front**. These points all have in common that they are *non-dominated*. In short, it means that no other solution exists where any of the objectives are strictly better than those on the Pareto front without some other objective being equal or worse. Figure 3.2, taken from Paper IV, illustrates the principles of Pareto optimality. The objectives along the x and y axes are both to be minimised. The solutions 1, 13, 9, 5 and 17 all belong to the first Pareto front. Solution 4, however, is said to be dominated by solution 5 and therefore does not belong to the Pareto front. Not taking the first Pareto front into account, another, inferior non-dominated set of solutions can be found. This set is called the second Pareto front. In the same way a number of Pareto fronts can be found. From Figure 3.2 it is evident that the two objectives are in conflict with each other. This is typical for multi-objective optimisation problems. Should the objectives not be in conflict, at least one dimension could be omitted. In the two-dimensional case illustrated above, this would lead to a single-objective optimisation problem.

3.2 Stochastic optimisation techniques

The search methods employed by stochastic optimisation algorithms depend, in part, upon computational procedures generating a random outcome. Therefore these algorithms produce different paths towards the optimal solution each time they are run, and in the general non-linear case, convergence cannot be guaranteed. However, in most practical applications, proof of optimality is not the most important aspect; Instead, finding a solution better than any presently available one is usually sufficient.

One of the most widely used stochastic optimisation techniques is the **genetic algorithm** (GA) [85, 86, 87]. This algorithm is inspired by biological evolution. In a GA, a population of candidate solutions to the problem at hand, referred to as **individuals**, is maintained. Each individual contains a **chromosome** that is a representation of a potential solution to the problem. The chromosome can, for example, consist of a string of discrete (e.g. binary) or decimal numbers. Mixed

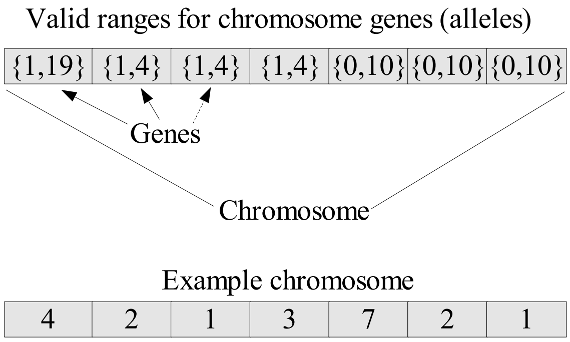

Figure 3.3: An encoding scheme for a genetic algorithm (GA) in which discrete numbers are used. An example of a chromosome is shown at the bottom of the figure.

representations exist as well, in which the chromosome contains both discrete and decimal numbers. An example of an encoding scheme used in Paper II can be seen in Figure 3.3. Each part of the chromosome is called a **gene**, and each gene may take different values, referred to as **alleles**. In this example, only discrete numbers are used. Since the problem is combinatorial, i.e. consists of a number of discrete alternative equipment sizes for a refueling station, it is natural to use a discrete encoding scheme. The problem also contains the time for investment, which is deliberately encoded as a discrete number in order to decrease the size of the search space, for faster convergence.

After the initial population is created (usually randomly), all individuals are evaluated. This involves a calculation of the fitness measure, which is used to rank individuals with respect to their performance. Usually, the calculation of fitness values is the most time-consuming part of the algorithm. The way the fitness measure is calculated depends entirely on the problem at hand. Two examples of calculating fitness measures are given in Papers III and IV.

When all individuals have been assigned fitness values, generational replacement is performed. First, the best individual is transferred unchanged to the next iteration (referred to as a *generation*), and then the remaining individuals are created from *selection*, *crossover* and *mutation*. The selection, usually of two individuals, is carried out in proportion to fitness. The selected two individuals then generate two new individuals by blending genes from both of them, a procedure known as crossover. In the simple case the genes are exchanged between chromosomes by cutting the latter at a random crossover point. The mutation is a random, low probability change to individual genes in the chromosome. Crossover and mutation must normally be tailored to the specific problem. A flow chart for a simple genetic algorithm can be seen in Figure 3.4.

In the problem considered in Paper IV, gradient information was very hard

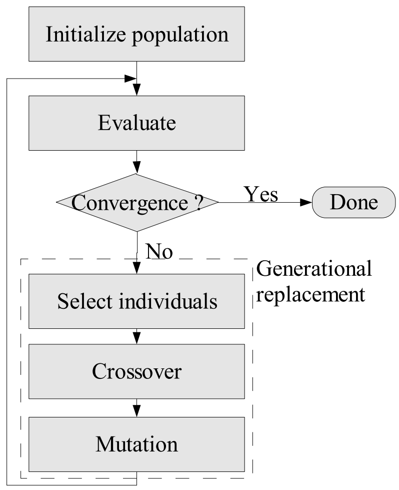

Figure 3.4: Flow chart of a genetic algorithm.

to find algebraically. Alternatively, numerical differentiation can be used; such a technique was employed in connection with the deterministic optimisation carried out in Paper II. However, in that paper it was shown that for longer optimisation time periods, the deterministic optimisation algorithm, in which numerical differentiation is an important part, led to unacceptably long computational times and was therefore intractable. Therefore, in Paper IV, a GA was used instead.

One significant advantage with using a GA is that it does not need any gradient information. In fact, GAs only need the fitness measure and can thus be applied to any optimisation problem where fitness can be quantified. In addition, GAs do not introduce any requirements on the function that is to be optimised (for example, it need not be convex), but it should be kept in mind that extra precautions may have to be taken for strongly non-linear and discontinuous functions. One such technique is to increase the mutation rate at the beginning of the evaluation in order for the solution not to get stuck on a local optimum but instead find the global one [85]. In all, the GA is a very flexible and easy-to-use optimisation algorithm. However, there are some drawbacks. One is the above-mentioned need for tailoring the encoding scheme, and the operators for crossover and mutation. Another, perhaps more serious, drawback is that since the search for better solutions is stochastic, so is the evaluation time. Occasionally, it may be better to stop the current calculation and start from the beginning by creating a new random population again. Also, there is no guarantee that the found solution indeed is the global optimum. However, in practice, these drawbacks are rarely significant.

The need for implementing extra operators is well compensated by the simplicity of the algorithm. Since true global optimisation is such a hard task, not even the most advanced deterministic algorithms can guarantee optimality in the general case. Considering this, the GA is a good candidate for real-world optimisations.

GAs have been extended to the multi-objective case [88]. The resulting algorithms are collectively known as multi-objective evolutionary algorithms (MOEA). These algorithms aim at finding the first Pareto-optimal front discussed above. In Paper II, a particular type of the above MOEA, called NSGA-II [89], is used. This is an elitist non-dominated sorting GA that uses an explicit diversity-preserving mechanism to keep solutions separated from each other. Since solutions are spread along the Pareto front, some measures need to be taken for the solutions not to clog together in the same spot. This is done by calculating the distance to the nearest neighbour, called the *crowding distance*. The new population is filled with solutions from one front at a time and in ascending order of fronts. First solutions from front number one is used, then solutions from front number two etc. If not all solutions from a front can be used (i.e. if the population is about to be filled), the remaining available positions in the new population are filled with the solutions having the highest crowding distance, i.e. lying furthest apart from each other. The NSGA-II algorithm can be summarized as follows

1. Randomly generate parent $P_t,\ (|P_t| = N)$ and offspring $Q_t,\ (|Q_t| = N)$ populations.

2. Combine parent and offspring populations to form $R_t = P_t \cup Q_t$.

3. Evaluate the combined population R_t and sort it into a number of non-dominated fronts $\mathcal{F}_i,\ i = 1, 2, \ldots, r$.

4. Iteratively create a new population $P_{t+1} \leftarrow P_{t+1} \cup \mathcal{F}_i,\ |P_{t+1}| + |\mathcal{F}_i| \leq N,\ i = 1, 2, \ldots$

5. Carry out a crowding distance sorting on the remaining fronts not included in P_{t+1} and include the most widely spread solutions until $|P_{t+1}| = N$.

6. Create offspring population Q_{t+1} from P_{t+1} by crowded tournament selection, crossover and mutation.

7. Iterate Steps 2-6 until convergence.

3.3 Dynamical optimisation

The **dynamical optimisation** problem is defined as the problem of minimising a cost function J over a given time period by finding the optimal control trajectory

$\boldsymbol{u}$. Thus, this type of problem is also referred to as an optimal control problem (OC) [90, 91, 92]. Common cost functions include energy, fuel, and time. The dynamical system can be mechanical, electrical or any other type that can be described mathematically. In this thesis, investment problems are considered. The continuous-time deterministic optimal control problem can be defined generally as

$$\begin{aligned} \min_{\boldsymbol{u}(t)} J, \quad \text{where} \quad & J = \Phi(\boldsymbol{x}(t_f)) + \int_{t_0}^{t_f} L(\boldsymbol{x}(t), \boldsymbol{u}(t), t)\mathrm{d}t, \\ \text{s.t. } \dot{\boldsymbol{x}} \quad = \quad & \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}, t), \\ \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{u}, t) \quad \leq \quad & 0, \end{aligned} \tag{3.12}$$

where J is the objective function, f are the state equation constraints, c are the path constraints and u is the control vector. The objective function consists of two parts: Φ, a cost based on the final time and state, and an integral depending on the time and state histories. In addition there may be simple bounds on the state and control variables, i.e.

$$\begin{aligned} \boldsymbol{x}_l \leq \quad & \boldsymbol{x} \quad \leq \boldsymbol{x}_u \\ \boldsymbol{u}_l \leq \quad & \boldsymbol{u} \quad \leq \boldsymbol{u}_u, \end{aligned} \tag{3.13}$$

and also boundary conditions on $\boldsymbol{x}$ and $\boldsymbol{u}$.

The above problem also has a discrete version, in which the integral is replaced by summation. The problems in Papers II and IV are both expressed in the discrete form, mainly due to the type of data available and for simplicity of calculation.

The optimal control problem may be solved by any of the following four methods: *dynamic programming*, the indirect method, the direct method, or simulation-based optimisation.

The dynamic programming approach makes use of Bellman's principle of optimality to solve the problem by backward induction [93]. The resulting partial differential equation is very hard to solve, except in very fortunate cases.

An indirect method aims at fulfilling the necessary conditions for an optimum, the Euler-Lagrange equations and the adjoint equations, using variational calculus. Finding these expressions requires calculation of gradients and Hessians, which usually is cumbersome. In addition, the indirect method is sensitive to the choice of starting point, i.e. the first estimate. A poor starting point may result in divergence or wildly oscillating trajectories.

A direct method [90] uses a sequence of points to approximate the state and control variables. The sequence may be a piecewise polynomial expansion. When these approximations are inserted into the objective function and constraints, the result is a static optimisation problem that can be solved using the methods discussed in Sections 3.1 and 3.2. Using the direct method [90], the integral in the objective function in Eq. (3.12) can be treated as an additional state $\dot{\boldsymbol{x}}_{n+1} = L(\boldsymbol{x}, \boldsymbol{u}, t)$ with the initial condition $\boldsymbol{x}_{n+1}(t_0) = 0$. It is thus possible to replace the original objective function with one of the type $J = \Phi(\boldsymbol{x}(t_f))$. Now the interval t_0 to t_f is divided into n_s segments where h_k is the time span of one segment. Furthermore, letting $M = n_s + 1$ be the number of points in the interval, the state equations can be approximated with any numerical integration method, i.e. Euler, Trapezoid and Runge-Kutta. For the simplest case using the Euler method, one may define $\boldsymbol{\zeta}_k = \boldsymbol{x}_{k+1} - \boldsymbol{x}_k - h_k \boldsymbol{f}_k$, and the original optimal-control problem in Eq. (3.12) can then be expressed as an NLP problem in each point $1, 2, 3 \ldots M$ of the time segments in the following way

$$\begin{aligned} \min_{(\boldsymbol{u}_1, \boldsymbol{y}_1, \ldots \boldsymbol{u}_M, \boldsymbol{y}_M)} J, \quad \text{where} \quad & J = \Phi(\boldsymbol{x}_M) \\ (\boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2, \ldots, \boldsymbol{\zeta}_{M-1}) \quad = \quad & 0 \\ (\boldsymbol{c}_1(\boldsymbol{x}_1, \boldsymbol{u}_1, t_1), \boldsymbol{c}_2(\boldsymbol{x}_2, \boldsymbol{u}_2, t_2), \ldots, \boldsymbol{c}_M(\boldsymbol{x}_M, \boldsymbol{u}_M, t_M)) \quad \leq \quad & 0. \end{aligned} \tag{3.14}$$

In this equation, the $\boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2, \ldots, \boldsymbol{\zeta}_{M-1}$ are the deviations, also referred to as the defects, for the dynamics (augmented with the integral in the objective function in Eq. (3.12)) approximated by the numerical integration method at each point. $(\boldsymbol{c}_1(\boldsymbol{x}_1, \boldsymbol{u}_1, t_1), \boldsymbol{c}_2(\boldsymbol{x}_2, \boldsymbol{u}_2, t_2), \ldots, \boldsymbol{c}_M(\boldsymbol{x}_M, \boldsymbol{u}_M, t_M)) \leq 0$ are the original inequality constraints expressed at every point. The result of the optimisation is M control and state vectors $\boldsymbol{u}$ and $\boldsymbol{y}$.

This optimisation problem is of the static NLP type and can be solved with the techniques discussed in the previous sections. The problem does, on the other hand, have $M - 1$ times more variables than the original dynamic optimal control problem. For the case of equality constraints and boundary conditions, the number of variables equals $M - 1 + M + 2 = 2 \times M + 1$. The method presented in Eq. (3.14) is also referred to as the multiple shooting method. In the case where $n_s = 1$, it is called a single shooting method. In the case of a long interval $t_f - t_0$ and small time constants, the resulting static problem will become hard to solve. In Paper II the above direct transcription method was used; see Chapter 5 for a further discussion.

The simulation-based approach uses a totally different technique to arrive at an optimisation problem that can be treated as a static one. Here, the system under study is simply simulated for the entire simulation period, during which the cost J is also calculated. Based on the value of J a static optimisation algorithm adjusts the control vector $\boldsymbol{u}$ in the direction of lower cost. The simulation-based technique can be described as follows

1. Find a feasible control vector $\boldsymbol{u}$.

2. Simulate the system using the control vector $\boldsymbol{u}$ and calculate the cost J.

3. Change the control vector for lower cost J using a static optimisation algorithm.

4. Repeat Steps 2-3 until convergence.

The static optimisation technique in Step 3 can be of any kind. However, a GA, as described in section 3.2, is particularly suitable.

3.4 Stochastic dynamical optimisation

In any real system, noise is present. In the systems discussed in this thesis, noise is represented as an uncertainty about future development. This fact motivates the usage of **stochastic dynamical optimisation** techniques [94, 95, 96], which is a dynamical optimisation technique, as discussed above, applied to a problem under the influence of a disturbance. The disturbance can be realized as a stochastic variable with a predefined probability distribution. The discrete-time stochastic optimal control problem can be defined generally as

$$\begin{aligned} \min_{\boldsymbol{U}} \; J(\boldsymbol{U}), \quad \text{where} \quad & J(\boldsymbol{U}) = \sum_{k=0}^{N-1} \gamma(k, \boldsymbol{X}_k, \boldsymbol{U}_k, \boldsymbol{W}_k) + \Gamma(\boldsymbol{X}_N, \boldsymbol{W}_N) \\ \text{s.t. } \boldsymbol{X}_{k+1} \quad = \quad & \boldsymbol{f}(k, \boldsymbol{X}_k, \boldsymbol{U}_k, \boldsymbol{W}_k) \\ \boldsymbol{c}_k(\boldsymbol{X}, \boldsymbol{U}) \quad \leq \quad & 0 \,\forall\, k = 1, \dots N, \end{aligned} \tag{3.15}$$

where $\boldsymbol{W}$ is an independent random disturbance, $\gamma(k, \boldsymbol{X}_k, \boldsymbol{U}_k, \boldsymbol{W}_k)$ is the cost associated with each time step k, $\Gamma(\boldsymbol{X}_N, \boldsymbol{W}_N)$ is the terminal cost and $\boldsymbol{c}_k(\boldsymbol{X}, \boldsymbol{U})$ represents simple limits of the state and control variables.

The above perturbed optimisation problem can be solved by methods analogous to those used for the unperturbed problem in Section 3.3, that is by dynamic programming, **stochastic programming** or the simulation-based approach. The solution methods generally work in the same way as in the unperturbed case.

The differences compared with the unperturbed case are that in the perturbed case the objectives are optimised with respect to expected values. The result is one control strategy $\boldsymbol{U}$ that minimises the expected value (the mean value) of the objectives. The definition of the disturbance can either be analytical, i.e. using data from the distribution used, or scenario-based, i.e. using a number of **samples** from, e.g. a probability distribution. In the former case the optimisation is done analytically and in the latter case it is done numerically. In Paper IV, several scenarios were used for generating samples after which the scenario-based optimisation method was applied. Using this technique, each sample corresponds to one possible future development of the disturbance, i.e., in this case, the number

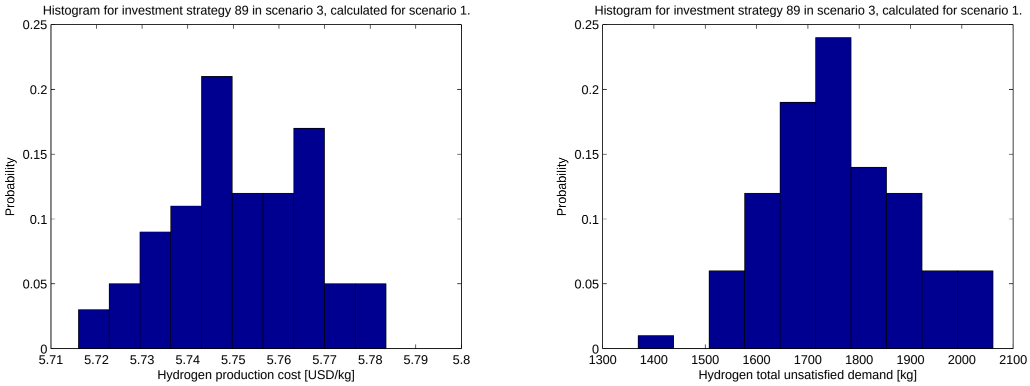

Figure 3.5: Examples of histograms representing the hydrogen production cost (left panel) and unsatisfied demand for hydrogen (right panel) for a given solution. The histograms were generated using 100 samples.

of vehicles arriving at the refueling station. The solution is the expectation value of the optimum for all samples.

In Paper IV, the problem is two-dimensional and, therefore, so is J. Applying all samples in a given scenario[2] will result in a distribution of the two-dimensional objective function J. In essence, for each solution $\boldsymbol{U}$ and set of samples there is one distribution for each dimension in the objective function J. In Figure 3.5 an example from the hydrogen and hythane refueling case is shown. The two objectives are hydrogen production and total hydrogen unsatisfied demand[3]. Each quantity has been calculated for one solution $\boldsymbol{U}$, and for all available samples.

[2] In Paper IV, 100 samples were generated for each scenario.
[3] As shown in [97], the occurrence of an unsatisfied demand is not uncommon.

Chapter 4

Assessing the future

This thesis focuses on long-term planning and optimisation, processes that require an assessment of the future. Such assessments can be obtained in different ways, and in this thesis (see Papers II and IV) the preferred method has been to generate a number of possible outcomes, referred to as *scenarios*. A number of probability distributions are associated with each scenario. Thus, once a scenario has been defined, a large number of samples can be generated, each representing one possible future outcome. Needless to say, such scenarios will always have a certain degree of arbitrariness.

Since the long-term effects of a scenario often may depend strongly on what happens during the first few time steps, short term prediction of time series, based on past data, is certainly relevant. Thus, time series prediction (TSP), considered in Paper III, can be used for reducing the prediction uncertainty

4.1 Forecasting

Forecasting time series is common in economics [23, 98]. In the technical domain it is part of system identification [99]. The underlying assumption is that the data series have an internal structure that can be identified. After identifying this structure, a procedure known as model fitting, a prediction of the future can be made. In practice, the model is selected first, after which the data sets are used to estimate its parameters. Clearly, this requires that the model *can* represent the data. If this is not the case, another model has to be found through structure selection, i.e. by finding a model with a more suitable internal structure, which can then be tuned by adjusting the values of the internal parameters so as to reduce the error over the data set.

Another issue is the amount of noise present. White noise can, by definition, not be predicted. Other types of noise can, to a certain and often limited degree, be predicted. In this case one can use models that have a noise part allowing for multi-step predictions[1] [99]. For one-step prediction the expected increment is zero in case of white noise, and the estimate is equal to that obtained from a model without noise. However, the genuine information part of the time series is deterministic and can, provided a good model is found, be subject to successful prediction.

Traditionally, methods like *the naive method*, *exponential smoothing* and *auto-regressive integrated moving averages* (ARIMA) have been used for time series prediction [22, 52]. The naive method estimates the next value in the time series by the present one. For very noisy time series, it is hard to beat the trivial prediction obtained from the naive method [100]. The ARIMA techniques consist of three parts: an auto-regressive part, an integrating part and a moving average part. Exponential smoothing is a special type of ARIMA model. More recently, artificial neural networks (ANNs), of which feedforward neural networks (FFNNs) and recurrent neural networks (RNNs) are examples, have been used in TSP [25, 101].

In Paper III, a novel kind of recurrent ANNs called *discrete-time prediction networks* (DTPNs) was developed for **time series prediction**. This study was a continuation and an improvement of earlier work on TSP using neural networks [26]. A DTPN contains inter-neuron connections as well as connections to the inputs. In a DTPN, any neuron may be connected to any other neuron, and to itself. Furthermore, each neuron has an individual squashing function σ which is (in principle) arbitrary. In Paper III the logistic function

$$\sigma_1(z) = \frac{1}{1 + \mathrm{e}^{-cz}}, \tag{4.1}$$

where c is a positive constant, and the hyperbolic tangent

$$\sigma_2(z) = \tanh cz, \tag{4.2}$$

have been utilized. Since no gradient information is needed in the training procedure, no restrictions exist on the functions that can be used. Therefore the squashing functions

$$\sigma_3(z) = \mathrm{sgn}(z), \tag{4.3}$$

and

$$\sigma_4(z) = \begin{cases} \tanh(z + c) & \text{if} \quad z < -c \\ 0 & \text{if} \quad -c \leq z \leq c \\ \tanh(z - c) & \text{if} \quad z > c \end{cases} \tag{4.4}$$

were also used. In addition, the function

$$\sigma_5(z) = \frac{cz}{1 + (cz)^2}, \tag{4.5}$$

[1] A multi-step prediction is defined as $x(t-n), x(t-n+1), \ldots, x(t) \to \hat{x}(t+k),\ k > 1$.

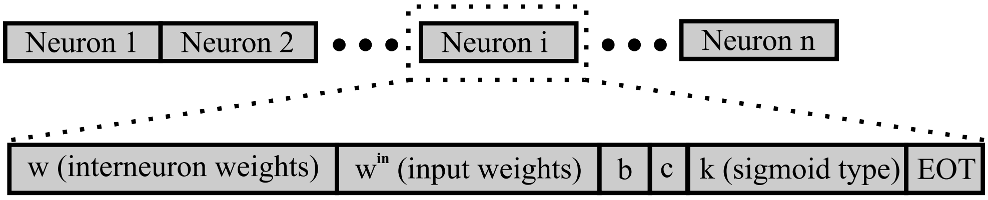

Figure 4.1: A chromosome encoding a DTPN as used in Paper III.

was used. Even though DTPNs have arbitrary connections between neurons, the order in which the neurons are updated is fixed, and given by so called evaluation order tags (EOTs), one for each neuron. In each time step, the neurons with lowest EOT are updated first according to

$$x_i(t+1) = \sigma\left(b_i + \sum_{j=1}^{n_{\text{in}}} w_{ij}^{\text{in}} I_j(t) + \sum_{j=1}^{n} w_{ij} x_j(t)\right), \tag{4.6}$$

where w_{ij}^{in} are the input weights, w_{ij} the interneuron weights, and b_i is the bias term. I_j are the inputs to the network which, in the case of time series prediction, consist of earlier values of the time series $Z(t)$, i.e. $I_j(t) = Z(t-j+1)$ For neurons with the second lowest EOT, the equations look the same, except that $x(t)$ is changed to $x(t+1)$ for neurons with lowest EOT etc. Finally, the output neuron (arbitrarily chosen as neuron 1) gives the following output

$$x_1(t+1) = \sigma\left(b_1 + \sum_{j=1}^{n_{\text{in}}} w_{1j}^{\text{in}} I_j(t) + w_{11}x_1(t) + \sum_{j=2}^{n} w_{1j} x_j(t+1)\right), \tag{4.7}$$

since, at this stage, all neurons except neuron 1 have been updated. Like other RNNs, DTPNs are capable of short-term memory, a feature which is important in time series prediction (see also Paper III).

The optimisation of DTPNs is carried out by means of a genetic algorithm (GA), which evolves not only the parameters of the network, but also its structure, i.e. the number of neurons and their EOTs. The encoding scheme used for evolving DTPNs is shown in Figure 4.1. Note that the sigmoid type σ_k is encoded by the integer k in the chromosome.

In Paper III, DTPNs were evolved for one-step prediction of the Fed Funds interest rate and US GDP, after first rescaling the data to the range $[-1, 1]$. A summary of the results is given in Table 4.1. As can be seen in the figure, the prediction results (average prediction errors) for the DTPNs were better than those of the other methods tested.

The DTPNs have been used for one-step predictions only. Of course, multi-step predictions are possible, in principle, but will inevitably result in inaccurate predictions due to the effects of cumulative errors [51, 102].

Data set	e_{N}	e_{ES}	e_{ARMA}	e_{DTPN}
Fed funds interest rate	0.2018	0.1901	0.1887	0.1837
GDP	0.1771	0.1490	0.1473	0.1305

Table 4.1: Average errors for one-step predictions carried out for two macroeconomic time series: the Fed funds interest rate and the US GDP. The table shows the minimum errors over the *validation* part of the data set, obtained using naive prediction (e_{N}), exponential smoothing (e_{ES}), ARMA (e_{ARMA}), and DTPNs (e_{DTPN}). Only the results for the very best DTPN are shown.

Also investigated were predictability measures, i.e. measures of the accuracy of an individual prediction. Several empirical measures were investigated, as well as one analytical measure. The empirical measures involved different ways of augmenting the DTPNs to incorporate the predictability. The amount of genuine information in a single time series can be analytically estimated using random matrix theory [103, 104]. If the original observations are contained within the Tx1 vector $x(t)$, a $T - m \times N$ delay matrix Z can be formed where the columns are delayed observations, i.e. $x(t)$, $x(t-1)$, $x(t-2)\ldots x(t-m)$. The parameter m represents the maximum delay and should be chosen to cover the time period of any cyclic behaviour. In the process of forming the delay matrix, m rows at the end of Z will lack values and hence only $T - m$ rows can be further used in Z. The number of columns, N, equals the maximum delay number, m, plus one initial column. In order to use Z, each column has to be normalised to zero mean and variance 1, which is done using

$$Z_{m,n} \leftarrow a\, Z_{m,n} + b, \tag{4.8}$$

where

$$a = \sqrt{\frac{T-m}{\sum_{i=1}^{T-m} Z_{i,n}^2 - 1/(T-m)(\sum_{i=1}^{T-m} Z_{i,n})^2}} \tag{4.9}$$

and

$$b = -a\frac{\sum_{i=1}^{T-m} Z_{i,n}}{T-m}. \tag{4.10}$$

The correlation matrix, C, is then defined as

$$C = \frac{1}{T} Z^T Z. \tag{4.11}$$

Furthermore, the eigenvalues of C can be used to estimate the information content by comparing with the eigenvalues of a random matrix with the same dimensions.

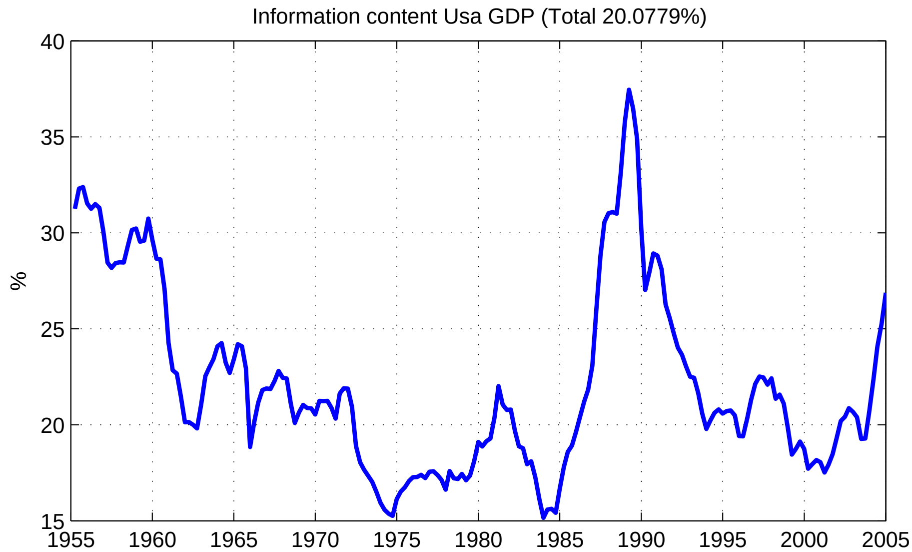

Figure 4.2: Information content in the US GDP time series using random matrix theory [104]. The remaining part is noise. For the above case the delay $m = 12$ and the window size 32. The total information content is calculated based on the eigenvalues for the full, non-windowed, correlation matrix C.

Such a matrix, $X\ [m \times n]$, will, if it is scaled according to Eq. (4.8), have a density of eigenvalues according to

$$\rho(\boldsymbol{\lambda}) = \frac{Q}{2\pi} \frac{\sqrt{(\boldsymbol{\lambda}_{\max} - \boldsymbol{\lambda})(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\min})}}{\boldsymbol{\lambda}} \tag{4.12}$$

for $\boldsymbol{\lambda} \in [\boldsymbol{\lambda}_{\min}, \boldsymbol{\lambda}_{\max}]$, and zero otherwise, in the case where $m, n \to \infty$, and where $Q = n/m \geq 1$ [105]. In Eq. (4.12), the minimum eigenvalue is $\boldsymbol{\lambda}_{\min} = \sigma^2(1 - 1/\sqrt{Q})^2$ and the maximum eigenvalue $\boldsymbol{\lambda}_{\max} = \sigma^2(1 + 1/\sqrt{Q})^2$. If the eigenvalues of C lie outside the range $[\boldsymbol{\lambda}_{\min}, \boldsymbol{\lambda}_{\max}]$, the time series $x(t)$ contains real information. A numerical estimate of the minimum and maximum eigenvalues for matrices of finite size, can be obtained by taking the minimum and the maximum eigenvalues obtained from a large number of generated random matrices of the same dimension as C.

A way of estimating the percentage of information content is by computing $100\boldsymbol{\lambda}_{\max}/N$, where $\boldsymbol{\lambda}_{\max}$ is the largest eigenvalue of the correlation matrix C. By making use of a moving data window, the local information content in time series may be estimated. Figure 4.2 shows such a calculation for the US GDP.

All results on the predictability measures were, however, negative. Comparison between the analytical and empirical candidate measures showed no correlations. The reason may be that the DTPNs do extract most of the information available in the time series.

4.2 Decision-making under uncertainty

Decision-making in industry as a scientific discipline can be regarded to be a part of operations research (OR) [106, 107, 108]. OR originates from the military sector, where it was used to make better decisions in, e.g. logistics and war tactics [109, 110]. Nowadays OR is widely used in the industry to raise efficiencies and optimise performance. Here it is also known as management science [111, 112]. The problems that occur in OR are real-world problems and are often hard to solve using traditional deterministic methods. Therefore it is not surprising that the efficiency of stochastic optimisation techniques was early recognised [113].

An important field where OR has contributed is decision-making under uncertainty. In the industry, strategic decisions have to be made and in all practical cases they are taken under uncertainty since they involve predicting, or guessing, what will happen in the future. Since it is generally very difficult, not to say impossible, to make correct long-term decisions intuitively, this is an area where much can be gained by applying advanced analytical techniques [114, 115, 116]. Application areas include logistics [117], financial instruments, investment planning [11], risk management [118], water pollution problems [119], water resource problems [120] etc. In all of the above areas, stochastic techniques, like GAs, nowadays are common ways of solving the resulting optimisation problem.

For an investment decision problem, each decision to invest will, in the optimisation framework, result in one decision period. In practical cases there is often a pre-defined number of occasions when investments are possible, e.g. once a month or once a year, something that leads to a *sequential decision problem*. The problems in Papers II and IV are both sequential decision problems. In addition, the problem considered in Paper IV is also stochastic. Furthermore, the decision-making can involve an inner loop where a number of decisions are made within each outer decision period, leading to two stages of decisions. For a production company, the first stage typically involve decisions on investments in production capacity and the second stage regards decisions concerning production planning given the resulting constraints from the first stage. The decision problem in Paper IV is also of the above two-stage type and is solved by the use of a pre-defined strategy for the first investment stage and a combination of closed-loop regulation[2] and a pre-defined strategy for the second production stage.

[2]The term closed-loop regulation is used in the standard way, as defined in control theory.

Decision-making under uncertainty can be modelled as a **Markov decision process** (MDP) [121]. In such a process, the decisions taken at a certain point depend only on the state at the previous time point and not on states further back in time. The MDP is a discrete-time stochastic control process that propagates through a series of states. For each state the decision-maker takes actions based on the information given by the previous state only. Next, a stochastic transition function determines probabilities for transition to the next state. For each state there is a reward, which depends on the new state. In Paper IV, the investment decisions are parametrised and calculated in an open-loop way, i.e. they are predefined. Uncertainties in the form of hydrogen and hythane demand are dealt with in the second stage, where the amount of stored hydrogen is kept at a constant level by adjusting the production. This second stage is a process of the Markov type.

The use of optimisation for finding optimal future investment strategies is a decision that has to be carefully considered for each individual case. As with all mathematical tools, optimisation methods also require a quantification of the input data, which is by no means trivial, since some data concern predictions of future sales, prices etc. Other factors such as availability of skilled personnel and data regarding the system under study also have to be taken into account. The methods used in Papers II and IV are, from a mathematical point of view, very robust. The sensitivities to disturbances can be determined by perturbation analysis, a technique used in Paper II. The quality of the optimisation results depends, of course, on the quality of the input data. On the other hand, the investment methods presented in Paper II and IV are meant to be used to update the investment strategy as soon as new and better predictions are found. In this case the optimal next investment decision can always be found, given the best available future estimates at the time of calculation. It should also be stressed that the use of GAs for investment planning, as in Paper IV, reduces the calculation effort since no gradient information is needed. It is the conviction of the author that, in the case of a complex system and as soon as the objectives are quantifiable, the presented methods are very powerful tools and will prove useful in many applications in addition to those discussed in this thesis.

Chapter 5

Case studies

This chapter provides a background to the case studies presented in Papers I, II and IV. Along with the general background, some details omitted from the papers are given as well.

The three cases are (1) the cement production model, (2) the hydrogen refuelling station infrastructure investment optimisation and (3) the combined hydrogen and hythane infrastructure investment optimisation.

5.1 The cement production case

In the cement production case considered in Paper I, a highly flexible model of a cement production factory has been built. The model has been used in several different calculations, including process optimisations and environmental assessment of new energy sources. The life cycle inventory analysis (LCI) model consists of a foreground system which defines the on-site production over which the company has full control, and a background system comprising purchased services and goods, see Figure 5.1. A more in-depth discussion of the production facility is given in Paper I and in [45].

The raw materials, i.e. different sorts of sand, are transported to the production site and ground depending on type. They are then mixed in relevant proportions and burnt to clinker in the *clinker production system*. For the burning process, fuel is, of course, required, and it may consist of coal, pet coke or an alternative fuel. All fuels are transported to the site, ground and mixed in correct proportions, before entering the burner. The produced clinker is then mixed with gypsum (and possibly other materials), further ground, and stored as cement.

The problem is to find the ratio of raw materials, fuels and the additional gypsum to produce cement of a certain quality. The quality is measured using the factors indicated in Table 5.1. In addition the approximate monetary costs throughout

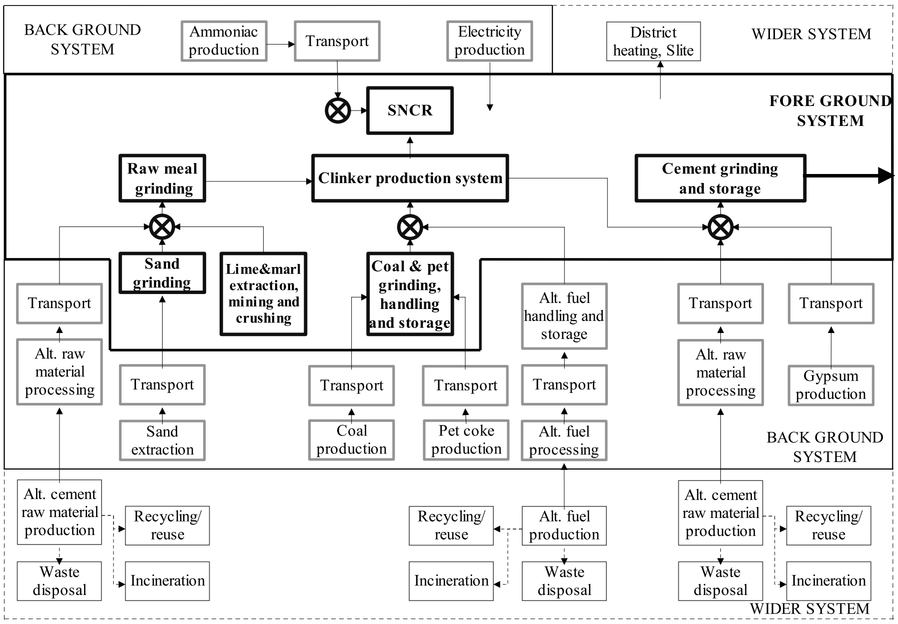

Figure 5.1: LCI model of the cement production line.

the production line must be calculated. Since the purchase costs of the raw materials and fuels are known, the production-related cost for each piece of equipment in the line can be estimated and added to the product flow. The model can be used as an aid in calculations for new types of raw materials, fuels and internal settings, and for changes in the layout of the production line. In addition to static solving, dynamic simulation and optimisation can be considered. It is therefore a requirement that the model should be modular and highly flexible.

One option would be to make a standard LCI model. When a standard LCI is carried out, the linear technology matrix model (A) described in Section 2.1 is sufficient for describing the technical production system, since the underlying production system is described as static and linear. Using this linear description, only one type of calculation is made in an LCI, which is the normalisation to the functional unit, obtained by solving a linear equation system. The developed mathematical LCI methods are designed to achieve *only* this normalisation [31, 32, 34], something that limits their usefulness. At times it is desirable to make extensions to this type of LCI model. One such occasion is when the inherent physical behaviour of the production system is strongly non-linear when seen as a mapping from resources and emissions to the product. A linear LCI model represents in this case a linearisation around a specified point and might lead to unacceptably large deviations in the calculated resource use and emissions released. Another

Table 5.1: Cement product quality indicators. The notation indicates weight percentage of the specified material.

Name	Symbol	Description
Lime saturation factor	LSF	$LSF = \frac{100CaO}{2.8SiO_3+1.1Al_2O_3+0.7Fe_2O_3}$
Silica ratio	SR	$SR = \frac{SiO_2}{Al_2O_3+Fe_2O_3}$
Alumina ratio	AR	$AR = \frac{Al_2O_3}{Fe_2O_3}$

occasion occurs when dynamic aspects are relevant, for example when closing down and starting up a production line in connection with maintenance. In the situations just described, another modelling approach, making use of non-linear and dynamic models, is needed. In addition, other types of calculations may be desirable as well. Examples include optimisation, simulation over time etc. In order to fulfill the requirements, one needs a higher degree of flexibility in the model than is given by the LCI model. In short, the modelling approach has provide the model with enough data to represent the underlying system in a correct way and this data has to be arranged in such a way that it is possible to make the desired calculations using the model.

In [122] the nature and effect of some different types of causality are discussed. The concept of causality is further applied to LCA in [50]. To recapitulate, there are two types of causality of interest: (1) physical causality and (2) computational causality. The physical causality is the cause-effect connection inherent in nature. The computational causality is the order in which an equation system is solved. While the former is governed by the laws of nature, the latter is the choice of the modeller. In [50], it was found that, by removing the computational causality from the model, advantages in flexibility can be achieved. The result is a so called acausal [122] or non-causal model. In effect, the entity that is normally regarded as the model can be split into three parts, namely:

- A computationally neutral (acausal) model, i.e. a model that maps the interpretation of the production system onto a mathematical formulation, but does not include any specific problem to be solved.

- A problem formulation, i.e. a description of which parameters should be calculated and an explicit list of which parameters should be held constant during a particular calculation as well as numerical values for each such constant parameter.

- A method of calculation. This part can be considered as a part of the problem formulation.

In addition it was found that the modularity of the model, i.e. the flexibility with regard to both change and exchange of parts within the model, can be enhanced by using an object-oriented modelling language in conjunction with physical entity modelling. The intention with the latter is to keep real physical entities together for ease of comprehension and transparency. This way of modelling also constitutes a natural way to keep parts that are separate in reality as separate objects in the model, so that the model resembles reality or a suitable representation of reality. To summarise, the following requirements are considered:

- A computational acausal model that contains the structure and constants of the system, but does not contain any information regarding computation.

- An object-oriented modelling language that makes use of encapsulation and inheritance[1].

- A physical property modelling approach that makes it possible to map the real physical structure onto a similar model structure.

However, there are drawbacks with using an acausal model. Any mathematical model consists of a number of equations. In the computationally causal case, e.g. block diagrams and state-space models, these equations are ordered in a specific way to achieve the desired result. In the computationally acausal case the equations are not ordered in any specific computational way. Instead they can be regarded mathematically as a number of equilibrium equations connected to each other, making them harder to understand. For models of physical systems which are based on **flow semantics**, i.e. correlation between the general variables intensity and flow, the model representation can be based on energy flow and is usually relatively easy to construct. For the type of flow models used in LCI there are also physical laws to consider, but not in the form of intensity-flow related connections. Under these circumstances acausal models can be structured in various ways depending on the application, and therefore such models are difficult to make both consistent and sufficiently general to reach a high degree of flexibility. Another disadvantage is that in order to use an acausal model, a dedicated software for sorting out the equations and ordering them computationally is needed. In practice this is rarely a limitation, since such software is available.

As an illustration of the use of acausal models, consider the simple resistor described by

$$u_R = R\, i_R. \tag{5.1}$$

[1]Encapsulation and inheritance are central concepts in object-oriented programming, see e.g. [123, 124, 125] for details.

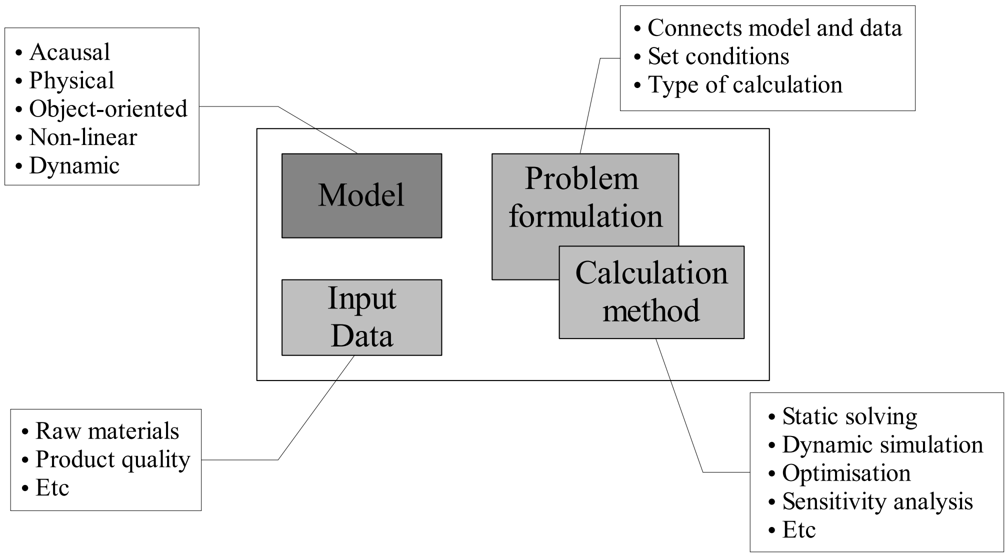

Figure 5.2: The separation of model and problem formulation that can be achieved by the use of acausal models.

Is it the current flowing through the resistor that causes the voltage drop or the voltage drop that causes the current? What is the physical causality of the resistor? Of course the order of calculation depends on the question at hand. If one is interested in the voltage drop, one would use the computational order given in Eq. (5.1). On the other hand, if one is interested in the current, one would re-order the equation accordingly. If Eq. (5.1) is interpreted as a statement of equilibrium, it can be regarded as an acausal model. A problem formulation might be to calculate the voltage drop while keeping the current at a constant value. A suitable method of calculation is then any static linear equation solver. Moreover, the above example is a physical system and is based on flow semantics. In this case the voltage is the intensity and the current is the flow [56]. For the simple example discussed, the computational aspects are obvious and need no further formalisation. However, in cases with more than, say, 100,000 equations, much time can be saved through the use of acausal modelling techniques.

When the project reported in Paper I was carried out (fall 1999), only a limited number of modelling languages and software programs for calculation were available and able to fulfill the requirements. Among them there were OmSim (Omola) [126], Dymola (MODELICA) [48] and Ascend [46]. OmSim and Dymola are specially made for modelling of physical systems and have a built-in support for flow semantic. Since the system considered does not have any intensity-flow dependency, it was decided not to use these programs (languages). Ascend is both a calculation software and a modelling language and was originally developed for applications within chemistry. However, it can best be described as a mathematical system modelling tool and is very flexible in defining connections and hence the structure of the system modelled, which is the main reason for using it.

The model was built in a bottom-up manner according to Paper I. It should be noted that the model is deliberately made redundant. In most cases redundancy has a negative effect, but here it is used to enhance the flexibility. The numerical parameters in a calculation can be divided into the following categories:

- Constants. These are set, once and for all, when the model is built.
- Locked variables. Parameters set to a constant numerical value for a certain calculation.
- Free variables. Parameters that will be calculated by the numerical algorithm.

The number of parameters in each category depends on the specific calculation considered. Providing information regarding these settings is part of the problem formulation. In the model, the information needed for specifying one parameter can be supplied in a number of ways. An example is the ingredients in raw meal composition. These can be set by specification of absolute masses or relative masses (percentage). The model contains the necessary mathematics to relate these parameters at the time of calculation. At any given time, only one of the two ways of specifying the parameter is used. The result, presented in Paper I, is a highly flexible calculation tool for the cement production process that has been used by Cementa AB, for several different purposes. It should be noted that the entire model of the cement production line was later transferred to MODELICA [127].

5.2 The hydrogen infrastructure case

The main task for the hydrogen refuelling station is to dispense hydrogen to vehicles. Since the incentives for using hydrogen are environmental, an important question to consider is where the hydrogen is to be produced. Producing the hydrogen is probably best done at large, centralised production facilities. It is then easier to take care of the created emissions, e.g. CO_2. The problem is to distribute the hydrogen to the local refuelling station. In order to do so efficiently, the hydrogen gas has to be highly pressurised, which is expensive and can also be dangerous. Another consideration is the vulnerability both to sabotage and to accidents. In this thesis an alternative solution comprising local production of hydrogen using a **hydrogen reformer**, i.e. a device that produces hydrogen from hydrocarbons, is investigated. The input to the reformer can be any type of methane gas and may originate from fossil or renewable resources. One disadvantage is that the reformer will produce considerable amounts of CO_2 which will not be easy to take care of. Probably it has to be released into the atmosphere. When the natural gas comes from a renewable source of energy the net contribution of CO_2 is nil. One obvious advantage with local production is that natural gas is considerably easier to transport than hydrogen gas. In fact there is already a rather small but growing number of natural gas refuelling stations in Sweden [128]. A hydrogen production and refuelling part can then be added to the already existing natural gas refuelling station. With such a refuelling station, it is also possible to dispense natural gas as an intermediate alternative.

If the refuelling station is equipped with fuel cells, it can also be used as a local electrical power station. This alternative might be useful in remote locations. When hydrogen is produced from renewable energy sources, it might also be an environmentally friendly alternative. If the refuelling station is located in a place where electricity from the grid is cheap, it can be equipped with an electrolysis part that can produce hydrogen gas directly from electricity. In this case it is important to keep track of how the electricity is produced. To begin by producing electricity from coal and then using electrolysis to produce hydrogen is not, however, a good environmental solution. In addition to the hydrogen reformer, the refuelling station layout that is considered in Paper II also has a local fuel cell and an electrolysis plant. Figure 5.3 illustrates options investigated in this thesis. The result is a refuelling station that is very flexible in terms of resource use and energy production.

The equipment for a hydrogen refueling station with the above layout is more expensive than present-day petrol station parts. In addition, not all of the configurations are suitable for specific conditions. Under these circumstances it is important to find the most profitable configuration for the specific location, the estimated number of customers, and general technical and economical development. The problem is to find the most profitable configuration. As described in Paper II, this problem is equivalent to finding the least expensive mean production cost for hydrogen. In Paper II, only the core parts (the parts within the shaded area in Figure 5.3) are part of the optimisation. The remaining parts can be dealt with separately, as discussed in Paper II.

In reality the choice of equipment is limited by supply. Let the set of available equipment, which consists of a finite number of sizes for each equipment type, be denoted by $\mathbf{C}$ and the control sequence $\mathbf{u}(t)$ be a vector of equipment sizes such that $\delta\mathbf{u}(t) \in \mathbf{C}$ and $\mathbf{u}(t+\delta t) \geq \mathbf{u}(t),\ \forall t$ where δt is a small time step. The

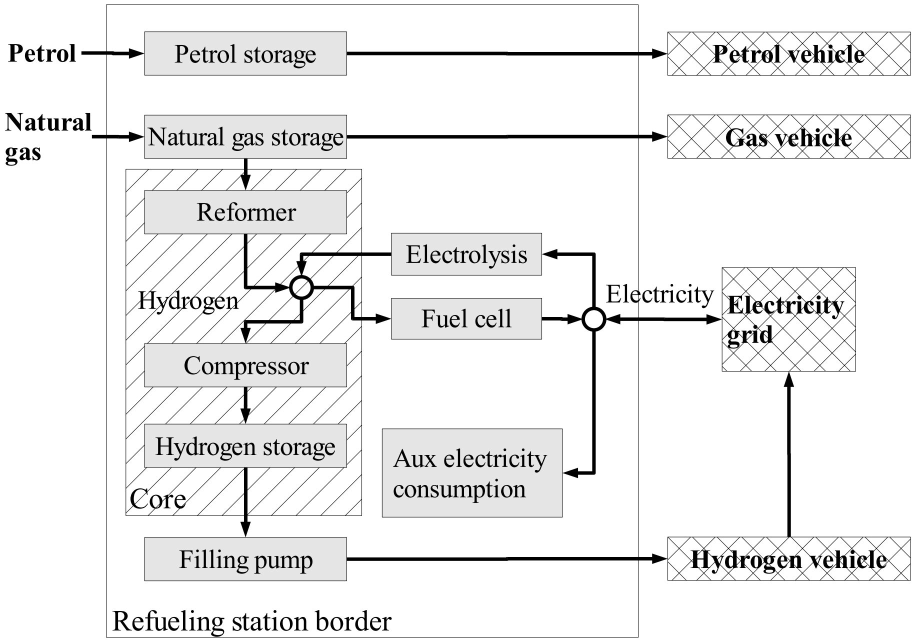

Figure 5.3: Refueling station layout. Natural gas is reformed to hydrogen at the site and stored for delivery to vehicles. It is also possible to produce hydrogen from electricity by electrolysis or electricity from hydrogen using a fuel cell.

implication is that $\mathbf{u}$ is only allowed to increase and to do so only with specific increments, namely those in $\mathbf{C}$. Further let $f(\mathbf{u}, \mathbf{x}, \mathbf{w})$ be the description of the core of the refuelling station in state-space form where $\mathbf{x}$ is accumulated volume in each piece of equipment and $\mathbf{w}$ is the hydrogen refuelling demand. The most general form of the problem of finding the most profitable configuration is, in the continuous case,

$$\begin{aligned} \min_{\mathbf{u}(t)} J &= \bar{c}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{w}(t)) \\ \text{s.t. } \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{w}(t)) \\ 0 &\leq \mathbf{x}(t) \leq \mathbf{u}(t), \end{aligned} \tag{5.2}$$

where $\bar{c}$ is a cost function described in Paper II and further discussed in Section 2.1 in this thesis. There are two major difficulties in solving this problem:

1. The problem is defined over the entire investment period of 20 years. At the same time the assumed filling curve for hydrogen has a time step of one hour. Dividing the interval of 20 years into one hour segments would lead to $2 \times M + 1 = 350,401$ variables, as is discussed in Section 3.3. This would make numerical solving of the resulting non-linear optimisation problem hard, not to say impossible.

2. The control sequence $\mathbf{u}$ can only increase in steps that are part of $\mathbf{C}$. This would make the problem discrete in $\mathbf{u}$. Discrete problems are combinatoric and in general harder to solve than continuous ones [129].

In order to solve the problem stated in Eq.(5.2) it is observed that, to be able to satisfy the hydrogen demand, the first investment has to take place initially, at $t = 0$. Consecutive investments can be divided into separate cases. Since the desired output, the filling curve f_w, is given for one week (168h) and then scaled using the S-curve R, it is sufficient to consider only one week for each investment. The S-curve is a purely exogenous estimate of the number of hydrogen vehicles using the refuelling station and is defined as

$$R(t) = \frac{1}{1 + \mathrm{e}^{-B(t-T_x)}}, \tag{5.3}$$

where t is the time from year 2010, T_x the S-curve inflection point and B the slope. For values of the constants T_x and B, see Paper II. The week to consider for each investment is when utilisation is at its maximum, namely the week right before the next investment. At these points in time, the equipment is used at its maximum capacity and, in order to satisfy the increasing demand, a new investment in capacity has to be made. By parametrising the set $\mathbf{C}$ using a scaling function $p_{eq}(s_{eq})$ (explained in Paper II), where s_{eq} is the size of equipment, the problem will become continuous in $\mathbf{u}(t)$.

The driving signal for the fast dynamics is the filling curve flow f_w. This curve is given for one week with the time step of one hour. The integral in the objective functions in Section 2.1 can therefore be replaced by a sum. Also, the discrete version of Eq. (5.2) can be used.

Using the direct transcription method in Section 3.3, the resulting NLP problem (see Section 3.1) becomes, in the single investment case

$$\begin{aligned} \min_{\mathbf{u}_k} J &= \bar{c}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{w}_k) \\ \text{s.t. } \zeta_k &= \mathbf{x}_{k+1} - \mathbf{x}_k - \mathbf{f}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{w}_k) = \mathbf{0} \\ \mathbf{0} &\leq \mathbf{x}_k \leq \mathbf{u}_k, \; k = 1, \ldots, M-1, \end{aligned} \tag{5.4}$$

where ζ_k are the defect constraints and $M = 168$ the number of steps. Note that in Eq. (5.4), the step length is one hour. Considering that the dynamics involved is of the first order and is stable, the multiple shooting method can be replaced by a single shooting one, which would make the problem easier to solve numerically.

The above defect constraints can be replaced by a cumulative summation, giving

$$\begin{aligned} \min_{\mathbf{u}_k} J &= \bar{c}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{w}_k) \\ \text{s.t. } \mathbf{x}_k &= \sum_{p=1}^{k} \mathbf{x}_p \\ \mathbf{0} &\leq \mathbf{x}_k \leq \mathbf{u}_k, \ k = 1, \ldots, M-1, \end{aligned} \tag{5.5}$$

This NLP problem can be solved using the methods in Section 3.1.

In Paper II two cases are considered: (1) variable utilisation as in Eq. (5.5) with extra requirements on initial amount of hydrogen stored and periodic maintenance and (2) constant utilisation, which is a special and simpler case of variable utilisation. In the variable utilisation case, the chosen special conditions are 100 kg hydrogen storage initially and at the end, and a weekly stop for maintenance from hour 75 to 87 during the week. Optimisations are done for the cases of one and two investments during the investment period. The resulting problem formulation is

$$\begin{aligned} \min_{\mathbf{u}_k} J &= \bar{c}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{w}_k) \\ \text{s.t. } \mathbf{x}_{hs,k} &= \sum_{p=1}^{k} (x^i_{hs,p} - x^o_{hs,p}) \\ 0 &= \sum_{p=75}^{87} x^o_{hr,p}. \\ x_{hs,1} &= 100 \\ x_{hs,1} &= x_{hs,M} \\ \mathbf{0} &\leq \mathbf{x}_k \leq \mathbf{u}_k, \ k = 1, \ldots, M-1, \end{aligned} \tag{5.6}$$

The data resulting from the optimisation are (1) the size of the equipment, (2) the running pattern of the facility, and (3) the price and utilization curve for the hydrogen produced. Figs. 5.4, 5.5 and 5.6 show some of the results in the case of two investments. The complete results are given in Paper II.

The problem in Paper II is on the edge of what is possible to solve. If the number of investments becomes too large (> 2 in the variable utilisation case), the computational time becomes prohibitively long.

5.3 The hythane infrastructure case

The **hythane** and hydrogen refueling station is a development of the previously discussed hydrogen refueling station. The differences in the layout is the absence

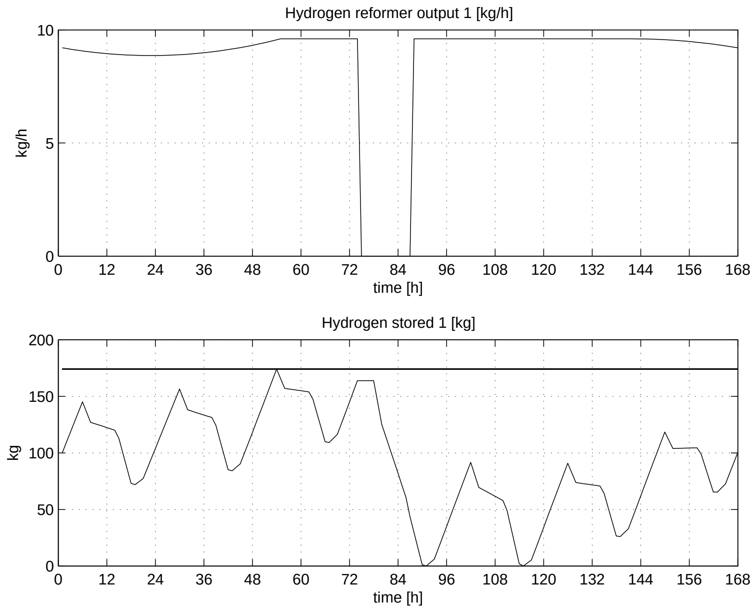

Figure 5.4: Variable utilisation case, two investments; throughput and stored hydrogen: Investment 1 at t=0.

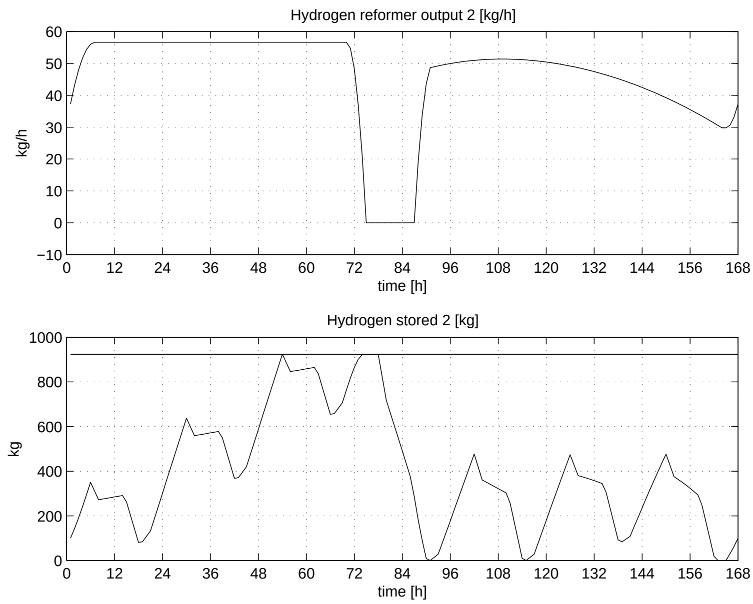

Figure 5.5: Variable utilisation case, two investments; throughput and stored hydrogen: Investment 2 at t=5.4.

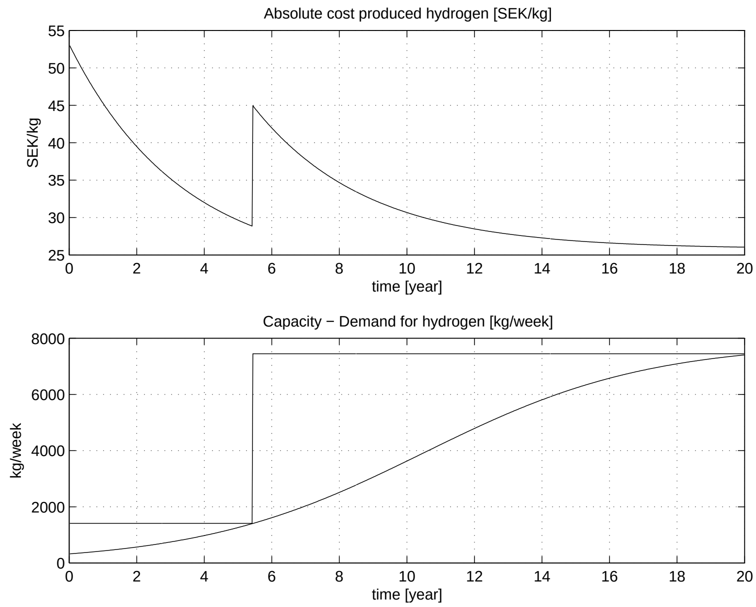

Figure 5.6: Variable utilisation case, two investments; hydrogen production cost and capacity-demand.

of the fuel cell for electricity production and, of course, the presence of a hythane dispenser, as can be seen in Figure 5.7. The major advantage with the above layout is that hythane can be used as an intermediate alternative fuel and, possibly, help introducing hydrogen by taking on some of the costs for the reformer, electrolysis and hydrogen storage.

In this study, the investment strategy is optimised with the objectives of minimising production cost for hydrogen as well as the requested amount of hydrogen that could not be satisfied, also called hydrogen unsatisfied demand. The optimisation method is described in Section 3.4. It should be noted that, in Paper IV, the results are expressed as Pareto fronts for the two objectives involved.

In Paper IV, the optimisation of the hydrogen and hythane station was carried out using a GA (see Section 3.2). In the evaluation of each solution candidate (individual), between one and 10 investments are allowed. This is accomplished with a variable chromosome length, see Figure 5.8. Since the first investment is mandatory at year 1, no timing is needed. Instead the demand priority policy υ, is defined. Demand can exceed supply and the demand priority governs how the available hydrogen is used to satisfy the demand at the hythane and hydrogen dispensers. Following υ in the chromosome, is the size of each piece of equipment for the refuelling station in investment 1. For consecutive investments, the demand priority policy is replaced by the time for the investment.

The selection, crossover and mutation operators are specially designed to cope

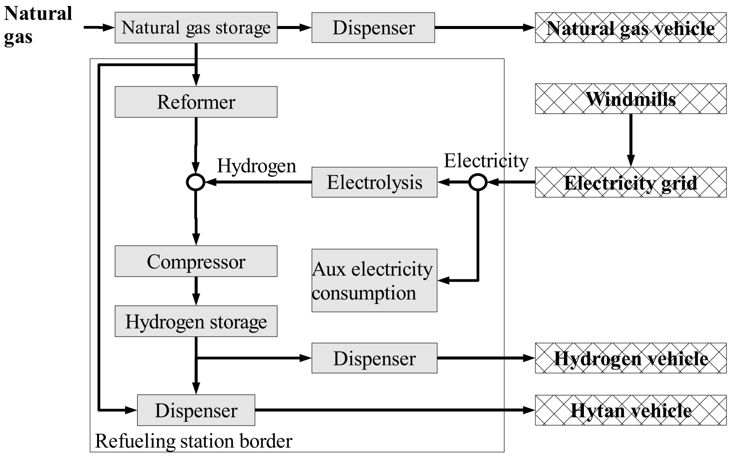

Figure 5.7: Hythane and hydrogen refueling station layout. Natural gas is reformed to hydrogen on-site and stored for delivery to vehicles. It is also possible to produce hydrogen from electricity by electrolysis. In Paper II, only the parts within the refueling station are considered.

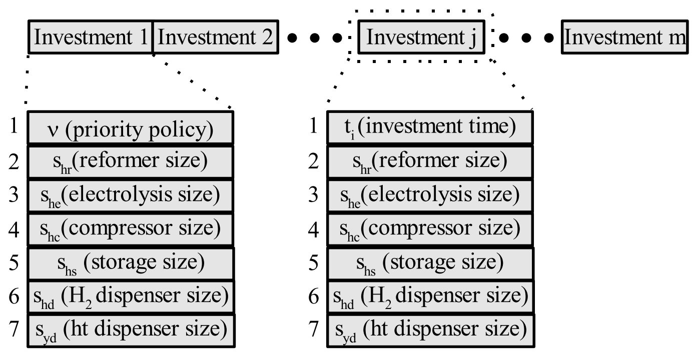

Figure 5.8: The encoding scheme used for the genetic algorithm in Paper IV. The priority policy υ, reformer size S_{hr} etc. are genes. Allowed values for genes (alleles) are given in Paper IV. The grouping of genes in the figure is only done for clarification.

with the problem at hand, the variables of which are implemented in chromosomes of the kind shown in Figure 5.8. The selection operator is of the crowded tournament selection type [88] where fitness is replaced with the inverse crowding distance within each Pareto front. The crowding distance is the mean distance to the nearest neighbour solutions. In this way the solutions lying furthest from each other are retained and a better spread of solutions within the front is achieved. The crossover operator is of the one-point type, in which a crossover point is chosen randomly within the shortest mutual length of the chromosomes. This will allow crossover between chromosomes of different length, i.e. different number of investments. An upper limit of 10 investments was set. In the mutation operator, the number of investments is changed with a low probability.

Traditionally, the control u is expressed as one vector for each decision period [93]. The above approach is a parametrization where investments not used are not part of the control. This is done in order to reduce the variable space and achieve a faster convergence.

The optimisations in Paper IV are all two-dimensional. Some experiments were also made with three-dimensional optimisations, i.e. optimising three objectives at the same time. Even though it is possible to extend the above algorithm to any dimensionality, there are practical limitations governed by the calculation time. Evaluation of one individual takes 75 s, using all scenario samples. Scenarios and sample generation are explained in Paper IV. In the two-dimensional case, the population R_t to be evaluated consists of 80 individuals. This number of individuals is needed to populate the Pareto front curve. The evaluation thus takes 1.7 hours. In the three-dimensional case at least $80 \times 80 = 6,400$ individuals would be needed to populate the generated Pareto surface, implying an evaluation time of 5.7 days per generation. Since at least 200-300 generations are needed, the whole optimisation would take approximately four years!

Each optimisation will give 40 solutions along the Pareto front for the objectives *hydrogen production cost* and *total hydrogen unsatisfied demand*. Each solution is optimised for the lowest expected values of each objective, given 100 samples from one of three scenarios, and can therefore be expressed as a distribution, as discussed in Section 3.4. In addition there are four other performance measures defined in Paper IV. These are unsatisfied demand for hydrogen $x_{h,u}$, production cost per kg for hythane p_{yf}, unsatisfied demand for hythane $x_{y,u}$ and flexibility $p_{h\Delta}$. All of the above measures can be calculated for the two scenarios not part of the optimisation (the passive scenarios). Also investigated was the variance of all the above measures. In all, this represents a large amount of data to take into consideration before making a decision. One way to handle the decision process could be to follow the procedure:

1. Find a reasonable solution regarding hydrogen production cost and unsatis-

fied demand while checking that the distribution of each variable is not too wide.

2. Check the location of the selected solution in the hythane production cost curve and the variance of the selected solution in the histogram.

3. Check flexibility, i.e. the result that would be obtained if another scenario should become reality. This can either be done with the defined flexibility measure, or in more detail, by calculating, e.g. production costs and distributions for the found solutions by applying the passive scenarios.

4. If production costs, unsatisfied demands and flexibility are all within reasonable limits, choose the solution. If not, go back to step 1.

Chapter 6

Concluding remarks

A number of techniques involving optimisation of industrial transition processes have been explored. In particular the problem of finding optimal long-term investment strategies taking economic an environmental considerations into account has been considered.

The investment strategy optimisation methods described in Papers II and IV, have been successfully applied to two cases concerning hydrogen dispensing infrastructure change. The first optimisation method, presented in Paper II, comprises a simultaneous calculation of the long-term investment strategy and the short-term utilisation scheme for a deterministic demand. The method has been applied to the case of finding an investment strategy for minimising the production cost for a single hydrogen refuelling station. The problem was shown to be convex; thus the resulting solution is the global optimum. The second investment optimisation method, presented in Paper IV, uses stochastic demand scenarios and multi-objective optimal control to produce the Pareto front of the two conflicting objectives *expected production cost* and *expected unsatisfied demand*. This method was applied to the case of finding the optimal investment strategy for a combined hydrogen and hythane refuelling station. Due to the uncertainty of the stochastic demand function, satisfying all demand would require a production capacity well above the mean demand, which would be very costly to maintain.

New ways for modelling joint economic-environmental systems and predicting future key parameters have been developed, in order to enhance the applicability and accuracy of structural optimisation methods. The findings are presented in a production system modelling case in Paper I and a time series prediction case in Paper III. The results obtained in Paper I have been applied in industry, by Cementa AB, in the evaluation of the consequences of using new fuels in cement production.

6.1 Future work

The optimisation method in Paper II was tested on the hydrogen refuelling station case, which was shown to be convex. Other algorithms for solving the resulting NLP problem could be investigated, e.g. *interior point* or *cutting plane* [72] methods, which are efficient for convex problems. It would also be interesting to test the developed method on a non-convex case and still try to obtain a global solution. The performance of the method in the described hydrogen refuelling case can most probably be improved. In case 2 with variable utilisation (see paper II) the computational time is unrealistically high for more than two investments. Since the most favourable solution probably lies between three and five investments, this limitation must be overcome. Even though computer hardware is constantly gaining speed, this does not mean that efforts to improve optimisation techniques should be neglected. On the contrary, in the author's opinion, the improvement of such techniques is more rewarding and useful than merely waiting for computers to become faster.

Due to the sampled nature of the refuelling curve, the investigated test case contained only time discrete dynamics. It would be interesting to try the method in a continuous dynamic case, i.e. where all the driving signals are continuous. Also, in order for the objective function to become more realistic, it should also incorporate, for example, the cost of labour for the hydrogen part of the refuelling station.

The investment problem in Paper IV was modelled as an open-loop system in the sense that the entire investment strategy was decided upon in advance. Such a system can, optimally, perform equally well as a closed-loop system [93]. However, in order to increase robustness, a closed-loop strategy could be used. This would allow for the strategy to change in accordance with revealed uncertainty in the demand. Furthermore, the large amount of data from stochastic multi-objective optimisations can be a problem. Efficient use of the method for decision support requires a higher degree of aggregation of the results than that done in Paper IV.

In both Paper II and Paper IV, the environmental measures are implicit, i.e. present through the use of an environmentally friendly technique. Another option would be to have explicit environmental figures in the objective functions. In Paper IV, which is a multi-objective problem solved with a GA, such objective functions could easily have been used. If explicit environmental measures can be derived and parametrised for different investment times, the techniques from Paper IV can be applied.

Different options in the scenario generation procedures can be explored. At present, a Poisson distribution is used to generate samples from the scenarios. Other methods, e.g. ARIMA models or neural networks, could also be evaluated.

Another possibility is to merge the three existing scenarios into one where the long-term behaviour in terms of the number of vehicles is governed by a set of stochastic variables. These variables can be tuned in accordance to expectations regarding the future development.

Chapter 7

Summary of appended papers

7.1 Paper I

In cement manufacturing, according to the law, the effect of any change to the production process must be investigated before the modified process is implemented. Such changes might involve type of sand, fuel or additives. Recently, Cementa AB, a major cement producer in Sweden, started to investigate alternative, more environmentally friendly types of fuel. In addition the company also started to improve the understanding of the involved physics and chemistry, which turned out to be complex. Today the verification comprises a calculation of produced emissions, but in the future other types of calculations would be needed.

In this paper a flexible model is developed which fulfills the requirements above. A computationally acausal model made it possible to separate the model describing the cement manufacturing process from the problem formulation. The model was built in ASCEND [46], which is an object-oriented, mathematically based modelling language as well as a multi-purpose simulation and calculation environment. In order to further enhance flexibility, the model was designed with a high degree of redundancy, so that the quantity of one physical property is expressed through a number of linked equations. This gives the user freedom to choose how to assign the physical property. In addition the model also fully traces the total cost throughout the production line.

7.2 Paper II

Running vehicles on hydrogen rather than petrol could lead to less environmentally hazardous emissions in a global perspective, especially if the hydrogen is made from renewable energy. Techniques for producing and storing the hydrogen, as well as fuel cells to convert the hydrogen into electricity, are constantly being improved. One of the most significant difficulties in the introduction of hydrogen vehicles today concerns the infrastructure that must be built. Considering the fact that all present refuelling stations for petrol need to be replaced, the total investment is huge. In this situation it is crucial to employ the most profitable investment strategy, given the probable future development.

In this paper the lowest production cost for a set of investments over a period of 20 years for an individual hydrogen refuelling station is found. For flexibility and convenience of transportation, the refuelling station utilises an on-site reformer for natural gas. The first case investigated assumes a constant production of hydrogen and will yield the minimal cost, whereas the second one can be used when special considerations like periodic stop for maintenance of the hydrogen reformer need to be taken into account. Both optimisation problems are shown to be convex and hence produce the global optimal point. The result is a hydrogen production cost of 4-6 USD/kg, comparable to the results of other studies. The major difference is that this study uses an increasing function to estimate the number of hydrogen vehicles refuelling at the station, and the estimated production cost is obtained as a time average. In other studies, the cost has been based on maximum utilization.

7.3 Paper III

In this paper, discrete-time prediction networks (DTPNs), a novel type of recurrent neural networks, are introduced and applied to the problem of macro-economic time series prediction. The DTPNs are optimized using a genetic algorithm (GA) that allows both parametric and structural mutations. Due to the feedback couplings present in the DTPNs, such networks are capable of a rudimentary short-term memory.

The results from applications involving two time series, namely the Fed Funds interest rate and US GDP, indicate that DTPNs are capable of one-step prediction with higher accuracy than several other benchmark methods. Thus, even though the data sets contain a large amount of noise, the study in Paper III indicates that there is more information available in the time series than can be extracted using, e.g. feedforward neural networks or ARIMA models.

In addition, an investigation of predictability was carried out. Here, the DTPNs were required not only to make a one-step prediction, but also to provide an estimate of the accuracy of the prediction. However, it was found that the discrepancy between the predictions obtained from the DTPNs and the actual data points in the time series consisted of noise, indicating that the DTPNs indeed extract almost all the available information from the time series.

7.4 Paper IV

Paper IV concerns the problem of finding the optimal investment strategy for a single hydrogen and hythane refuelling station giving the minimum production cost while trying to match the hythane and hydrogen capacity to a demand generated from three future stochastic scenarios over a 20-year period. Hydrogen is a promising fuel for vehicles. However, one of the major barriers is the lack of a hydrogen infrastructure. An important component of the hydrogen infrastructure is the individual hydrogen refuelling station. The long-term profitability of the hydrogen filling station is a key issue for the success of the transition to a hydrogen infrastructure. The resulting minimal expected production cost lies between 2-6 USD/kg for hydrogen and 1-1.5 USD/kg for hythane, depending on preferences for unsatisfied demand, flexibility etc. The results are meant to be used as decision support when planning new refuelling stations.

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Paper I

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The design and building of a life cycle-based process model for simulating environmental performance, product performance and cost in cement manufacturing

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Abstract

State of the art Life Cycle Inventory (LCI) models are typically used to relate resource use and emissions to manufacturing and use of a certain product. Corresponding software tools are generally specialised to perform normalisation of the flows to the functional unit. In some cases it is, however, desirable to make use of the LCI model for other types of environmental assessments. In this paper, an alternative modelling technique resulting in a more flexible model is investigated. We exemplify the above by designing and building a model of a cement plant. The commissioner's, in this case Cementa AB, requirements on a flexible model that generates information on environmental performance, product performance and the economic cost were seen as important. The work reported here thus has two purposes; on the one hand, to explore the possibility for building more flexible LCI models, and on the other hand, to provide the commissioner with a model that fulfils their needs and requirements. Making use of a calculational a-causal and object-oriented modelling approach satisfied the commissioner's special requirements on flexibility in terms of modularity and the types of calculations possible to perform. In addition, this model supports non-linear and dynamic elements for future use. The result is a model that can be used for a number of purposes, such as assessment of cement quality and environmental performance of the process using alternative fuels. It is also shown that by using the above modelling approach, flexibility and modularity can be greatly enhanced.

Keywords: Life-cycle-simulation; Predict; Consequences; Process model

1. Introduction

The interest in environmental issues, as well as the pressure on industries to develop more environmentally preferable products and processes, is constantly increasing. This drives product and process development towards more sustainable practices. However, products, processes and production systems are always developed taking cost and product performance into consideration. Thus, there is a growing need for tools to predict and assess both the environmental performance and the economic cost and the product performance of alternative production operations.

The purpose of this paper is to describe how we designed and built a flexible model for process and product development in the cement industry. The model predicts the environmental performance, the economic cost and the product performance by simulating different operational alternatives for producing cement. The needs and requirements were specified by the cement industry. These are outlined in Section 3. We give our interpretations as a conceptual model in Section 4. We chose the modelling approach and simulation tool and describe how we designed and built the model in Section 5. We end Section 5 by testing the tool in two real cases. The

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results of these tests show that the modelling approach used can generate a potentially powerful tool.

A life cycle perspective ("cradle to gate") was used to assess the environmental consequences of process and product changes, in order to avoid sub-optimisation. The conceptual model represents the cement manufacturing process from cradle to gate. However, the model in this paper, the construction of and test of we describe in detail, represents the gate to gate part of the manufacturing process. Environmental performance is described in terms of environmental load (resource use and emissions). Economic cost is described in terms of the company's own material cost and production cost. Product performance is expressed as cement composition. The product performance is used to determine whether or not the operational alternative is feasible. Environmental load and economic cost have to be related to a feasible operational alternative and product.

Cementa AB, the cement manufacturer in Sweden and the commissioner of the study, has previous experience of Life Cycle Assessment (LCA) through a Nordic project on Sustainable Concrete Technology [1]. In that project, several LCA studies were carried out on cement, concrete and concrete products [2,3,4,5,6]. One conclusion drawn from the project was that life cycle assessment is a tool, with the potential for improvement, to be used to avoid sub-optimisation in the development of more environmentally adapted cement and concrete products and manufacturing processes [1]. Several other LCA's of cement, concrete and concrete products have also been carried out [7,8,9,10].

However, there are limitations with today's LCA. One important limitation, from an industrial perspective, is that social and economic benefits of industrial operations are not taken into account. Another limitation of present LCI modelling is its limited capability to perform different types of simulations. There are limits on the possibility of changing process variables without changing the underlying model. Usually a new model is built for each operational alternative simulated. In addition, LCI models are usually defined as linear and time independent.

2. Background

2.1. Cement manufacturing and related environmental issues

The cement manufacturing process, shown in Fig. 1, consists of the following main steps: limestone mining, raw material preparation, raw meal grinding, fuel preparation, clinker production, cement additives preparation and cement grinding. Clinker is the intermediate product in the manufacturing process. The following description is based on the manufacturing process at Cementa's Slite plant. The cement manufacturing process at the Slite plant is described in detail in the report "Cement Manufacturing — Process and Material Technology and Related Environmental Aspects" [11].

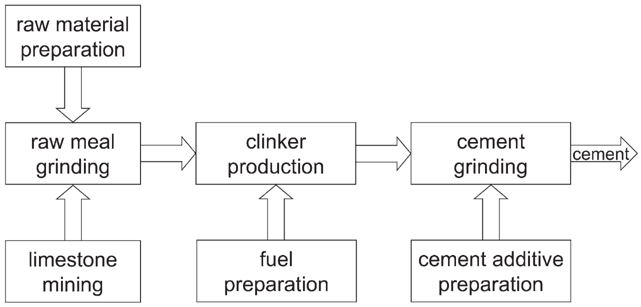

Fig. 1. Cement manufacturing process.

Limestone, the main raw material is mined and crushed. Other raw materials used may be sand, iron oxide, bauxite, slag and fly ash. The raw materials are prepared and then proportioned to give the required chemical composition, and ground into a fine and homogeneous powder called raw meal.

Various fuels can be used to provide the thermal energy required for the clinker production process. Coal and petroleum coke are the most commonly used fuels in the European cement industry [12]. A wide range of other fuels may be used, e.g. natural gas, oil and different types of waste, e.g. used tyres, spent solvents, plastics, waste oils. The fuels are processed, e.g. ground, shredded, dried, before being introduced into the process.

Clinker production is the "heart" of the cement manufacturing process. The raw meal is transformed into glass-hard spherically shaped minerals clinker, through heating, calcining and sintering. The raw meal enters the clinker production system at the top of the cyclone tower and is heated. Approximately half of the fuel is introduced into the cyclone system, and at about 950° C the carbon dioxide bound in the limestone is released, i.e. the calcination takes place. The calcined raw meal enters the rotary kiln and moves slowly towards the main burner where the other half of the fuel is introduced.

Raw materials and fuels contain organic and inorganic matters in various concentrations. Normal operation of the kiln provides high temperature, a long retention time and oxidising conditions adequate to destroy almost all organic substances. Essentially all mineral input, including the combustion ashes, is converted into clinker. How metals entering the kiln behave depends largely on their volatility. Most metals are fully incorporated into the product, some precipitate with the kiln dust and are captured by the filter system, and some are present in the exhaust gas.

Inter-grinding clinker with a small amount of gypsum produces Portland cement. Blended cement contains, in addition, cement additives such as granulated blast furnace slag, pozzolanas, limestone or inert filler. Depending on their origin, the additives require different preparations.

The exhaust gases leaving the clinker production system are passed through a dust reduction device before being let out through the stack. The dust is normally returned to the process. The clinker production system is the most important part of the manufacturing process in terms of environmental issues. The main use of energy is the fuel for clinker production. Electricity is mainly used by the mills and the exhaust fans. The emission to air derives from the combustion of fuel and the transformation of raw meal into clinker. Apart from nitrogen and excess oxygen, the main components of kiln exhaust gas are carbon dioxide from the combustion of fuel and the calcination of limestone and water vapour from the combustion process and raw materials. The exhaust gas also contains dust, sulphur dioxide, depending on sulphur content of the raw materials, small quantities of metals from raw material and fuel, and remnants of organic compounds from the raw material.

The emissions to air from the clinker production system largely depend on the design of the system and the nature and composition of the raw material and fuel [11]. The raw material and fuel naturally vary in composition and the content of different compounds have a different standard deviation. The emissions of metals depend on the content and volatility of the metal compound in the raw material and fuel. The metal content varies over time and consequently so does the metal emission.

The Nordic study “LCA of Cement and Concrete — Main Report” points out emissions of carbon dioxide, nitrogen oxides, sulphur dioxide and mercury, and the consumption of fossil fuel as the main environmental loads from cement production [6]. According to the European Commission, the main environmental issues associated with cement production are emissions to air and energy use [13]. The key emissions are reported to be nitrogen oxides, sulphur dioxide, carbon dioxide and dust.

2.2. Means and work done to minimise negative environmental impact

The negative environmental impact from cement manufacturing and cement can be minimised in numerous ways. These can be grouped into four categories:

- Substituting input, raw materials, fuels and cement additives, to the process.
- Process development; optimise and develop the existing process.
- End-of-pipe solutions; adding emission reduction systems.
- Product development; develop new products or change cement composition and performance.

Many of these solutions have consequences outside the actual cement manufacturing plant, both upstream as well as downstream. Therefore, the life cycle perspective is necessary to assess the environmental consequences of process and production changes in order to avoid sub-optimisation.

Examples of environmental improvement measures taken at the Slite plant in recent years are given in the following, in order to give examples of technical devices and measures the model should be able to deal with.

Different types of waste are used, e.g. used tyres, plastics, spent solvents, waste oils, as substitutes for traditional fuels to reduce the consumption of virgin fossil fuels and the emission of carbon dioxide. The goal is to replace 40% of the fossil fuel with alternative fuel [14] by 2003. Cementa is also looking into the possibility of using alternative raw materials, i.e. recovered materials, to substitute for traditional, natural raw materials. The alternative raw materials can either be used as raw material in the clinker production process or as cement additives, i.e. to substitute for clinker in cement grinding.

In 1999 a new type of cement, “building cement”, was introduced on the Swedish market. Building cement is a blended cement with about 10% of the clinker replaced with limestone filler. The environmental benefits of substituting limestone filler for clinker are a reduction in the amount of raw meal that has to be transformed into clinker, and consequently less environmental impact from the clinker production process, raw material and fuel preparation. The environmental impact per ton cement has been reduced by 10% [15].

The use of alternative material and fuel at the cement plant requires pre-treatment, transport and handling, and affects the alternative treatment of waste and by-products. New materials and fuels lead to new combinations and concentrations of organic and inorganic compounds in the clinker production system, which in turn lead to new clinker- and exhaust gas compositions.

As an end of pipe-solution, a Selective Non Catalytic Reduction system (SNCR) to reduce nitrogen oxide emissions was installed at the Slite plant in 1996. In 1999, a scrubber was taken into operation to reduce sulphur dioxide emissions. In the scrubber, SO_2 is absorbed in a slurry consisting of limestone and water. The separated product is used as gypsum in the cement grinding.

3. The commissioner’s needs and requirements on the model

The commissioner’s, Cementa AB, needs and requirements, as interpreted from discussions with representatives from different departments, are outlined in this section.

Cementa AB needs a tool to predict and assess product performance, environmental performance and economic cost of different operational alternatives for producing cement. The tool is to be used to support company internal decisions on product and process development and strategic planning through generating and assessing operational alternatives. Another specific use is as a basis for government permits. To get permits for test runs of new raw materials and fuels, information on the expected outcome is needed.

Cementa intends to learn about the system and the system's properties regarding product performance, environmental performance and economic cost and the relations between these parameters. The life cycle perspective is seen as important. Cementa wants to be able to simulate combinations of raw materials, fuels and cement additives in combination with process changes and end-of-pipe solutions. For all tested combinations, information about the system's predicted properties should be generated and assessed in relation to feasibility criteria, such as product performance, emission limits and economic cost. Product performance is regarded as the most important criterion.

The commissioner gave the following two examples of how to use the tool. They asked for specific and detailed information about the predicted consequences for each alternative.

A Produce a given amount of cement, given the raw material mix, the fuel mix and fuel demand, and the cement additive mix. What is the product performance of the cement, the environmental performance and the economic cost?
B Produce a given amount and type of cement, given the fuel mix and fuel demand, the cement additive mix and the available raw materials. What raw material mix is required? What are the environmental performance and the economic cost?

Concrete with different strength developments needs different amounts of cement. Therefore, it should be possible to state the amount of cement produced in the operational alternative simulated. The environmental performance should be described as environmental load, i.e. as resource use, emissions to air and water, and waste. The composition of the kiln exhaust gas from clinker production should be described. The composition of all raw material, fuel, intermediate products and products should be described and possible to evaluate. The product performance should be described with three ratios; the lime saturation factor (LSF), the silica ratio (SR), and the alumina ratio (AR), used in the cement industry as measures of cement composition. The ratios describe the relation between the four main components and are shown in Table 1. The total material and production cost in "SEK" per amount cement produced should be calculated. The accumulated material and production cost should be available to study after each step in the cement manufacturing process; both as cost per amount cement produced and as cost per kilo of the intermediate product.

Cementa produces cement at three plants in Sweden. The different plants use the same main production process as described in Section 2.1. However, there are variations between the plants, especially in the design of the clinker production system. Variations are mainly due to the nature of the available raw material, when the plant was built, modifications done and the installation of different emission reduction systems. It should be easy to adapt the tool to represent any of the commissioner's cement manufacturing processes, although the first model was intended to represent the Slite plant.

The content of metal compounds in the raw material, and the standard deviation of the metal content, vary depending on the location of the plant. Thus, the emissions of metals to air vary from one plant to another. Emission of metals from clinker production should be included in the first model, but they are not in focus. However, in the next stage, when site-specific models of each plant are developed, the level of detail with which metal emissions are described, should be further increased.

The cement manufacturing process is by nature non-linear and dynamic. The tool should describe stable state conditions and describe the static and linear transformation of raw material and fuel into clinker. The tool has to have development potential to include the non-linear transformations in the process. In addition, there should also be the potential to simulate dynamic behaviour, e.g. during start-up and shut down of the kiln.

4. Conceptual model and system boundary

Based on the commissioner's requirements, a conceptual model was constructed, as presented in the following:

To avoid sub-optimisation, the model was to be from a life cycle perspective. The raw material, fuel and cement additives used are to be traced upstream to the point where they are removed as a natural resource. Alternative raw materials, fuels and cement additives are by-products or waste from other technical systems. The production of these alternative products is not to be included. However, the additional preparation, handling and transport to make them fit the cement industry is to be included. The cement is to be followed to the gate of the cement plant.

The cement manufacturing system has been divided into a background system and a foreground system [16]. The foreground system represents Cementa's "gate to gate" part of the system. Cementa can, in detail, control and decide on processes in the foreground system, but can only make specifications and requirements on pro-

Table 1
Product performance (cement-, clinker-, raw meal ratios)

Ratio	Denomination	Formula
Lime saturation factor	LSF	LSF=(100CaO)/(2,8SiO_2+1,1Al_2O_3+0,7Fe_2O_3)
Silica ratio	SR	SR=(SiO_2)/(Al_2O_3+Fe_2O_3)
Alumina ratio	AR	AR=(Al_2O_3)/(Fe_2O_3)

Note: CaO, SiO_2, Al_2O_3 and Fe_2O_3 are all expressed in weight percentage.

ducts from the background system. Depending on whether the additional preparation, handling and transport is done by Cementa or not, the processes are either in the foreground system or the background system. The conceptual model, in Fig. 2, shows the foreground and background systems, and in addition a wider system. The wider system shows consequences of actions taken at the cement plant, which exist, but are not modelled.

The foreground system was divided into the following processes:

- Lime- and marlstone extraction, mining and crushing;
- Sand grinding;
- Raw meal grinding;
- Coal and petroleum coke grinding;
- Clinker production;
- Cement grinding and storage.

Between each one of these processes, intermediate homogenisation, transportation and storage might take place and, where applicable, are accounted for.

The background system consists of the following processes:

- Production and transport of sand and other raw material;
- Additional preparation of alternative raw materials and transport to the cement plant;
- Production and transport of traditional fuels;
- Additional preparation of waste to convert them into fuels for cement manufacture and transport to the cement plant;
- Production and transport of cement additives;
- Additional preparation of alternative cement and transport to the cement plant;
- Production of electricity.

The plant in Slite produces waste heat used for district

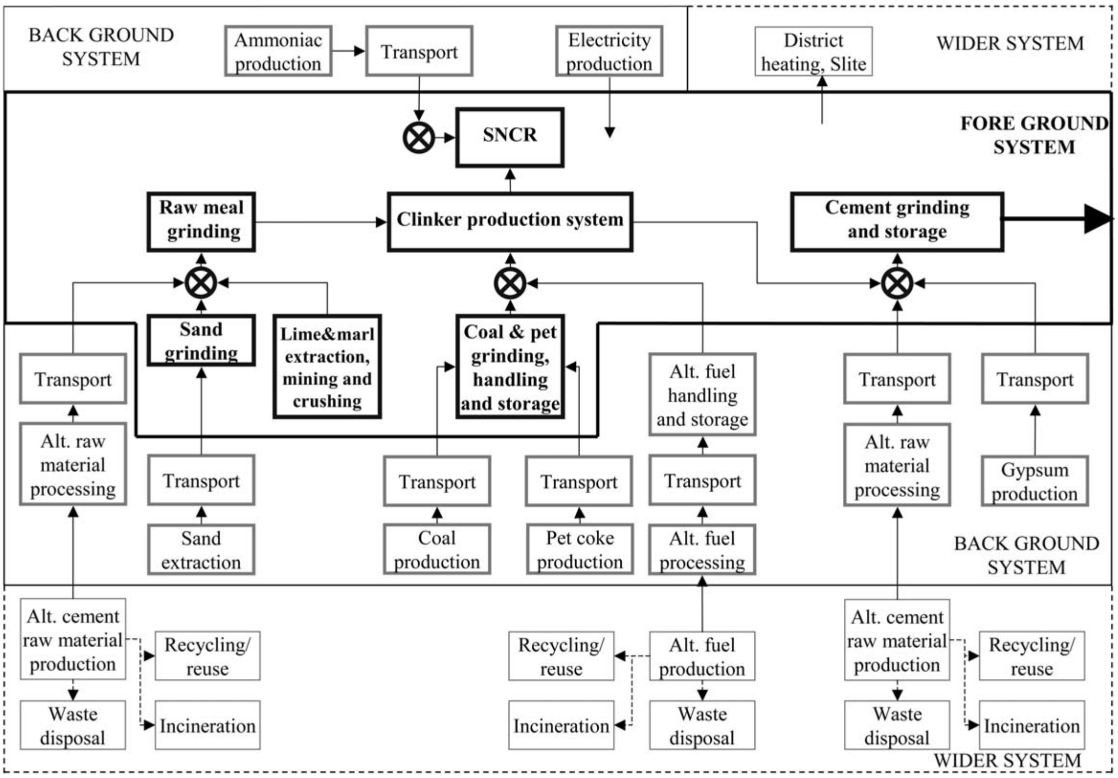

Fig. 2. Conceptual model.

heating in Slite. The waste heat is accounted for as an output, a product, but no credit is given to the cement production through allocation or system enlargement. In the same way, when alternative raw materials and fuels are used in cement manufacturing, the amount of waste thus disposed of is accounted for, but no allocation is made. These consequences of the cement manufacturing process are placed in the wider system in the conceptual model.

Not considered are:

- Production and maintenance of capital equipment for manufacturing and transport;
- Extraction and production of alternative raw materials, fuels and cement additives;
- Working material, such as explosives, grinding media and refractory bricks;
- Iron-sulphate used in the cement milling to reduce chromium;
- Offices.

The two systems were modelled with different techniques and level of detail. The foreground system model was built according to the techniques described in the next section. For the background system, traditional life cycle inventory (LCI) techniques [17] were used. Product performance and economic cost were taken into account by assigning the products entering the foreground system a chemical composition and a cost. Subsequently, flows entering the foreground system are described as a flow of mass (kg/s), cost (SEK/s) and thermal energy content (MJ/s) with a composition according to Table 2, and in accordance with the purchase deal. Flows of material in the background system are defined and described as a flow of mass (kg/s).

The environmental load (resource use and emissions) was described according to the parameters in Table 3. The kiln exhaust gas from the clinker production system was described using the parameters in emission to air in Table 3. The transport was expressed both in ton kilometres and as the related environmental load, according to the parameters in Table 3.

Table 3
Environmental load, resource use and emissions to air and water

Resource use	
Raw material, kg	
Alternative raw material, kg	
Fuel, kg and MJ	
Alternative fuel, kg and MJ	
Water, kg	
Emission to air	Hg, mercury
CO_2, carbon dioxide	Mn, manganese
NO_x, nitrogen oxides (NO and NO_2 as NO_2)	Ni, nickel
SO_2, sulphur dioxide	Pb, lead
CO, carbon monoxide	Sb, antimony
VOC, volatile organic compounds	Se, selenium
Dust	Sn, tin
As, arsenic	Te, tellurium
Cd, cadmium	Tl, thallium
Co, cobolt	V, vanadium
Cr, chromium	Zn, zinc
Cu, copper	
Emission to water	
BOD, biological oxygen demand	
COD, chemical oxygen demand	
Total N, total nitrogen content	
Non elementary in-flow, "flows not followed to the cradle"	
Alternative raw material and fuel	
Non elementary out-flows, "flows not followed to the grave"	
Industrial surplus heat, MJ	

Table 2
Material and fuel composition

Compound	Unit	Compound	Unit
CaO	weight-share	As, arsenic	weight-share
SiO_2	weight-share	Cd, cadmium	weight-share
Al_2O_3	weight-share	Co, cobolt	weight-share
Fe_2O_3	weight-share	Cr, chromium	weight-share
MgO	weight-share	Cu, copper	weight-share
K_2O	weight-share	Hg, mercury	weight-share
Na_2O	weight-share	Mn, manganese	weight-share
SO_3 (sulphides and organic in raw material)	weight-share	Ni, nickel	weight-share
SO_3 (sulphates in raw material)	weight-share	Pb, lead	weight-share
SO_3 (in fuel)	weight-share	Sb, antimony	weight-share
Cl	weight-share	Se, selenium	weight-share
C (in traditional fuel)	weight-share	Sn, tin	weight-share
C (in alternative fuel)	weight-share	Te tellurium	weight-share
C (in raw material)	weight-share	Tl, thallium	weight-share
Organic (in raw material)	weight-share	V, vanadium	weight-share
Moist (105° C)	weight-share	Zn, zinc	weight-share

5. Modelling and simulation

This section starts by interpreting the commissioner's requirements in a system technical context. Only the foreground system is considered in the following. The result is a set of decisions on the modelling and the simulation techniques. This is followed by a description of how the model was built in accordance with these techniques and, finally, how the constructed model was validated.

5.1. System technical interpretation

To predict the performance of the desired type of operational alternatives it was concluded that we had to simulate them, i.e. perform calculations on a model representing the cement manufacturing plant. A model is, here, a mathematical description of any real subject. A simulation is then any kind of mathematical experiment carried out on the model.

The requirements on the model indicate the necessity of keeping these simulations flexible in the sense that it should be possible to predict a number of aspects of the plant, depending on the situation. Examples of static equilibrium calculations that are given in Section 3 include:

A Setting the percentage of each raw material in the raw meal and each fuel in the fuel mix used. Then calculating the percentage of raw meal mix and fuel mix, the produced cement quality, emissions and economic cost under the constraint that the fuel provides all the thermal process energy. This means we give all the materials necessary to produce cement and then watch what comes out of the process.

B Setting properties of the produced cement and each fuel in the fuel mix used. Then calculating the percentage of each raw material in the raw meal mix, the percentage of raw meal mix and fuel mix, emissions and economic cost under the constraint that the fuel provides the process thermal energy. This means we want to control properties of the cement produced and calculate the proportions of the raw materials, under the same constraint for the fuel to provide enough thermal heat.

In a mathematical model, numerical parameters can be divided into the following categories:

- Constants. Are set when the model is built and then remain.
- Locked variables. Parameters set to a numerical value throughout a certain simulation, in accordance to input data.
- Free variables. Parameters that will be calculated in the simulation. Some of these are internal variables in the model and others are the ones we want to calculate; the output.

The difference between the above cases is which parameters are locked and which are free. This controls how the simulation is carried out, i.e. how the equations for simulation are formulated. The two static equilibrium cases above will result in different sets of equations. A simultaneous solving of a respective set of equations will render the result. It is indeed possible to make these calculations with any general mathematical package available. If so, each of the cases has to be treated separately. The result is a well functioning simulation for the specific case that cannot, however, be used for other different simulations. If so, the equations need to be re-formulated. Since a specific requirement was flexibility in the calculations that are possible to perform, we will refine our modelling method by a separation of the model, or what is normally thought of as the model, into three parts, namely:

- A neutral model. Only the model, i.e. a description of our system, in which the connecting equations are expressed in a neutral form. The model maps our interpretation of the plant onto a mathematical formulation, but it does not include any specific problem to be solved, hence it is called neutral.
- A problem formulation. An explicit list of which parameters to lock and a value with which to designate each of them.
- A simulation method, which is the calculation method chosen, can also be considered to be a part of the problem formulation.

The most powerful way to achieve this separation is to remove the calculational causality (CC) from the model [18]. The CC determines the order in which the equations included in a simulation are calculated. This is merely a technical consideration and affects only the order in which the calculations are done and does not imply any restrictions or special considerations regarding the nature or contents of the system behind the model. The resulting model is said to be a-causal, or non-causal, in that nothing is said about the order of calculation in future simulations with the model. The model can be regarded mathematically as a number of equilibrium equations connected to each other.

Another important aspect of flexibility for the model is modularity. In order to be truly flexible, according to the requirement regarding adjustments to represent different cement plants, the model has to be easy to rebuild. In most practical cases, changes would probably be limited to assigning different inputs and performing different kinds of simulations, which would already be part of the problem formulation. In some cases, this is not enough and the underlying model structure needs to be altered. Changing the number of raw materials or fuels is one such case, and adopting it to fit a cement manufacturing plant with different designs is another. A step to create modularity has already been taken by making the model a-causal. This is merely a theoretical prerequisite and will not, in itself, produce a flexible model. On the other hand, if this is combined with an object oriented modelling language, we will end up with a practical, easily re-combinable model. The paradigm of object orientation is something that affects the language the model is expressed in. This includes a natural way to keep parts that are separate in reality as separate objects in the model, so that the model resembles reality, or a suitable picture of reality. Usually this feature is used to group sub-parts of the model into objects, but it is also useful to group flow entities together. Flows that are made up of a number of substances can thus be treated as an entity to enhance the transparency and ease of comprehension.

The cement manufacturing process contains both parts that vary over time and parts which cannot always be sufficiently described with a linear relation. One of the requirements was to make it possible to account for these properties in the future, so it must be possible to include both dynamic and non-linear elements. The first model which is covered in this paper does not, however, contain any dynamic or non-linear elements.

In addition to being able to include the above dynamic elements of the model, we also need to perform dynamic solving, i.e. calculate and trace (all) the variables in the model over a certain time span. This simulation type can be used for environmental predictions when, e.g., starting up, shutting down or changing parameters in the cement production process. The starting point for such a simulation can be given values for a set of variables, such as the start conditions for the plant when performing a start up simulation. It can also be from a state of equilibrium, which is the case when simulating a shut down situation. In the latter case, we need a method to determine this state of equilibrium, e.g. perform a steady state solving. The steady state solving can, of course, also be used on its own to find stable points of operation for the production plant. It is then equivalent to what in LCI is generally called "normalisation of the life cycle" or, specifically in ISO 14041 [17], "relating data to functional unit". In addition, another simulation type which is mentioned for future use, is optimisation.

In summary, we have found that in order to fulfil the requirements of the commissioner the model needs to be flexible in terms of:

- Simulation — type of predictions that can be made: static equilibrium, dynamic solving, etc.;
- Modularity — ease of combination into models of other cement plants by re-arrangement of the parts;
- Transparency — all governing equations and resulting figures readily available to the user, even the internal ones;
- Comprehension — easy to grasp and understand.

We have, thus, found that the following modelling approach is needed:

- Calculational non-causal used to separate a neutral model and the problem formulation;
- Physical modelling to keep physical entities together in the model;
- Object oriented modelling language to enhance the reusability of the model.

In addition, the model needs to support:

- Dynamic elements;
- Non-linear elements.

Simulation types the software tool needs to support:

- Steady state solving;
- Dynamic solving;
- Optimisation.

Not all of the requirements above are fulfilled with state-of-the-art LCI techniques [19]. In LCI, it is generally enough to describe the life cycle with such a resolution that it is sufficient with a static and linear model. Moreover, current LCA tools normally provide normalisation of the life cycle to the reference flow as the only simulation alternative. Consequently, there are no LCA related software tools available that can perform the desired types of simulations. In the field of general simulation there are, however, a large number of tools that can be used. Some equivalent examples include OmSim [20], DYMOLA [21] and ASCEND [22]. These software are of the kind that use computational non-causal models and allow a number of types of simulations to be performed. For this application, ASCEND was chosen based on the following criteria:

- It was possible to run on a PC, hence convenient (DYMOLA, ASCEND);
- It had plug-in modules allowing user made simulation types, hence flexible (OmSim, DYMOLA, ASCEND);
- It was freeware, hence economical (OmSim, ASCEND).

5.2. Model construction

Building a model with the specifications and techniques discussed above is more a matter of generalisation than specification. Most of the core components in the model will hence reflect the general behaviour of an “object” or “function”. Later, these will be specialised to the specific case, here the cement manufacturing plant. This technique of extracting layers of behaviour is well suited for object oriented implementation where the mechanism of inheritance can be used for that purpose. The general behaviours are implemented in base classes and the more specific in inherited ones.

The first step when building the model was to find the objects contained in our perception of the cement manufacturing plant. This was already done in the conceptual model. These objects then needed to be abstracted into their general behaviour. Usually, this reveals that a number of objects follow the same basic rules, which then means that they can inherit from the same base object.

First, the general functionality of parts in the conceptual model was extracted. Then, a number of general objects were built to host the functionality. Focus was put on the mechanisms behind the general functionality and the correspondence with reality for the more specific one. From the conceptual model, we found the objects given in Table 4.

In the following, a detailed explanation of some of these objects is given. The syntax used is based on the ASCEND IV model language [22] but has been simplified to only include the contents (semantic). All code is given in another font (**model**). The word **composition** thus means the model (object) composition as declared in Table 5.

Table 5
Syntax used in declaration of objects

Syntax	Explanation
MODEL xyz	Start declaration of the object xyz
Declarations:	Part of object where declarations are given
abc IS_A xyz;	Declares abc as of type xyz
abc[n] IS_A xyz;	Declares abc as an array with *n* number of elements of type xyz
Assignments:	Part of object where constants are initiated
Rules:	Part of object where the equations are given
FOR i IN abc END FOR;	Loop where *i* get the contents of each member in abc
SUM[abc]	Compute the sum of all elements in abc
=	Neutral equality. Used to express equilibrium, i.e. that two expressions are numerically equal. It is not an assignment and does not imply any order of calculation, e.g. left to right.

5.2.1. Composition

This object is used to represent any kind of composition of a mixture. A list is used to contain the name of each component in the mixture (**compounds**). The weight share of each component is given as a fraction with the range of 0 to 1 (**y[compounds]**). To be able to handle redundant descriptions (where the weight of the parts differs from that of the whole), no limitation is put on the fractions to sum up to 1.0. The object also contains the cost (**cost**) and heat content (**heat**) per mass unit of the total mixture. The typical usage of this object is to declare the contents of a material, such as a raw material, fuel or a product.

Table 4
Total listing of objects in the model

Name	Inherits from	Role
composition	–	Any kind of composition of a mixture
mass_stream	–	Flow of material
materialfuel_stream	**mass_stream**	Flow of raw materials and fuels
kilnexhaustgas_stream	**mass_stream**	Flow of exhaust gas
chemical_analyser	–	Test probe for specific cement ratios
materialfuel_mixer	–	Mixer for *n* number of material fuel streams
rawmeal_mixing	**materialfuel_mixer**	Specific raw meal mixer at Slite
fuel_mixing	**materialfuel_mixer**	Specific fuel mixer at Slite
rawmealfuel_mixing	**materialfuel_mixer**	Specific raw meal fuel mixer at Slite
cement_mixing	**materialfuel_mixer**	Specific cement mixer at Slite
materialfuel_grinder	–	General grinder for a material fuel stream
rawmeal_grinder_slite	**materialfuel_grinder**	Specific grinder for raw meal at Slite
sand_grinder_slite	**materialfuel_grinder**	Specific grinder for sand at Slite
lime_grinder_slite	**materialfuel_grinder**	Specific grinder for lime at Slite
marl_grinder_slite	**materialfuel_grinder**	Specific grinder for marl at Slite
coalpetcoke_grinder_slite	**materialfuel_grinder**	Specific grinder for coal and pet coke mixture at Slite
cement_grinder_slite	**materialfuel_grinder**	Specific grinder for cement at Slite
clinker_production	–	General clinker production
clinker_production_slite	**clinker_production**	Specific clinker production at Slite
cement_model_slite	–	Top level model over the Slite plant

```
MODEL composition
Declarations:
        compounds        IS_A set OF
                         symbol_constant;
        y[compounds]     IS_A fraction;
        cost             IS_A cost_per_mass;
        heat             IS_A
                         energy_per_mass;
```

Note: The contents of the **compounds** list is not yet specified.

5.2.2. *Mass stream*

The mass stream is a flow of material where the content is declared by a **composition** (**state**). The flow rate is expressed both as total flow (**quantity**) and flow of each of the contained components (**f**). For convenience (easier access at higher levels), the list of components in the flow is repeated (**compounds**). It is, then, declared equivalent to the one already present within **state** to prevent deviating values.

The two ways of describing the flow can be expressed in terms of each other and, thus, are not independent of each other. In fact, for all components the flow of each component equals the total flow times the fraction for the component in question (**f[i]** = **quantity∗state.y[i]**).

```
MODEL mass_stream
Declarations:
    compounds                  IS_A set OF
                               symbol_constant;
    state                      IS_A composition;
    quantity,f[compounds]      IS_A mass_rate;
Rules:
    compounds,                 ARE_THE_SAME;
    state.compounds
    FOR i IN compounds         f_def[i]: f[i] =
    CREATE                     quantity*state.y[i];
    END FOR;
```

5.2.3. *Material–fuel stream*

The material–fuel stream is a specialisation of the mass-stream declared above. It represents the flow of raw materials and fuels in the cement manufacturing process. It takes all relevant materials into account, as defined in Table 2, and permits these to be described either as a share or mass per time. Here, the share option is used to declare the weight share of each component. The material–fuel stream also carries the associated cost and heat.

```
MODEL materialfuel_stream REFINES
mass_stream
Declarations:
        cost           IS_A cost_per_time;
        heat           IS_A energy_rate;
Assignments:
        Compounds:=    [‘CaO’,‘SiO2’,‘Al2O3’
                       ,‘Fe2O3’,‘MgO’,‘K2O’
                       ,‘Na2O’,‘SO3sulphides’
                       ,‘SO3sulphates’,‘SO3fu
                       el’,‘Cl’,‘Ctrad’,‘Calt’
                       ,‘Craw’,‘Moist’,‘Organi
                       c’,‘As’,‘Cd’,‘Co’,‘Cr’
                       ,‘Cu’,‘Hg’,‘Mn’,‘Ni’
                       ,‘Pb’,‘Sb’,‘Se’,‘Sn’,‘Te’
                       ,‘Tl’,‘V’,‘Zn’];
Rules:
        cost =         quantity*state.cost;
        heat =         quantity*state.heat;
```

5.2.4. *Kiln exhaust gas stream*

The exhaust gas from the clinker production system is modelled as a flow representation of its own. The components are specified with the mass flow, e.g. kg/s. The components are defined in Table 3. The kiln exhaust gas stream is a specialisation of the mass-stream, to which the appropriate compounds have been added as described below.

```
MODEL kilnexhaustgas_stream REFINES
mass_stream
Assignments:
        Compounds:=    [‘CO2raw’,‘CO2trad’
                       ,‘CO2alt’,‘CO’,‘VOC’
                       ,‘NOx’,‘SO2’,‘vapour’
                       ,‘As’,‘Cd’,‘Co’,‘Cr’,‘Cu
                       ’,‘Hg’,‘Mn’,‘Ni’,‘Pb’
                       ,‘Sb’,‘Se’,‘Sn’,‘Te’,‘Tl’
                       ,‘V’,‘Zn’];
```

5.2.5. *Chemical analyser*

A chemical analyser is a sort of test probe for product performance. It describes the product performance in the ratios used in the cement industry, i.e. Lime Saturation Factor (LSF), Silica Ratio (SR) and Alumina Ratio (AR). Definitions of these are given in Table 1.

The analyser is modelled as a stand-alone object and can be connected to any material fuel stream *composition* object in order to measure the performance.

```
MODEL chemical_analyser
Declarations:
        state      IS_A composition;
        LSF        IS_A factor;
```

```
        SR      IS_A factor;
        AR      IS_A factor;
Rules:
        LSF =   100*state.y['CaO']/(2.8*state.y['SiO2']+1.1*state.y['Al2O3']+0.7*state.y['Fe2O3']);
        SR =    state.y['SiO2']/(state.y['Al2O3']+state.y['Fe2O3']);
        AR =    state.y['Al2O3']/state.y['Fe2O3'];
```

The analyser can also be used to control the ratios of a certain material–fuel stream. In such a case, the ratios' parameters (LSF, SR and AR) can be set and thereafter locked.

5.2.6. Material–fuel mixer

A mixer object transforms two or more inflows of material into one outflow and thus is an *n*-to-1 junction for material–fuel streams. It can be used to mix a number of material–fuel streams in fixed percentages or to have these percentages calculated, depending on settings. The number of inputs (**n_inputs**) must be set before the object is used. The number of fractions (**mix_part[1..n_inputs]**) equals the number of inputs. Independent of the number of inputs, there is only one output (**out**). The list of components (**compounds**) in the inputs and the output are equivalent. For each component, the output flow is the sum of the inputs (**out.f[i] = SUM[in[1..n_inputs].f[i]]**), or

$$f_{out} = \sum_{i=1}^{n\_inputs} f_{in(i)}$$

The mass balance for each individual component must be maintained. (**in[j].quantity = mix_part[j]*out.quantity**). An additional constraint is that the input fractions must sum up to 1.0 (**SUM[mix_part[1..n_inputs]] = 1.0**). The heat contents and economic cost thus must be calculated separately. Here, they are both expressed so that the respective cost and heat for the output equals the sum of the input cost and heat.

```
MODEL materialfuel_mixer
Declarations:
        n_inputs                IS_A integer_constant;
        in[1..n_inputs], out    IS_A materialfuel_stream;
        mix_part[1..n_inputs]   IS_A fraction;
Rules:
        in[1..n_inputs].compounds, out.compounds    ARE_THE_SAME;
        FOR i IN out.compounds CREATE    cmb[i]: out.f[i] = SUM[in[1..n_inputs].f[i]];
        END FOR;
        FOR j IN [1..n_inputs] CREATE    mix[j]: in[j].quantity = mix_part[j]*out.quantity;
        END FOR;
        SUM[mix_part[1..n_inputs]]=1.0;
        out.cost=SUM[in[k].cost | k IN [1..n_inputs]];
        out.heat=SUM[in[k].heat | k IN [1..n_inputs]];
```

5.2.7. Material–fuel grinder

The material–fuel grinder represents grinding raw meal, clinker, etc., and transforms one inflow of coarse material into one outflow of ground material. Grinding consumes electrical energy according to the mass ground. The energy constant (**ED**) is used to calculate total electrical power consumption (**electricity_consumption**). The quantity decreases due to dust generation that is given by a dust-generating constant (DG) defined as a fraction of the out quantity. A total cost adding is modelled as a fixed cost per mass unit (**COST**) to cover maintenance and operation plus the cost of electricity. This total cost is then added to the cost for the material entering the grinder so that the specified material cost always corresponds to the cumulated production cost at the specified location.

The compositions of the input and output material–fuel stream (in and out) are the same. The heat content is not changed during grinding.

```
MODEL materialfuel_grinder
Declarations:
        in, out                   IS_A materialfuel_stream;
        electricity_consumption   IS_A energy_rate;
        dust_generation           IS_A mass_rate;
        cost_adding               IS_A cost_per_mass;
        ED                        IS_A energy_per_mass_constant;
        DG                        IS_A mass_per_mass_constant;
        COST                      IS_A cost_per_mass_constant;
        ELECTRICITY_COST          IS_A cost_per_energy_constant;
Rules:
        in.compounds,             ARE_THE_SAME;
```

out.compounds
in.state.y, ARE_THE_SAME;
out.state.y
dust_generation = out.quantity * DG;
out.quantity = in.quantity -
dust_generation;
electricity_consumption = out.quantity *
ED; (* cost/s *)
cost_adding = COST +
ELECTRICITY_COST * ED; (*
cost/kg *)
out.state.cost = in.state.cost +
cost_adding; (* cost/kg *)
out. state.heat = in.state.heat;

5.2.8. Clinker production

The clinker production transforms one inflow of material and fuel into one outflow of material and one outflow of kiln exhaust gas. The module contains relations and constants for cost adding, electricity-consumption and dust-generation.

Clinker production requires a specified amount of heat per mass unit that must be supplied by the fuel. In this model, a constant value per mass unit clinker entering the clinker production is used. This amount was therefore calculated and set as a requirement on the heat contents in the fuel entering the clinker production.

The clinker production object contains equations that relate input mixture, output clinker and emissions to each other. From a modelling technique point of view, clinker production does not contain any additional concepts beyond what has already been discussed.

5.2.9. Cement plant

When all the objects were defined, they were connected to form a model of the foreground system: the cement manufacturing plant at Slite. To start with, all the necessary objects were instantiated and some of the constants within them were set, such as the number of inputs for all mixers and site specific values. Then they were connected in accordance to the structure of the conceptual model, which resulted in the model in Fig. 3.

5.3. Problem formulations

The model built is neutral in the sense that it does not include any specific problem to be solved. Such a problem formulation, consequently, needs to be done separately. The formulation contains the following:

- A distinction between what to treat as locked variables and what to treat as free variables, depending on the desired solution and the calculation method chosen.
- A connection between input data and the model. Usu-

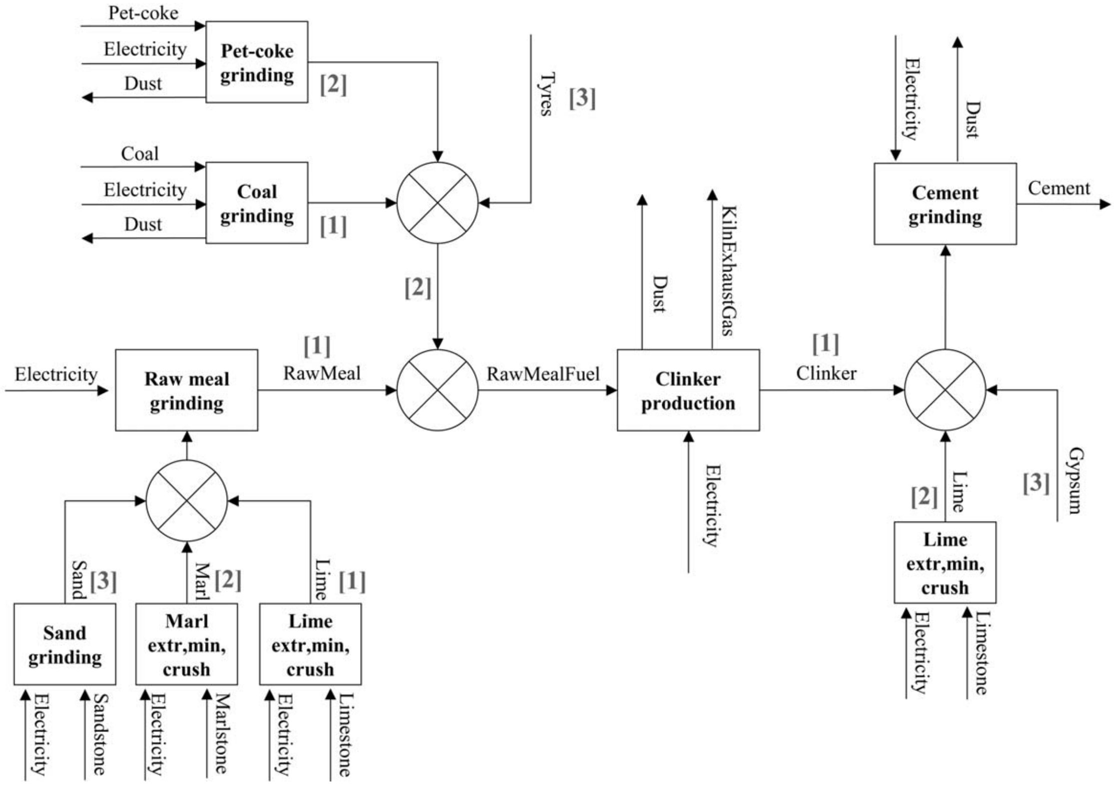

Fig. 3. Foreground system model.

ally locked variables are initiated with suitable input data.
- The calculation method to use, which sorts equations and calculates the result by invoking a mathematical algorithm.

Problem formulations will, in the following, be exemplified for the two specific operational alternatives discussed in Section 3. To be able to find a solution, the number of constraints (equations) needs to equal the number of free variables. The number of equations is a consequence of the model, and thus, the parts of the model and how these are connected. Initially, all variables in the model are free. In the problem formulation, some of them are locked so the desired simulations will be possible to perform.

5.3.1. Case A

The requirements in Section 3, further interpreted in Section 5.1, result in the locked variables, according to Table 6. These variables are set to the values indicated, which represent the input. With this problem formulation, the number of variables will equal the number of equations and the system, thus, becomes possible to solve. The used solver in ASCEND is QRSlv, which is a non-linear algebraic equation solver [23].

5.3.2. Case B

Here, variables are locked according to Table 7 and constants are set to the values indicated. Even here the number of variables will equal the number of equations and the system will thus be possible to solve.

5.4. Model validation and simulation

To use the model, i.e. to predict the environmental load, the product performance and the economic cost, a prerequisite is that the model acts as the system it represents. Before using the model and accepting the information generated, the model has to be validated. It has to be determined whether or not the model gives a good enough description of the system's properties to be used in its intended application. When satisfactory correspondence between the situation, the model and the modelling purpose has been attained, then the use and implementation are appropriate. However, validation of the model will continue throughout the user phase. Once a future operational alternative has been tested and implemented, the simulated information will be compared with the observations of the real system. It is then possible to improve the model. Consequently, the validity and relevance of the model may be continuously improved.

Validation is an intrinsic part of model building and the validity of the model has to be assessed according to different criteria. Technical validation of the foreground system model, i.e. to ensure that the model contains or entails no logical contradictions and that the algorithms are correct, was done as the model was built.

To validate the foreground-system-model, and in

Table 6
Constants and input data for Case A

Variable to lock	Initiated data	Comment
Quantity of cement	1000 kg/s	Product quantity
Fraction gypsum for cement grinding	0.052	
Fraction limestone for cement grinding	0.044	Implies 90.4% clinker for cement grinding
Fraction pet-coke in fuel mix	0.20	Implies 80% coal in fuel mix
Fraction sand in raw meal	0.02	
Fraction marlstone in raw meal	0.71	Implies 27% limestone in raw meal
Heat required by clinker production	3.050 MJ/kg	Related to the inflow of raw meal fuel

Table 7
Constants and input data for Case B

Variable to lock	Initiated data	Comment
Quantity of cement	1000 kg/s	Product quantity
Fraction gypsum for cement grinding	0.045	
Fraction limestone for cement grinding	0.04	Implies 91.5% clinker for cement grinding
Fraction pet-coke in fuel mix	0.23	
Fraction tyres in fuel mix	0.22	Implies 55% coal in fuel mix
Clinker LSF quality factor	97	
Clinker SR quality factor	2.9	Only two out of three quality factors can be set
Heat required by clinker production	3.050 MJ/kg	Related to the inflow of raw meal fuel

addition show examples of model usage and results, we performed simulations on two real operational alternatives. These have actually been used at the plant, and hence there were measurements to validate against. The simulations are those given in Sections 3 and 5.1 and are illustrated in Figs 4 and 5, respectively.

For each of the two operational alternatives, data generated with the model was compared with observations and measurements of the real system. The simulated values were related to the real values. A selection of simulated values as a percentage of measured values is shown in Figs 6 and 7 for the two real operational alternatives, respectively.

The two simulations show that the model can simulate the desired operational alternative and generate the desired information. The simulated and calculated information shows, in comparison with the real system's properties, satisfactory correspondence. We have a valid general model of the Slite plant that can be used to predict product performance, the economic cost and environmental load.

For metals, the model has been technically validated. But due to large variations in metal content in raw material and fuel and insufficient empirical data to describe the emissions of metals we did not achieve total correspondence between simulated and real metal emissions.

6. Discussion and future research

It has been shown that the modelling approach used, i.e. a calculational non-causal model, physical modelling and an object oriented modelling language can greatly enhance modularity, flexibility and comprehensiveness. Together with an appropriate simulation tool, e.g. ASCEND IV, this technique provided a flexible and general-purpose model of a cement manufacturing process for process and product development purposes.

The tool generates the desired information, i.e. predicts the environmental load, product performance and economic cost, by simulating the desired operation alternative. For the two operational alternatives tested, the model generated information which shows satisfactory agreement with the real system's properties. We are of the opinion that since all entities are described independent of each other, they can easily be combined and connected to represent another plant or manufacturing process.

To avoid sub-optimisation, the model was to use a life cycle perspective. The cement manufacturing process from cradle to gate was divided into a foreground system, the "gate to gate" part, and a background system. To complete the model in the life-cycle aspect, the background system model, which is modelled using normal LCI technique [17] and stored in the SPINE [24] format,

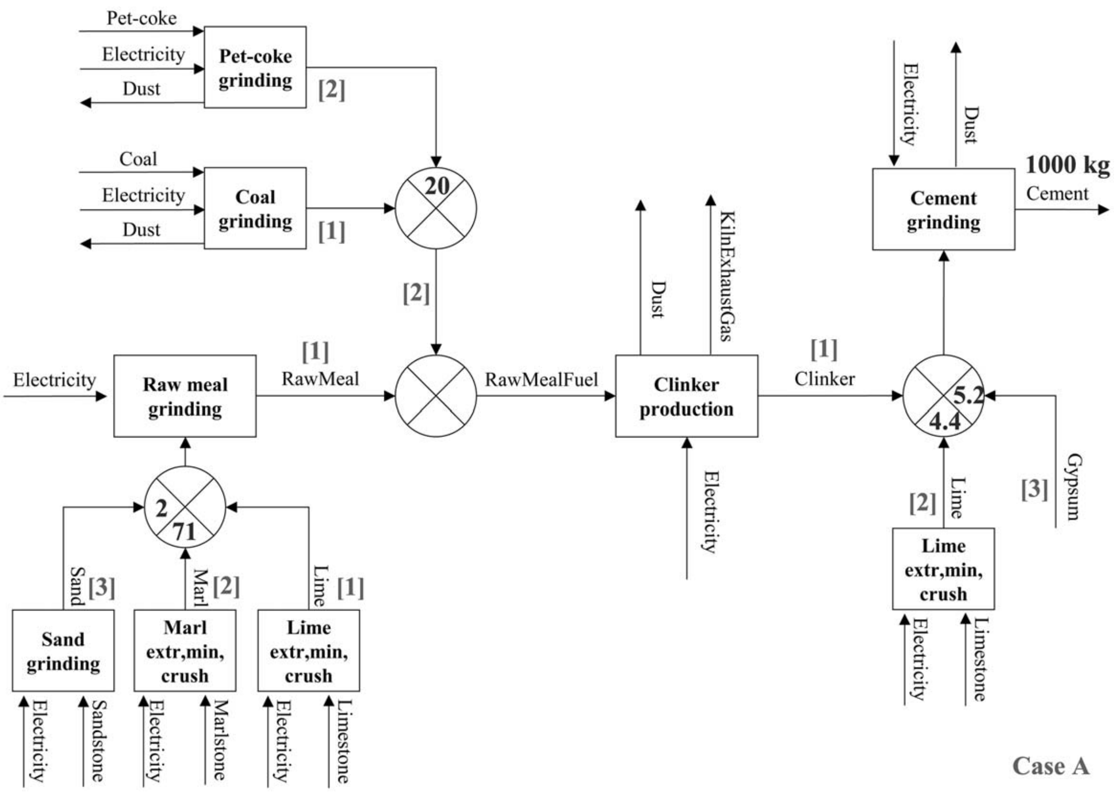

Fig. 4. Real operational alternative A to be simulated.

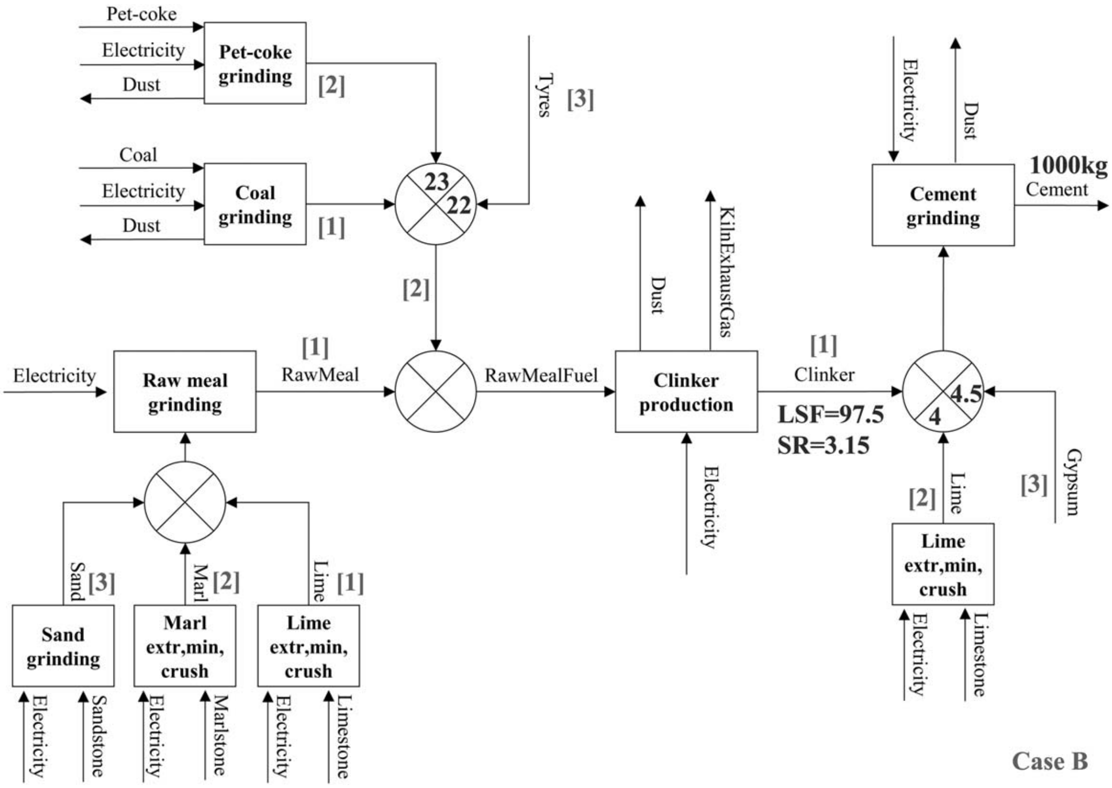

Fig. 5. Real operational alternative B to be simulated.

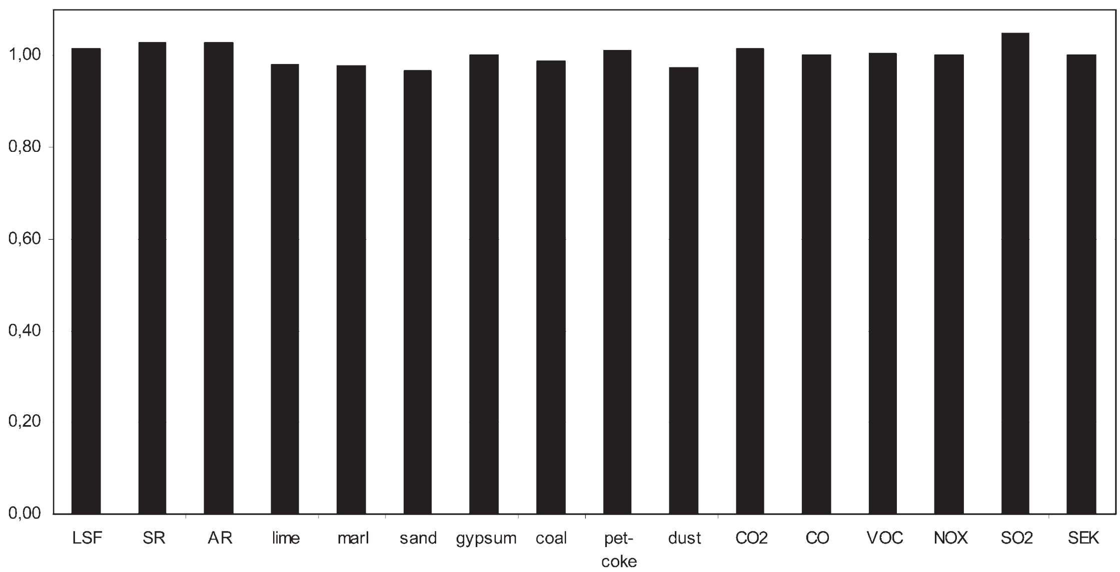

Fig. 6. Simulated values as a percentage of measured values. A selection for operational alternative A.

needs to be connected to the foreground model. Since the background model is both linear and time independent (static) it can be expressed with the techniques and tools discussed in this paper.

As a result of the chosen modelling approach and simulation tool the model, as such, has potential for development. One especially interesting area for future research is to develop the model and the problem formulations so that it will be possible to perform optimisation with the model. The library of re-usable problem formulations and model parts can be developed and extended. Other modelling developments would be adding non-linear and dynamic relations which transform input into output, and increase the level of detail in the model, where applicable.

Naturally, the validation process of the cement model

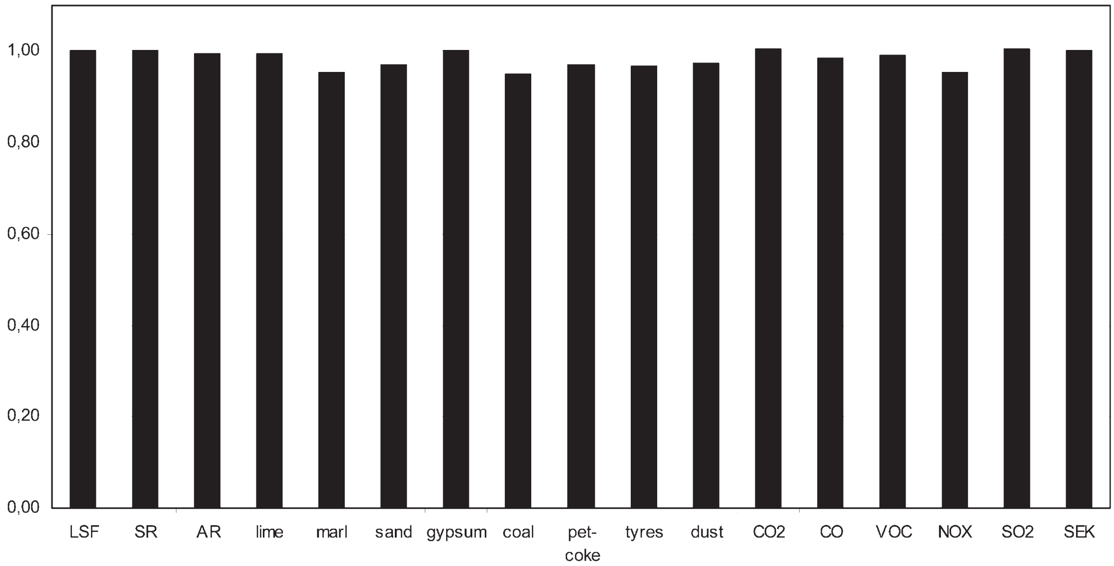

Fig. 7. Simulated values as a percentage of measured values. A selection for operational alternative B.

will continue to increase the validity and extend the interval for which the model is valid. The next step thus will be to use and implement site specific models, including the emission of metals, in the cement industry.

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Paper II

On optimal investment strategies for a hydrogen refueling station

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On optimal investment strategies for a hydrogen refueling station

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Abstract

The uncertainty and cost of changing from a fossil-fuel based society to a hydrogen based society are considered to be extensive obstacles to the introduction of Fuel Cell Vehicles (FCVs). The absence of existing profitable refueling stations has been shown to be one of the major barriers. This paper investigates methods for calculating an optimal transition from a gasoline refueling station to future methane and hydrogen combined use with an on site small-scale reformer for methane. In particular, we look into the problem of matching the hydrogen capacity of a single refueling station to an increasing demand. Based on an assumed future development scenario, optimal investment strategies are calculated. First a constant utilization of the hydrogen reformer is assumed in order to find the minimum hydrogen production cost. Second, when considerations such as periodic maintenance are taken into account, optimal control is used to concurrently find both a short term equipment variable utilization for one week and a long term strategy. The result is a minimum hydrogen production cost of $4-6/kg, depending on the number of re-investments during a 20 year period. The solution is shown to yield minimum hydrogen production cost for the individual refueling station, but the solution is sensitive to variations in the scenario parameters.

Keywords: Hydrogen; Infrastructure; Investment; Optimization; Refueling station

1 Notations

Table 1 shows the symbolic conventions used in this paper. The letters c, f etc. are variables and constants, which may be further specified using sub and superscripts. The symbol $c_{hr,w}$ indicates, for example, the weekly capacity of the hydrogen reformer. Additional scenario parameters starting with a capital letter are discussed in section 3.2 below. The currency used is USD ($).

Table 1: Symbolic conventions.

Type	Name	Description	Unit
Variables, constants	c	Capacity	kg, kg/time unit
	f	Factor	-
	l	Lifetime	yr
	p	Cost, price	$
	r	Profit	$/time unit
	s	Size	kg, kg/time unit
	u	Consumption	kg/time unit
	t	Time	yr
	x	Flow	kg/time unit
	η	Efficiency	-
Subscripts	a	Annuity	
	d	Daily, per day	
	e	Electricity	
	eq	Equipment, any/all part(s)	
	f	Filling, refueling	
	fc	Hydrogen fuel cell	
	fp	Hydrogen refueling pump	
	g	Methane	
	h	Hydrogen	
	hc	Hydrogen compressor	
	he	Hydrogen electrolysis	
	hf	Hydrogen refueling	
	hr	Hydrogen reformer	
	hs	Hydrogen storage	
	i	Investment	
	k	Peak demand to average	
	m	Maintenance	
	n	Nominal	
	p	Progress ratio	
	s	Scale, scaling	
	t	Technology development	
	w	Weekly, per week	
	x	Inflexion point	
Superscripts	i	Input flow	
	o	Output flow	

2 Introduction

Hydrogen is considered a promising future fuel for vehicles [1, 2, 3]. Three main arguments are used to support this assertion: the potential of reducing greenhouse gases from the transport sector; greater energy supply security, i.e. hydrogen can be produced from many energy sources and hence the risk of shortage of supply may be reduced; the potential of zero local emissions with the use of fuel cells.

The absence of a hydrogen infrastructure is seen as a major obstacle to the introduction of hydrogen fuel cell vehicles. A full-scale hydrogen infrastructure with production facilities, a distribution network and refueling stations is costly to build. The venture of constructing a hydrogen refueling infrastructure constitutes a long-term, capital-intensive investment with great market uncertainties for fuel cell vehicles. Therefore, reducing the financial risk is a major objective of any long-term goal to build a hydrogen infrastructure [4].

Ogden [5] has described several hydrogen supply options. Investigations have also been made for large scale production of hydrogen [6]. A number of studies of cost and technology for a hydrogen infrastructure have also been carried out [7, 8, 9]. However, to the knowledge of the authors, no studies aimed at finding the most profitable investment strategy for the individual refueling station have been done.

There are several reasons to focus on the individual hydrogen refueling station. Car owners are used to accessing a network of stations. For the ordinary car owner to accept a hydrogen-refueling infrastructure, accessibility of service stations will be crucial [10]. Therefore, a network of hydrogen stations will need to be built in order to reach the target of about 15-20% of the total number of refueling stations having a hydrogen fuelling option for consumers. In the EU, the estimated need is 15-20,000 refueling stations by 2020 (a maximum of 100,000 stations are predicted by 2020 for EU15[1]) [11]. At present there are only about 110-120 hydrogen stations around the world, some of which are quite small [12]. Several researchers have proposed that small-scale reforming of methane could be a feasible transition strategy for the introduction of hydrogen fuel [13, 14].

This study aims at finding the most economic investment strategy, i.e. the lowest cost for the hydrogen produced, for an individual hydrogen refueling station featuring on site small-scale reforming of methane. The question is to what extent and when to build the parts of the station, satisfying an increasing demand of hydrogen. The method developed may be used to find optimal investment strategies in other cases in which the number of dynamic states is reasonably low. Our calculations begin in 2010 and cover 20 years, until 2030.

3 The refueling station

Methane is chosen as the main energy carrier for the refueling station since:

1. Methane can be produced from fossil fuel, which is, and will probably continue to be, one of the cheapest production sources for hydrogen in the short term.

2. Methane can be produced from renewable resources, e.g. from different types of wood and plants.

3. Methane is relatively easy to transport and can be re-formed into hydrogen gas.

4. It is possible that running vehicles directly on methane might be a favourable alternative as an intermediate step toward hydrogen usage.

After reforming, the produced hydrogen gas can be compressed and stored, or used directly in fuel cells on site for either local consumption or distribution on the electricity grid when electricity prices are high. On the other hand, when electricity prices are low it might be more profitable to produce hydrogen by electrolysis using grid electricity. Taking this into consideration, a large number of station configurations are possible, including the one indicated in figure 1. The model developed does, however, only consider the core components, i.e. reformer, compressor and hydrogen storage. The model is flexible with respect to refueling station types, e.g. car, truck or bus, and refueling station locations, e.g. central, suburb or countryside.

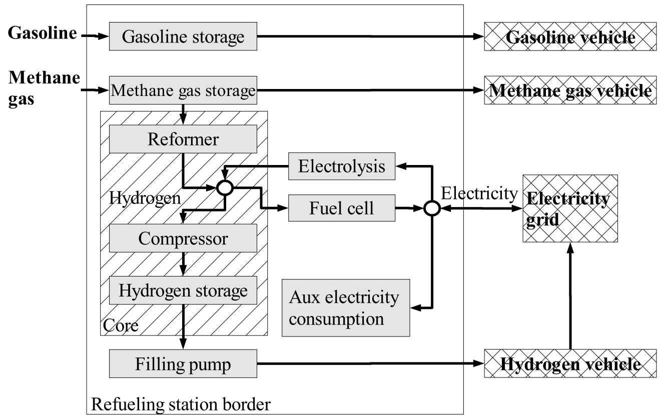

Figure 1: Possible refueling station configurations. Methane is reformed to hydrogen at the site and stored for delivery to vehicles. It is also possible to produce hydrogen from electricity by electrolysis or electricity from hydrogen using a fuel cell.

3.1 The parts of the refueling station

The parts of the refueling station, see figure 1, are considered to have the characteristics given in table 2. This table gives data on actual produced equipment in the year 2000. In this paper we have used figures from the Simbeck [15] study. Another comparable study is the GM Well-to-Wheel Analysis of Energy Use and Greenhouse Gas Emissions of Advanced Fuel/Vehicle Systems - A European Study (GM WtW) [16].

The purchase price is calculated using the scale function

$$p = p_n \, c_n^{1-f_s} s^{f_s}, \tag{1}$$

where f_s is a scale factor, further discussed in section 3.2. Using this function an existing piece of equipment with capacity c_n and purchase price p_n is scaled to any size (s) to obtain an estimated purchase price. The function (1) applies to all parts of the refueling station except the filling pump, which is not scalable but purchased on a piece-wise basis. Regardless of size, all equipment is considered to have a certain expected lifetime, l. Using the expected lifetime, the weekly annuity is calculated as

$$f_{a,w} = \frac{D}{52(1 - \frac{1}{(1+D/52)^{52\,l}})}, \tag{2}$$

where D is the real rate of interest. The total weekly equipment cost, including maintenance (f_m), is then

$$p_w = f_{a,w} \, p(1 + f_m). \tag{3}$$

In reality each part of the refueling station is chosen from a finite number of available brands and sizes. By using scaling

[1] The present 15 EU member states

Table 2: Refueling station parts data. Figures are from Simbeck [15] except lifetimes and progress ratio, which are assumed.

Part	Reformer	Compressor	H_2 store	Fill pump	Electrolysis	Fuel cell
Lifetime(l)	15 yr	15 yr	15 yr	20 yr	30 yr	11.4 yr
Nom. capacity(c_n)	42 kg/h	42 kg/h	263 kg	48 kg/h	42 kg/h	-
Nom. purchase cost(p_n)	38,774 $ h/kg	7,792 $ h/kg	592 $/kg	83,117 $/pc	25,665 $ h/kg	12,987 $/kW
Scale factor(f_s)	0.75	0.80	0.80	-	0.72	-
Maintenance cost(f_m)	0.05	0.06	0.05	0.05	0.02	0.1
Efficiency(η)	0.286 kg H_2/kg NG	0.99	0.99	0.99	0.02 kg H_2/kWh	18.33 kWh/kg H_2
Electricity use(f_e)	0.02	2.492	0	0	-	-
Progress ratio(f_p)	0.8	0.9	0.9	0.9	0.9	0.9

functions (1) for the purchase price, the set of available parts can be replaced with one continuous variable. Compared to evaluating a number of discrete alternatives, this represents a significant saving in computational complexity.

The efficiency in table 2 indicates the relation between the mass entering and leaving the equipment. In the case of the reformer, the substance entering is methane and that leaving is hydrogen.

3.2 Scenario parameters

The scenario parameters reflect assumed developments in the future and are given in table 3 together with their respective values.

Table 3: Scenario parameters. The electricity price is assumed to be higher during daytime (6 am-10 pm) than at night (10 pm-6 am).

Name	Description	Value	Unit
B	S-curve slope	0.3	-
D	Real rate of interest	0.05	1/yr
F_{cont}	Contingency cost factor	0.1	-
F_{eng}	Engineering permitting cost factor	0.1	-
F_f	Refueling characteristics factor		-
$F_{f,k}$	Refueling ratio peak-demand to average	1.12	-
F_{gen}	Include land cost factor	0.2	-
P_1	Cost of manufacturing 1^{th} unit	-	$
P_e	Electricity price vector (6am-10pm)	7.8	c/kWh
	Electricity price vector (10pm-6am)	3.9	c/kWh
P_g	Methane gas price[17]	47	c/kg
P_n	Cost of manufacturing n^{th} unit	-	$
$R(t)$	Relative number of hydrogen vehicles at time t	-	-
T_x	Inflection point of the S-curve	10	yr
$U_{h,d}$	Mean hydrogen consumption	1000	kg/day
V_n	Cumulative production at n^{th} unit	-	-
$V(t)$	Number of vehicles at time t	-	-
V_{tot}	Total nr of vehicles at t_{end}	-	-

The number of hydrogen vehicles refueling at the station is a crucial variable for optimization. It is probably also the most difficult parameter to predict. In this study the S-curve

$$V(t) = \frac{V_{tot}}{1 + \mathrm{e}^{-B(t-T_x)}} \tag{4}$$

is used. V_{tot} is the total number of vehicles using the refueling station, T_x the S-curve inflection point, and B the slope. The relative number of hydrogen vehicles at the station is thus

$$R(t) = \frac{1}{1 + \mathrm{e}^{-B(t-T_x)}}. \tag{5}$$

The function $R(t)$ is purely exogenous and therefore uncertain. This uncertainty will influence the results, as is discussed in section 6.

Figure 2 shows the refueling characteristics during 24 hours of operation for a typical gasoline station ($F_{f,d}$). Together with the daily mean hydrogen consumption ($U_{h,d}$) and ratio peak-demand to average ($F_{f,k}$), an absolute demanded refueling capacity is calculated. This sequence is the hydrogen demand when 100% of the vehicles use hydrogen. To adjust the demand to intermediate situations the sequence is scaled using the S-curve (5), which results in the daily maximum hydrogen demand curve

$$x_{h,f,d}(t) = R(t)\, F_{f,d}\, U_{h,d}\, F_{f,k}. \tag{6}$$

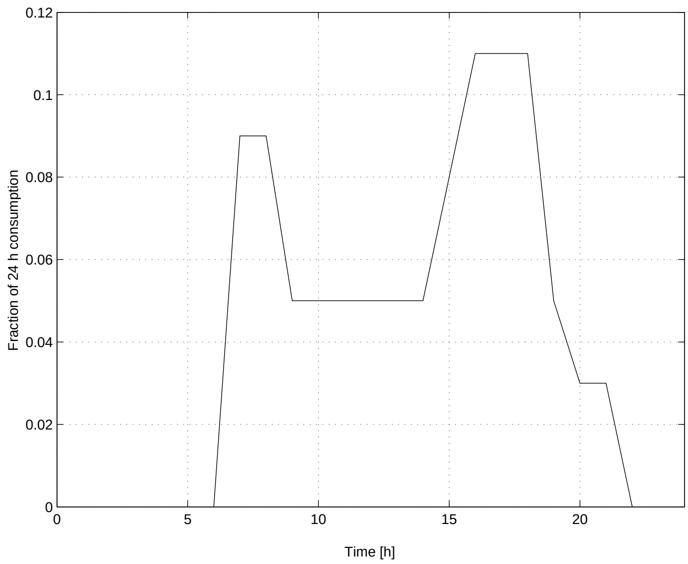

Figure 2: Refueling curve for 24 hours ($F_{f,d}$). This curve gives the distribution of hydrogen demand in fractions of the total consumption for one day. The figures are based on statistics for a typical gasoline refueling station. [15]

The demand also differs between weekdays according to table 4, which creates a periodic sequence of one week for the total hydrogen demand ($x_{h,f,w}$). Both the 24 hour refueling curve and the variations between weekdays are based on statistics for a typical gasoline refueling station. We assume that this behavior is independent of fuel type and therefore will persist when hydrogen is used in place of gasoline.

It is assumed that equipment becomes cheaper with increasing production and technology development, which is adjusted in the

Table 4: Distribution of hydrogen demand in fractions of the total consumption for one week ($F_{f,w}$). The figures are based on statistics for a typical gasoline refueling station. [15]

Day	Mon	Tue	Wed	Thu	Fri	Sat	Sun
Fraction	0.14	0.14	0.14	0.15	0.16	0.14	0.13

cost to manufacture the n^{th} unit P_n according to

$$P_n = P_1 \, V_n^{(\log f_p / \log 2)}, \tag{7}$$

where P_1 is the cost of manufacturing the first unit, V_n the cumulative production at n^{th} unit and f_p the progress ratio factor. It is assumed that the number of hydrogen refueling stations (cumulative production) will be 5,000 in 2010 and 50,000 in 2030, and will follow the S-curve (4). We have assumed an increase in the number of refueling stations using steam reforming from 5,000 to 50,000 in the world from the year 2010 to 2030. These numbers are based on the predictions about when the fuel cell vehicle market will open up and on the number of station needed. A report presented by E4tech [18] and funded by the UK Department of Trade and Industry and the Carbon Trust predicts that ”if the hurdles are overcome, the mainstream propulsion market is expected to open up after 2010”. Melaina [19] made a preliminary analysis of the sufficient number of initial hydrogen stations in the US, and concluded that between 4,500 and 17,700 hydrogen stations would be required in the US to initiate a hydrogen infrastructure for fuel cell vehicles. We justify our estimate of 50,000 hydrogen stations by the fact that we consider the whole world and in a later stage than do Melaina.

The total decrease in relation to the present-day purchase price owing to increased production and technology development is thus

$$\begin{aligned} f_{eq,t}(t) &= \frac{(50000R(t))^{(\log f_p / \log 2)}}{5000^{(\log f_p / \log 2)}} \\ &= (10R(t))^{(\log(f_p)/\log(2))}, \end{aligned} \tag{8}$$

where t is the time from year 2010. Within any real mass production-based learning process, there will be a trade-off between system standardization and modularity of system capacity. However, in this model we have used a simplification, as indicated in equation 8.

With respect to interest rates, future costs can be calculated from present day values using the Present Day Value Correction

$$pdc(t) = \frac{1}{(1+D)^t}. \tag{9}$$

3.3 Initial considerations

We assume that, from the outset, no economic costs, i.e. wages and rent for land, from the gasoline part of the refueling station are shared with the hydrogen part and vice versa. Hence, it does not matter if the gasoline refueling station is present or not when the hydrogen station is being built. In reality some resources can probably be shared between the gasoline and hydrogen parts of the refueling station.

The hydrogen part of the refueling station, see figure 1, can be divided into a number of units that can be optimized separately.

The question of whether or not the local fuel cell and electrolysis parts are profitable depends on the price of electricity and methane. If the total cost including maintenance (see (3)) is lower than the difference between produced and bought electricity and hydrogen respectively, it is profitable to invest in the respective equipment. For the fuel cell the profit is then

$$r_{fc} = p_e \, s_{fc} - \frac{p_g \, s_{fc}}{\eta_{hr} \, \eta_{fc}} - \frac{p_{fc,w} + \Delta p_{hr,w}}{168}, \tag{10}$$

i.e. almost linearly dependent on the investment, with no upper boundary. The same reasoning applies to the electrolysis. An intermediate situation may appear when the purchase price of electricity is high, whereas the selling price is low. It might then only be profitable to produce electricity for the consumption of the refueling station.

The methane storage facility is sized in accordance with how frequently the methane gas tank is filled at the refueling station. Since the estimated methane consumption is known, the periodic delivery can be calculated. A large volume of methane delivered at the same time would cost less per kg, but requires a larger storage tank. This is a separate problem that can be solved using optimization techniques. For the remainder of this study we therefore assume a constant delivery of methane from a pipeline or similar construction.

The refueling pump can be dimensioned according to the maximum amount refueled. The daily mean hydrogen consumption $U_{h,d}$ is distributed throughout the day corresponding to the refueling curve (figure 2). A maximum rate of 0.11 is reached between 3 pm and 5 pm. The busiest day of the week is Friday, reaching 0.16 of the weekly consumption. The ratio peak-demand to average ($F_{f,k}$), which is estimated to 1.12, should also be considered. All in all the number of refueling pumps required is

$$c_{fp}(t) = \text{ceil}(2.87R(t)), \tag{11}$$

where the function ceil rounds to the nearest integer greater than or equal to the operand.

The remaining parts of the refueling station are the ones within the shaded area in figure 1 and are collectively called ”the core”. This core consists of reformer, compressor and storage tank. Considering only the core, hydrogen is delivered to vehicles only. This means that all the hydrogen produced by the reformer will go through the compressor to the storage tank. The size of the reformer and compressor will thus have to be the same.

Owing to a non-linear price decrease in the equipment over time (7), the core problem cannot be further split into size distribution between reformer and tank, plus time and extent of investments. The relative cost between reformer/compressor and storage tank will change over time.

3.4 Core model

The model describing the core, see figure 1, is quite simple and includes only one state, the hydrogen storage. It can be described by

$$\begin{aligned}
\dot{x}_{hs} &= x_{hs}^i - x_{hs}^o \\
x_{hs}^i &= x_{hr}^i \eta_{hr}\eta_{hc} \\
x_{hs}^o \eta_{fp} &= x_{hf} \\
x_{hf} &= H f_w \\
x_{hr}^i &= x_{ng}
\end{aligned} \tag{12}$$

subject to the constraints

$$\begin{aligned}
0 &\leq x_{hr}^o \leq c_{hr} \\
0 &\leq x_{hc}^i \leq c_{hc} \\
0 &\leq x_{hs} \leq c_{hs} \\
0 &\leq x_{fp}^i \leq c_{fp}.
\end{aligned} \tag{13}$$

The rest of this paper addresses the problem of choosing the size of reformer/compressor versus storage volume over one or many investments over time for the core of the refueling station. The model developed will be used in the optimization in the subsequent section.

4 The optimization problem

Optimal control can be used to optimize a system over a certain time interval. Given a dynamic model of the system, an objective function, and constraints, a path from one state to another can be calculated where the objective function is at a minimum. Solving non-dynamic design problems using optimization techniques is common practice, see e.g. [20] or [21]. In the case where the model is static, i.e. does not change over time, such techniques are sufficient.

In this study, however, we are interested in investment planning and internal properties that change over time, such as utilization curves and transients for hydrogen generation. Therefore a dynamic optimization technique is used, see e.g. [22].

4.1 The objective function

The criterion function to be minimized is based on the total production cost for hydrogen, which consists of costs for equipment, methane and electricity. In addition the number of investments has to be taken into account.

The total weekly equipment cost is the sum of the cost for each part of the refueling station (p_w, see (3)), i.e

$$p_{eq,w}(s_{eq}, t_i) = \sum_{\forall\, eq} p_w(s_{eq})\; f_{eq,t}(t_i). \tag{14}$$

The loans are of the annuity type, which make the equipment cost independent of time.

Since consumption is given by the refueling demand ($x_{h,f,w}$), production during the given time frame can be calculated. The total weekly methane gas cost is then

$$p_{g,w}(t_w) = \sum_{t=1}^{168}(x_{g,w})\; P_g\; R(t_w) = \frac{\sum_{t=1}^{168}(x_{h,f,w}) P_g\; R(t_w)}{\eta_{fp}\; \eta_{hs}\; \eta_{hc}\; \eta_{hr}}, \tag{15}$$

where t_w indicates the time (in years) when the weekly cost is calculated.

For electricity the price varies throughout the day and needs to be evaluated on an hourly basis. The weekly cost is then scaled using the S-curve (5). The total weekly electricity cost is thus

$$p_{e,w}(t_w) = x_e P_e^T R(t_w) = \sum_{t=1}^{168}(x_{h,f,w}) \tag{16}$$

$$(f_{fp,e} + \frac{f_{hs,e}}{\eta_{fp}} + \frac{f_{hc,e}}{\eta_{fp}\eta_{hs}} + \frac{f_{hr,e}}{\eta_{fp}\eta_{hs}\eta_{hc}} p_{el}^T R(t_w).$$

Note that both the methane and electricity costs are independent of the size of the equipment.

In this study the production cost for hydrogen is averaged over the whole investment period as

$$\overline{p_h} = \frac{1}{N} \sum_{t_w=1}^{N} \frac{\sum_{\forall\, s_{eq},t_i} p_{eq,w} + p_{g,w}(t_w) + p_{e,w}(t_w)}{\sum_{t=1}^{168}(x_{h,f,w})\; R(t_w)}, \tag{17}$$

where N is the number of weeks for the investment period. This production cost takes into account the timing of the investments, making the purchase cost of all parts of the refueling station decrease over time (8). It does not, however, correct future costs to present-day values (9). It is possible to calculate the hydrogen cost in other ways. One way is to use the formula above and add the Present Day Value Correction (9), which gives

$$\overline{p_h} = \frac{1}{N} \sum_{t_w=1}^{N} \frac{pdc(t_w) \sum_{\forall\, s_{eq},t_i}(p_{eq,w}) + p_{ng,w} + p_{el,w}}{\sum_{t=1}^{168}(x_{h,f,w}) R(t_w)}. \tag{18}$$

Another totally different approach is to distribute the total cost evenly over the whole investment period, i.e

$$\overline{p_h} = \sum_{t_w=1}^{N} \frac{\sum_{\forall\, s_{eq},t_i}(\sum_{\forall\, eq}(p_{eq}(1+f_m)pdc(t_w)))f_{a,w}}{\sum_{t=1}^{168}(x_{h,f,w}) R(t_w)}. \tag{19}$$

In this study the average production cost of hydrogen (17) is used to find the objective function. Expanding the function, it is clear that not all the terms are necessary to generate the shape of the production cost. The terms $p_{g,w}$ and $p_{e,w}$ can be summed up separately and are independent of size of equipment (s_{eq}) and time for investment (t_i), giving a constant contribution. In addition the sum over $x_{h,f,w}$ and N are constants. Omitting these constant terms yields the objective function

$$p_{obj}(t_i) \;=\; \sum_{t_w=1}^{N} \frac{\sum_{\forall\, s_{eq},t_i}(p_{eq,w})}{R(t_w)}. \tag{20}$$

Expanding the objective function, it can be written as

$$\begin{aligned}
p_{obj} \;\sim\; & \sum_{t_w=1}^{N}(1 + \mathrm{e}^{-B(t_w - t_x)}) \\
& \sum_{\forall\, s_{eq},t_i}((1 + \mathrm{e}^{-B(t_i - t_x)})^{C_1} \sum_{\forall\, eq} s_{eq}^{f_s}),
\end{aligned} \tag{21}$$

where C_1 is a constant. Since this is a sum over exponentials of convex functions, the objective function is also convex [23].

In the case when the objective function (20) does not provide enough information to find an unambiguous optimal point, it can be augmented , e.g. by variations in utilization of equipment.

This would result in a smoother utilization curve. Adding e.g. the quadratic variations in the hydrogen reformer output would then give

$$p_{obj2} = p_{obj} + \alpha \sum_{k=1}^{M-1} (x^o_{hr}(k) - x^o_{hr}(k+1))^2, \qquad (22)$$

where α is a weight factor and M the number of hours to consider.

4.2 The constraints

The constraints for the optimization problem are developed from (12) and (13). By integrating the first equation of (12), which controls the storage of hydrogen at the refueling station, the first constraint is found. Since consumption statistics for refueling are given on an hourly basis for one week, it is possible to use a time-discrete formulation where integration is replaced by summation. The model (12) becomes

$$\begin{aligned} x_{hs} &= \sum_{t_0}^{t_f} (x^i_{hs} - x^o_{hs}) \\ x^i_{hs} &= x_{ng}\eta_{hr} \\ x^o_{hs}\eta_{fp} &= x_{h,f,w}. \end{aligned} \qquad (23)$$

By assuming a periodicity of one week for all variables included, it is only necessary to take $7 * 24 = 168$ points (hours) into account.

The method of transcription used in the time continuous case to eliminate time [22] can be replaced in this discrete problem by cumulative summation. This results in the following constraints:

$$\begin{aligned} \sum_{t_0}^{t} (x^i_{hs} - x^o_{hs}) &\geq 0, \; t_0 \leq t \leq t_f \\ c_{eq} &\geq x_{eq}. \end{aligned} \qquad (24)$$

The first equation ensures that the stored amount of hydrogen does not become negative, while the second ensures that the flow through each piece of equipment does not exceed the capacity.

A way of extinguishing transients of the state variables is to require that the initial value equals the end value, i.e

$$x_{hs}(t_0) = x_{hs}(t_f). \qquad (25)$$

One inconvenience is that in order to precisely follow the calculated path, the storage containers have to be initially filled to a certain extent. In reality this is not very important since the initial transients decay rapidly.

Other requirements, e.g. periodical maintenance stops of reformer or required initial amount of hydrogen stored may also be taken into consideration by adding one or more constraints.

The optimizations in cases 1 and 2 are carried out for a one week operation for each investment. For intermediate investments, the demand is estimated using the S-curve ($R(t)$), and equipment is assumed to have decreased in price according to (7) with scenario parameters as in table 3. Note that the price decrease is faster for the reformer than for the rest of the equipment.

5 Results

This section presents the results from the optimization in the two cases discussed. Both cases are solved using Tomlab [24]. No gradients or Hessians are provided, instead estimates are made using numerical differentiation within the optimization method.

5.1 Case 1: constant utilization

In case 1, constant utilization of reformer and compressor is considered. The capacity of the reformer/compressor (c_{hr}) is determined from the weekly average demand and the hydrogen storage capacity by finding the minimum of the sum of net input to the hydrogen storage tank, see (26).

$$\begin{aligned} c_{hr} &= \frac{\sum_{t=1}^{168}(x_{h,f,w})}{168\eta_{hc}\eta_{hs}\eta_{fp}} \\ x_{hs}(t_0) &= -\min_t \sum_{t_0}^{t} (c_{hr}\eta_{hc} - x_{h,f,w}/(\eta_{fp}\eta_{hs})) \\ c_{hs} &= \max_t \sum_{t_0}^{t} (c_{hr}\eta_{hc} - x_{h,f,w}/(\eta_{fp}\eta_{hs})) + x_{hs}(t_0) \end{aligned} \qquad (26)$$

The result is an unconstrained optimization problem that can be described by

$$\min_{t_i} \quad p_{obj}(t_i). \qquad (27)$$

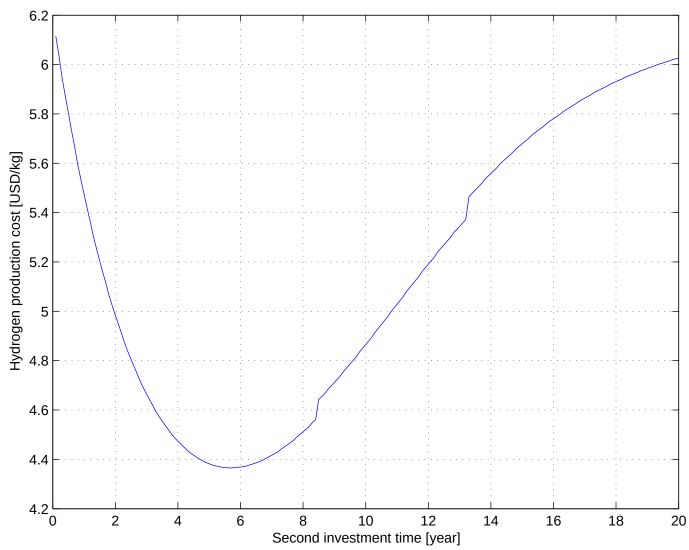

Figure 3: Case 1, 2 investments, hydrogen production cost as a function of second investment time. Note the discontinuities at times 8.5 and 13.2. These are caused by an increase in the number of refueling pumps (11).

If only one investment is made, the characteristics are calculated directly using (26) and no optimization is carried out. In the case of 2 or more investments, the curves in figures 3 and 4 illustrate the effect of investment time.

The problem in case 1 is solved using a quasi-Newton method implemented in the Tomlab function ucSolve. The results for 1-3 investments are as shown in table 6, figures 5 and 6.

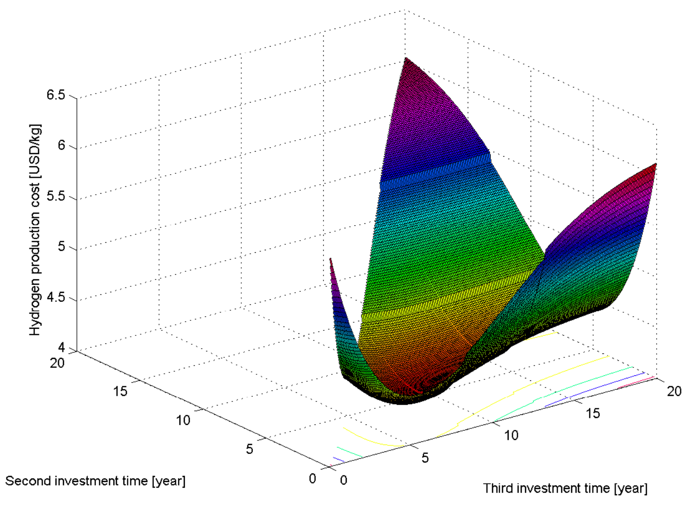

Figure 4: Case 1, 3 investments, hydrogen production cost as a function of second and third investment time.

Table 5: Result of optimization, case 1. The total cost is the cost for equipment, methane and electricity for the entire investment period. The mean distance cost is calculated from the use of 0.1kg H_2/10km for fuel cell vehicles.

No of investments	1	2	3
Investment time [yr]	0	0, 5.7	0, 3.9, 8.4
Cost equipment [$]	3,868,763	2,961,677	2,793,208
Total cost [$]	16,296,295	15,026,375	14,791,149
Mean cost hydrogen[$/kg]	6.03	4.37	4.14
Mean distance cost[$/10km]	0.60	0.44	0.41
Reformer size [kg/h]	45.47	9.2+36.3	5.8+10.9+28.7
Storage size [kg]	606	123+484	77+146+383
Initial storage [kg]	271	55,271	35,100,271
Refueling pump no [pcs]	3	1+2	1+0+2

The mean distance cost is based on a consumption of 0.1kg H_2/10km for a fuel cell vehicles. This is an estimate of the hydrogen consumption for a small fuel cell vehicle and is only used for comparison with petrol fueled cars.

Further investments have very little effect on the mean hydrogen production cost, as can be seen in figure 7.

5.2 Case 2: variable utilization

In Case 2 utilization of equipment is parametrized and determined by the optimization algorithm. The chosen special conditions in this study are 100 kg hydrogen storage initially and at the end of each week (periodic boundary conditions), and a weekly stop for maintenance from hours 75 to 87 during the week. Investments are done on 1 and 2 occasions during the investment period. Further investments have not been investigated for case 2, owing to the computational complexity and time involved. The

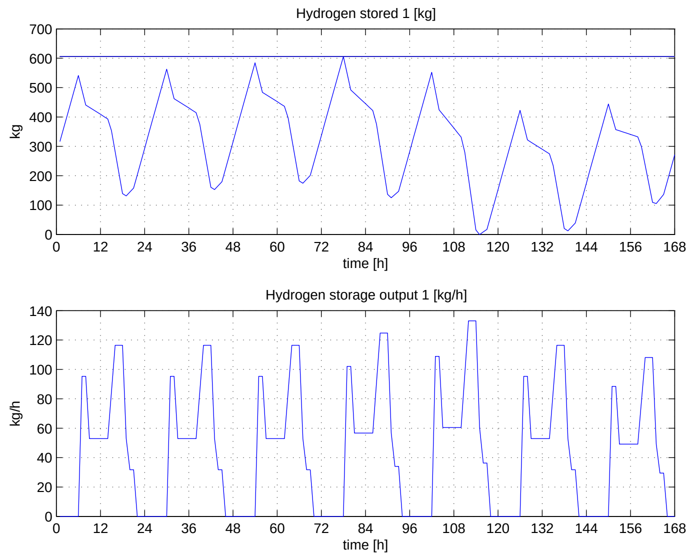

Figure 5: Case 1, 1 investment, stored hydrogen and storage output.

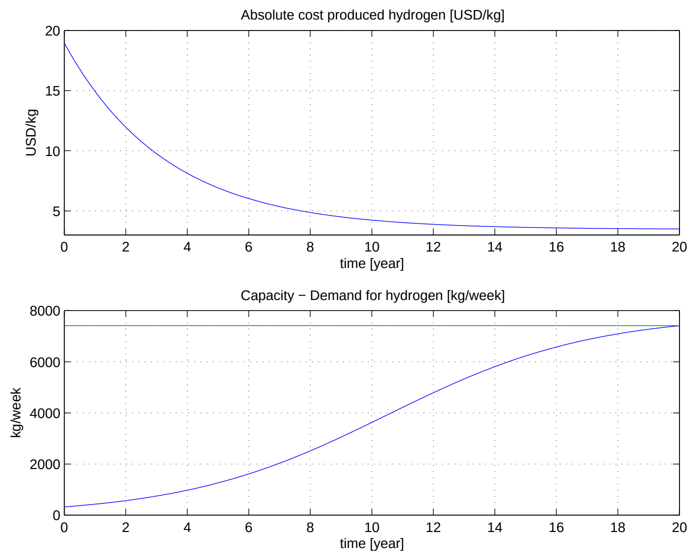

Figure 6: Case 1, 1 investment, hydrogen production cost and capacity-demand.

resulting constrained non-linear optimization problem

$$\begin{aligned}
&\min_{t_i, s_{hr}} \quad p_{obj2} \\
\text{s.t.} \quad \sum_{t_0}^{t}(x^i_{hs} - x^o_{hs}) &\geq 0, \; t_0 \leq t \leq t_f \\
c_{eq} &\geq x_{eq} \\
x_{hs}(t_0) &= x_{hs}(t_f) \\
x_{hs}(t_0) &= 100 \\
\sum_{t=75}^{87} x^o_{hr} &= 0, \qquad (28)
\end{aligned}$$

was solved using a Sequential Quadric Programming (SPQ) method [25], as part of the NPSOL [26] package running in Tomlab [24].

The results from the optimization give the size of equipment

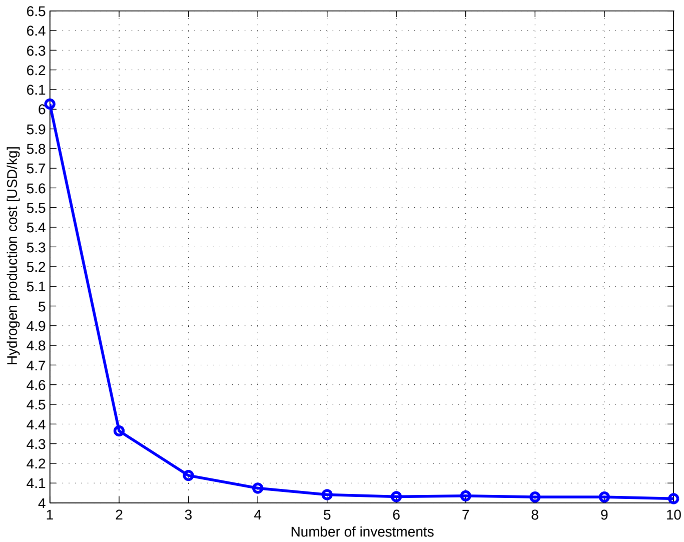

Figure 7: Case 1, hydrogen production cost for 1-10 investments.

(table 6), running pattern of the facility (figure 8) and produced hydrogen price and utilization curves (figure 9). The solution shows good utilization of storage; the stored hydrogen amount frequently drops to near zero.

Table 6: Result of optimization, case 2. The total cost is the cost for equipment, methane and electricity for the entire investment period. The mean distance cost is calculated from the use of 0.1kg H_2/10km for fuel cell vehicles.

No of investments	1	2
Investment time [yr]	0	0, 5.6
Cost equipment [$]	4,707,805	3,724,066
Total cost [$]	17,522,971	16,151,907
Mean cost hydrogen [$/kg]	6.74	4.72
Mean distance cost [$/10km]	0.67	0.47
Reformer size [kg/h]	57	10.0, 50.0
Storage size [kg]	939	199, 873
Initial storage [kg]	63	90, 64
Refuelling pump no [pcs]	3	1 + 2

5.3 Sensitivity of the solution

To evaluate the sensitivity of the solution in case 1 (with 2 investments) to changes in the scenario parameters, calculations were made with slightly changed values from the settings in table 3. Table 7 shows the results in relative sensitivities, i.e.

$$sens_y = \frac{\min_i(z + \delta z)}{\min_i(z)}, \tag{29}$$

where $sens_y$ is the relative sensitivity value with respect to property z. The optimization procedure is abbreviated $\min_i$.

Owing to the similarities in the objective function, the sensitivities also are valid for case 2.

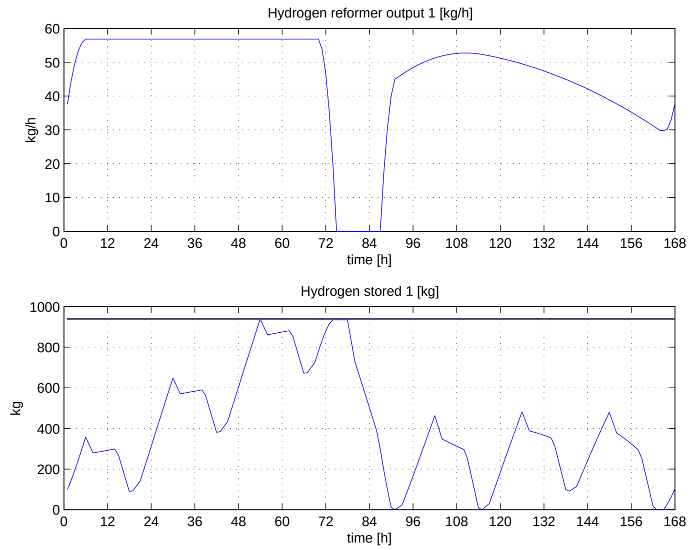

Figure 8: Case 2, 1 investment, throughput and stored hydrogen.

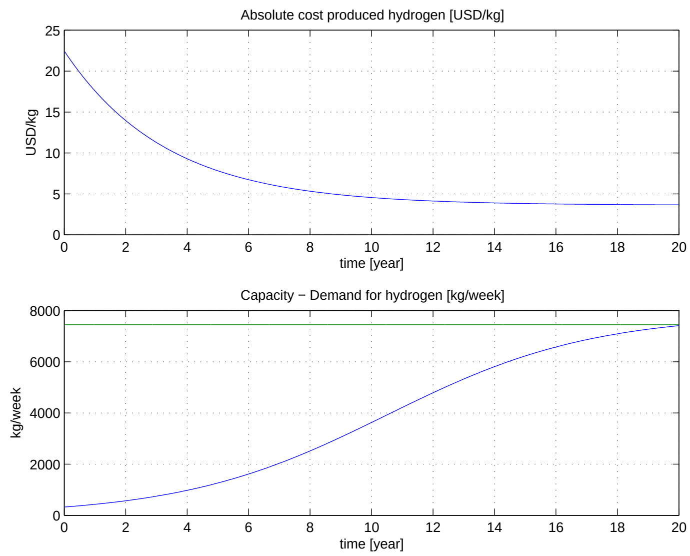

Figure 9: Case 2, 1 investment, hydrogen production cost and capacity-demand.

Table 7: Relative sensitivity at the optimal point, case 1 with 2 investments. The numbers given are relative sensitivity at the optimal point, see (29).

Property name	Investment time sensitivity	H_2 production cost sensitivity
Real rate of interest (D)	-0.04	0.10
Progress ratio (f_p)	0.26	0.85
S-curve slope (B)	-0.42	0.47
S-curve inflection point(T_x)	0.34	0.58
Total units at t_{end} (V_{tot})	0.02	-0.23
Mean hydrogen cons.($U_{h,d}$)	-0.01	0.002

6 Discussion

It is possible to use optimization and optimal control to determine optimal investment strategies for a hydrogen refueling station for

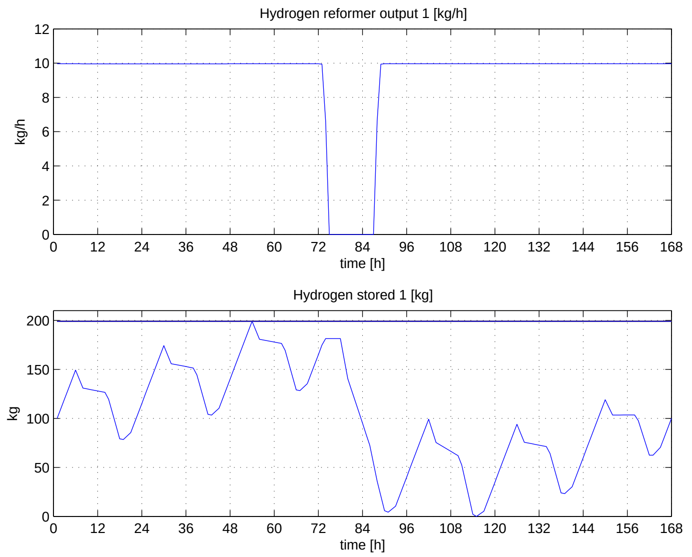

Figure 10: Case 2, 2 investments, throughput and stored hydrogen: Investment 1 at t=0.

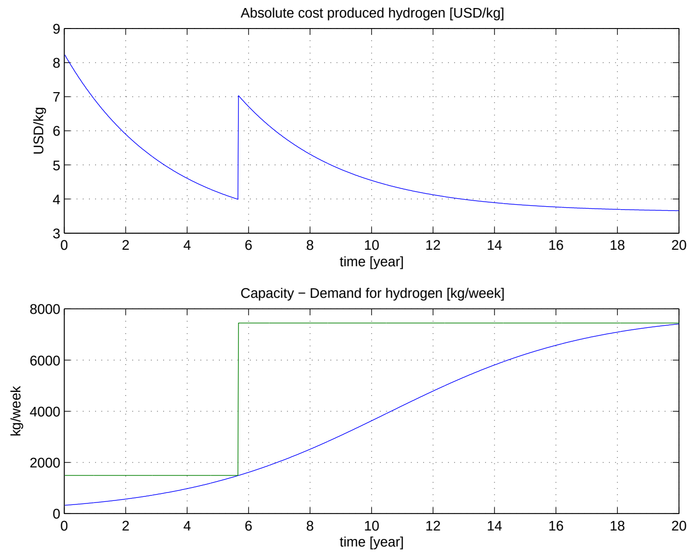

Figure 12: Case 2, 2 investments, hydrogen production cost and capacity-demand.

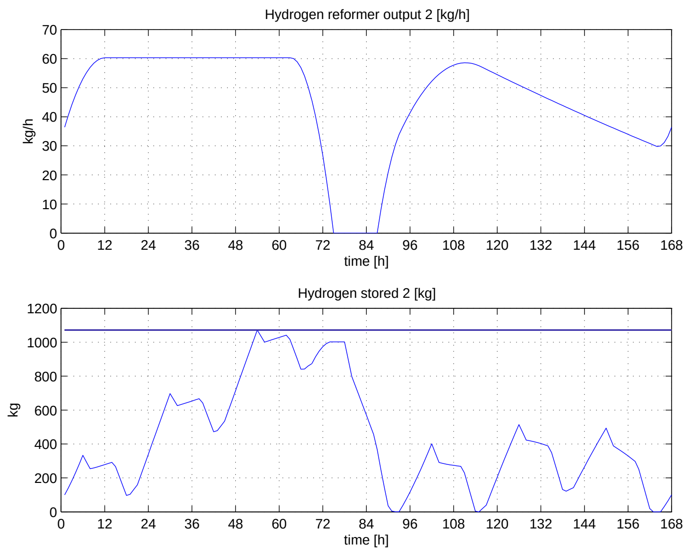

Figure 11: Case 2, 2 investments, throughput and stored hydrogen: Investment 2 at t=5.6.

Table 8: Other studies of on site reforming of methane

Study	$/kg	Size
Schoenung [27]	5.7	400 kg/d
Knight [4]	1.79	250 cars/d
Thomas [7]	11-2.2	180 - 2720 kg/d
Simbeck [15]	4.4	470 kg/d
Ogden [5]	1.7-5.6	400 cars/d

vehicles. The results indicate a hydrogen production cost at a refueling station with on site reforming of methane ranging from $4.1 to 6.0/kg, depending on the number of investments and special requirements of periodic maintenance, etc. This is in the same range as previous findings, see table 8. The main difference is that this study uses a function that increases over time (4) to estimate the number of hydrogen vehicles refueling at the station, which makes the estimated production cost an average over time. In other studies, the cost is based on maximum utilization. The idea underpinning the method developed is to be able to easily change assumptions and scenario parameters according to a given case. The method can then be used for investment planning in individual refueling station cases.

When one large investment is made, hydrogen produced will initially become very expensive. Although the production cost will have dropped to a more reasonable level after 10 years of production, the refueling station may not survive that long. A better approach would be to start with a smaller capacity, and then increase it over time. The results show that the most realistic economic production cost situation can be achieved at approximately 4 to 5 investments (figure 7) and that little is to be gained by further increasing number of investments. Increasing the number of investments can also be more favourable from a risk management point of view. It is then possible to adjust the investment plan before the next investment is made, using the same method but with more recent assumptions.

The sensitivity analysis shows that the H_2 production cost is quite sensitive to changes in some of the scenario parameters. The most sensitive one is progress ratio, i.e the price decrease for equipment. Since the progress ratio is not known in advance, large changes in the predicted production cost may result. One way of handling this situation is to add uncertainty estimates to all scenario parameters and make an optimization that takes these uncertainties into account.

Some factors in the cost function can be improved to make the results more realistic, e.g. maintenance of the equipment and resources split between the gasoline and hydrogen parts of the refueling station. Another area that can be improved is the efficiency factors for equipment, η_{eq}. In reality, efficiency is dependent on other factors, e.g. flow through the equipment. Also, in reality future development is not known. By using stochastic variables and make a stochastic optimization, uncertainties can be expressed in the result in terms of probability functions.

When the number of investments increases, so does the computational time. For case 2 with variable utilization, calculations with more than 2 investments already result in unrealistically long computational time. Since the problem is convex in the objective function (but not in the constraints), other more specialised optimization algorithms may be used. In addition, gradient and Hessian information can be provided to further reduce computational time.

The above model can probably also be used as a starting point when doing investment optimization for multiple refueling stations in a community. This optimization problem is not as straightforward as the one discussed in this paper: here factors such as local competition between refueling stations and how this affect sales (i.e. supply-demand curve) have to be taken into account. Another option would be to investigate under what circumstances the complete station layout (figure 1) would be profitable.

7 Summary and conclusions

1. With the assumptions made in this study, it is possible to produce hydrogen with on site reforming at a price ranging from \$6.0/kg for one investment to \$4.1/kg for 3 investments over 20 years when continuous production is considered.
2. Special requirements, e.g. specified storage in the beginning of the week and periodic maintenance stops of the reformer, can be accounted for but will make the produced hydrogen more expensive.
3. Investment timing is most sensitive (in order of magnitude) to changes in the scenario parameter S-curve steepness (B), S-curve inflection point (t_x) and progress ratio (f_p). It is less sensitive to changes in methane and electricity prices, interest rates (D) and S-curve total number of units at t_{end} (V_{tot}).
4. The hydrogen production cost is most sensitive (in order of magnitude) to changes in progress ratio (f_p), scenario parameter S-curve inflection point (t_x) and S-curve steepness (B). It is also quite sensitive to changes in S-curve total number of units at t_{end} (V_{tot}) and interest rates (D).
5. The method developed in this paper can be used for optimal investment planning in other areas with flow processes that can be described with state equations.

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Paper III

Macroeconomic and financial time series prediction using networks and evolutionary algorithms

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Macroeconomic time series prediction using prediction networks and evolutionary algorithms

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Abstract

The prediction of macroeconomic time series by means of a form of fully recurrent neural networks, called discrete-time prediction networks (DTPNs), is considered. The DTPNs are generated using an evolutionary algorithm, allowing both structural and parametric modifications of the networks, as well as modifications in the squashing function of individual neurons.

The results show that the evolved DTPNs achieve better performance on both training and validation data compared to benchmark prediction methods. The importance of allowing structural modifications in the evolving networks is discussed. Finally, a brief investigation of predictability measures is presented.

Key words: time series prediction, recurrent neural networks, evolutionary algorithms

1 Introduction

Prediction of time series is an important problem in many fields, including economics. Due to the high level of noise in macroeconomic time series, models involving two parts, one deterministic and one stochastic, are often used. One such method is ARIMA [1]. For one-step prediction, the results obtained by these simple predictive methods (such as exponential smoothing, which is a special case of ARIMA models), are difficult to improve much due to the high levels of noise present. However, even a small improvement can translate into considerable amounts of money for data sets that concern e.g. an entire national economy. The aims of this paper is (1) to introduce a class of generalized, recurrent neural networks and an associated evolutionary optimization method and (2) to apply such networks to the problem of deterministic prediction of macroeconomic time series, with the aim of extracting as much information as possible, while keeping in mind that the noise in the data introduces limits on the achievable performance.

2 Macroeconomic data

Two different data sets were considered, namely US GDP (quarterly variation, from 1947, first quarter to 2005, second quarter), and the Fed Funds interest rate (monthly values, from July 1954 to July 2005). The raw GDP and interest data were first transformed to a relative difference series, using the transformation

$$Z_{\mathrm{RD}}(t) = \frac{Z_{\mathrm{raw}}(t) - Z_{\mathrm{raw}}(t-1)}{Z_{\mathrm{raw}}(t-1)}. \tag{1}$$

Next, this series was further transformed using a hyperbolic tangent transformation

$$Z(t) = \tanh(C_{\mathrm{TH}} Z_{\mathrm{RD}}(t)). \tag{2}$$

For the GDP and interest rate series transformations, the values $C_{\mathrm{TH}} = 25$ and $C_{\mathrm{TH}} = 5$ were used, respectively. The aim of the hyperbolic tangent transformation was to make the data points as evenly distributed as possible in the range $[-1, 1]$.

Both data sets were divided into a training part with M_{tr} data points, and a validation part with M_{val} data points. During training, only the results (i.e. the error) over the training data set were used as feedback to the optimization procedure (see below). The rescaled GDP data set contained 233 data points. For training, steps 16-115 were used ($M_{\mathrm{tr}} = 100$) and for validation, steps 126-225 were used ($M_{\mathrm{val}} = 100$). During training, the first 15 steps were used to initialize the short-term memory of the DTPN. A similar initialization procedure was applied during validation. For the Fed Funds data set, with 612 data points, steps 26-475 were used for training ($M_{\mathrm{tr}} = 450$) and steps 486-605 ($M_{\mathrm{val}} = 120$) were used for validation.

3 Methods for prediction

3.1 Discrete-time prediction networks

Neural networks constitute a commonly used blackbox prediction model. In most cases, feedforward neural networks (FFNNs) are used. In such networks, the computational elements (neurons) are placed in layers. The input signals (i.e. earlier, consecutive values of the time series) are distributed to the neurons in the first layer, and the output signals of those neurons are then computed and used as input in the second layer etc. The output of a given neuron i is computed as

$$x_i(t+1) = \sigma\left(b_i + \sum_{j=1}^{N} w_{ij} y_j\right), \tag{3}$$

where b_i is the bias term, w_{ij} are the weights connecting neuron j in the preceding layer to neuron i, N is the number of neurons in the preceding layer, and σ is the squashing function, usually taken as the logistic function

$$\sigma_1(z) = \frac{1}{1 + \mathrm{e}^{-cz}}, \tag{4}$$

where c is a positive constant, or the hyperbolic tangent

$$\sigma_2(z) = \tanh cz. \tag{5}$$

Given a set of training data, i.e. a list of input vectors and their corresponding desired output, such networks can be trained using gradient-based methods, such as e.g. backpropagation.

However, there are fundamental limitations in the prediction that can be achieved using FFNNs, due to their lack of dynamic (short-term) memory. Stated differently, an FFNN will, for a given input, always give the same output, regardless of any earlier input signals [2], [3]. Thus, such networks are unable to deal with situations in which identical inputs to the network (at different times along the time series) require different outputs. Earlier work [2] has shown that dynamic short-term memory *does* make a difference in neural network-based time series prediction.

Furthermore, the requirement that it should be possible to obtain a gradient of the prediction error, in order to form the derivatives needed for updating the weights (during training), restricts the shape of the squashing functions. Without such restrictions, squashing functions such as e.g.

$$\sigma_3(z) = \mathrm{sgn}(z), \tag{6}$$

and

$$\sigma_4(z) = \begin{cases} \tanh(z+c) & \text{if} \quad z < -c \\ 0 & \text{if} \quad -c \leq z \leq c \\ \tanh(z-c) & \text{if} \quad z > c \end{cases} \tag{7}$$

could be used.

To overcome the limitations of FFNNs, it is possible to introduce feedback couplings in the networks, transforming them into recurrent neural networks (RNNs). Such networks have been used in many financial and macroeconomic applications, see e.g. [3], [4]. A problem with many standard training techniques for neural networks is that they require that the user should set the structure of the network (i.e. the number of neurons and their position in the network), a procedure for which one often has to rely on guesswork and rules-of-thumb [5]. An alternative training procedure is to use an evolutionary algorithm (EA) which, if properly designed, can handle both structural and parametric optimization [6].

In this paper, a new kind of network (and an associated evolutionary optimization method), well suited for the problem of time series prediction, will be used, with dynamical memory, arbitrary structure, and (in principle) arbitrary squashing functions. Each of the n neurons in these networks which, henceforth, will be called *discrete-time prediction networks* or DTPNs for short) contains arbitrary connections from the n_{in} input elements and from other neurons (including itself). In addition, each neuron has an *evaluation order tag* (EOT) such that, in each time step, the output of the neurons with the lowest EOT values is computed first, followed by the output of the neurons with the second lowest EOT values etc. The output neuron, i.e. the neuron with highest EOT (arbitrarily chosen as neuron 1) is evaluated last. Thus, the equations for neurons with the lowest EOT become

$$x_i(t+1) = \sigma\left(b_i + \sum_{j=1}^{n_{\mathrm{in}}} w_{ij}^{\mathrm{in}} I_j(t) + \sum_{j=1}^{n} w_{ij} x_j(t)\right), \tag{8}$$

where w_{ij}^{in} are the input weights, w_{ij} the interneuron weights, and b_i is the bias term. I_j are the inputs to the network which, in the case of time series prediction, consist of earlier values of the time series $Z(t)$, i.e. $I_j(t) =$

$Z(t-j+1)$. The number of inputs can thus be referred to as the *lookback* (L) of the DTPN. For neurons with the second lowest EOT, the equations look the same, except that $x(t)$ is changed to $x(t+1)$ for neurons with lowest EOT etc. Finally, the output neuron gives the following output

$$x_1(t+1) = \sigma\left(b_1 + \sum_{j=1}^{n_{\text{in}}} w_{1j}^{\text{in}} I_j(t) + w_{11}x_1(t) + \sum_{j=2}^{n} w_{1j}x_j(t+1)\right), \qquad (9)$$

since, at this stage, all neurons except neuron 1 have been updated. It is evident that the EOTs introduce the equivalent of layers. Thus, while most DTPNs will contain many recurrent connections, an FFNN is a special case of a DTPN. More precisely, a DTPN is equivalent to an ordinary FFNN if and *only* if (1) all squashing functions are of the same type (either σ_1 or σ_2), (2) only neurons with the lowest EOT values receive external input, and (3) w_{ij} (i.e. the weight connecting neuron j to neuron i) is equal to zero if $\text{EOT}(j) \geq \text{EOT}(i)$.

3.2 Benchmark predictions

In order to evaluate the results obtained using DTPNs, a comparison will be made with two standard prediction techniques, namely *autoregressive moving average* (ARMA) and *exponential smoothing*. The general simple ARMA(p,q) model

$$\phi(\Lambda)Z(t) = \theta(\Lambda)\epsilon(t), \qquad (10)$$

where Λ is the lag operator, ϵ is the disturbance $Z - \hat{Z}$, and

$$\phi(\Lambda) = 1 - \phi_1\Lambda - \ldots - \phi_p\Lambda^p, \qquad (11)$$

and

$$\theta(\Lambda) = 1 + \theta_1\Lambda + \ldots + \theta_q\Lambda^q, \qquad (12)$$

gives the one-step prediction $\hat{Z}(t+1|t)$

$$\hat{Z}(t+1|t) = \sum_{i=0}^{p} \phi_i Z(t-i) + \sum_{i=0}^{q} \theta_i\epsilon(t-i). \qquad (13)$$

ϕ_i and θ_i are parameters to be estimated in order to find the lowest error. The exponential smoothing technique (without trend) is described by the

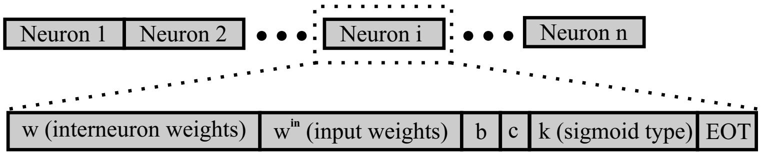

Figure 1: A chromosome encoding a DTPN.

ARIMA(0,1,1) equation

$$(1-\Lambda)Z(t) = (1-\theta_1\Lambda)\epsilon(t). \tag{14}$$

This model gives the prediction

$$\hat{Z}(t+1|t) = \frac{1-\theta_1}{1-\theta_1\Lambda}Z(t) = \theta_1\hat{Z}(t|t-1) + (1-\theta_1)Z(t). \tag{15}$$

As a special case, if $\theta_1 = 0$, the *naive prediction* $\hat{Z}(t+1|t) = Z(t)$ is obtained.

4 Evolutionary algorithm

The DTPNs were generated using an evolutionary algorithm (EA) [7]. The EA used here employed a non-standard chromosomal representation, shown in Fig. 1, in which each gene represented a neuron in the network, encoding its interneuron weights (w_{ij}), input weights (w_{ij}^{in}), bias term (b_i), sigmoid parameter (c), sigmoid type, and EOT. During the formation of new individuals, crossover was only allowed between individuals containing the same number of neurons. Several different forms of mutations were used, both parametric mutations modifying the values of the parameters (including the EOT) listed above, and structural mutations which could either add or subtract a neuron from the DTPN. No upper limit was set on the number of neurons. A lower limit of 2 neurons was introduced, however. In addition to the mutations just listed, a sigmoid type mutation was introduced as well, allowing a neuron to change its sigmoid type by randomly changing the index k of the sigmoid σ_k (see Sect. 3.1 and Eq. (17) below). Finally, in order to *allow* (not force) the EA to produce sparsely connected networks, some runs were carried out in which parametric mutations of interneuron weights, input weights, and biases not only could modify the value of the parameter in question, but also (with low probability) could set it exactly to zero. Thus, these mutations essentially functioned as on-off toggles, and were therefore called *zero-toggle mutations*. The number of input elements (and therefore the lookback L) was fixed in each run. The fitness measure F used by the EA was taken as the inverse of the RMS prediction error over the training set, i.e. $F = 1/e_{\mathrm{RMS}}$ where

$$e_{\mathrm{RMS}} = \sqrt{\frac{1}{M_{\mathrm{tr}}} \sum_{i=1}^{M_{\mathrm{tr}}} \left(Z(i) - \hat{Z}(i) \right)^2} \tag{16}$$

Note that the use of an EA implies that any form of sigmoid function can be used in the networks. In addition to the four functions $\sigma_1 - \sigma_4$, a fifth sigmoid, namely

$$\sigma_5(z) = \frac{cz}{1 + (cz)^2}, \tag{17}$$

was also allowed in the simulations reported below.

5 Prediction results

A large number of runs were carried out, using different number of inputs and different EA parameters in order to test the ability of the evolutionary algorithm to generate DTPNs with low prediction error for the two data sets under consideration.

The results are summarized in Table 1. The table shows the prediction error for the DTPN with lowest validation error. In addition, the prediction errors obtained using naive prediction, exponential smoothing, and ARMA (all with optimized parameter values), are shown.

As is evident from the table, the best DTPNs outperform the two other prediction methods. Table 2 gives a more detailed description of the best DTPNs, obtained with different values of n_{in}. For comparison, note that the best *training* errors obtained with exponential smoothing were $e_{\mathrm{ES}}^{\mathrm{tr}} = 0.2512$ for the GDP data and $e_{\mathrm{ES}}^{\mathrm{tr}} = 0.3477$ for the Fed funds data. Using the ARMA model, the best training errors were $e_{\mathrm{ARMA}}^{\mathrm{tr}} = 0.2108$ and $e_{\mathrm{ARMA}}^{\mathrm{tr}} = 0.3248$, respectively.

6 Predictability measures

The fact that the DTPNs outperform the benchmark prediction methods does not imply that these networks extract all the available information in the time series under study. One way of determining whether additional information can be extracted would be to devise a measure $P(t)$ of predictability such that, in addition to the prediction $\hat{Z}(t + 1)$ of the

Data set	e_{N}	e_{ES}	e_{ARMA}	e_{DTPN}
Fed funds interest rate	0.2018	0.1901	0.1887	0.1837
GDP	0.1771	0.1490	0.1473	0.1305

Table 1: Minimum errors over the *validation* part of the data set, obtained using naive prediction (e_{N}), exponential smoothing (e_{ES}), ARMA (e_{ARMA}), and DTPNs (e_{DTPN}). Only the results for the very best DTPN are shown.

Data set	n_{IN}	P_{zero}	n	n_L	$e^{\mathrm{tr}}_{\mathrm{DTPN}}$	$e^{\mathrm{val}}_{\mathrm{DTPN}}$
Fed funds, run 1	2	0.00	7	5	0.3072	0.1837
Fed funds, run 2	2	0.25	5	5	0.2968	0.1881
GDP, run 1	5	0.00	4	4	0.2095	0.1423
GDP, run 2	4	0.00	6	4	0.2173	0.1399
GDP, run 3	3	0.00	5	4	0.2131	0.1360
GDP, run 4	3	0.20	11	5	0.2094	0.1305

Table 2: Examples of the performance of evolved DTPNs. The second column shows the number of inputs to the network, and the third column shows the probability of a mutation being of the zero-toggle type, i.e. a mutation that sets the parameter in question to zero. The fourth column shows the (evolved) number of neurons, and the fifth column shows the (evolved) number of layers (n_L), i.e. the number of distinct EOT values in the evolved network. The two final columns show the errors over the training and validation parts of the data set.

next value in the time series, one would obtain an estimate of the error $e(t+1) = Z(t+1) - \hat{Z}(t+1)$. Ideally, the measure should be such that $P(t) = f(e(t+1))$ where f is a known, monotonous function.

Several different predictability measure can be formed. The amount of (local) information in a time series can, for instance, be estimated analytically using random matrix theory, based on the correlation matrix formed from the delay matrix D [8]. In addition, various empirical measures can

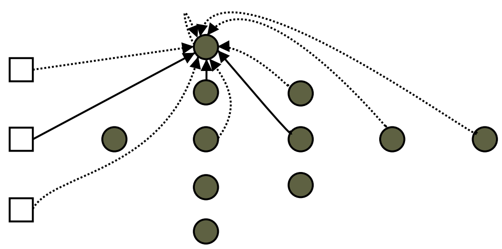

Figure 2: The best evolved network (run 4) for the prediction of the GDP series. Input elements are shown as squares and neurons as filled circles. The neurons are arranged in layers based on their EOT values. For clarity, only the inputs to one neuron are shown. Solid lines indicate positive weights and dotted lines negative ones.

also be generated, based on the prediction errors obtained in previous time steps. An investigation was made involving both the analytical measure and a few different empirical measures, applied to the rescaled difference series $Z(t)$. However, in all cases, the results were negative, i.e. the proposed predictability measure showed near-zero correlation with the actual prediction error, and therefore these measures will not be described further here.

7 Discussion and conclusion

This investigation has shown that it is possible to improve, albeit only slightly, the predictions obtained from standard prediction methods using a generalized version of neural networks (called discrete-time prediction networks, DTPNs) with the possibility of adding a short-term memory through feedback couplings.

In earlier work [2], continuous-time recurrent neural networks were considered for time series prediction. The DTPNs introduced here do not require continuous-time integration, i.e. the network output is obtained by discrete-time equations rather than differential equations, making the evaluation of the networks much faster, while still allowing a rich dynamical structure, including dynamic short-term memory.

The use of an EA for the optimization of the networks removes all restrictions regarding both the behavior of individual neurons as well as the structure of the network as a whole, while still allowing standard feedforward neural networks as a special case.

The importance of structural modifications in the network is illustrated by the fact that, in any given run, the structure of the current best network varied significantly during the run. The final networks often contained rather few neurons and used only a few input elements, illustrating another advantage of using recurrent networks: because of their ability to form a short-term dynamic memory, such networks need not use as many inputs as a feedforward network, thus also reducing the number of networks weights and hence the risk of overfitting.

The best network for prediction of the GDP series, shown in Fig. 2, had a slightly more complex structure. However, in the run generating that network, zero-toggle mutations were used, and indeed the resulting network was far from fully connected, and therefore had, in fact, a somewhat simpler structure than would have been suspected on the basis of the number of neurons involved.

The fact that the predictability measures all gave negative results was expected, and it indicates that the DTPNs really do extract all, or almost all, information available in the time series.

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Paper IV

Optimization of the investment strategy for a combined hydrogen and hythane refueling station

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Optimization of the investment strategy for a combined hydrogen and hythane refueling station

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Abstract

One of the major barriers to the widespread use of hydrogen is the lack of a hydrogen infrastructure, an important component of which is the individual hydrogen refueling station. The long-term profitability of the hydrogen filling station is a key issue for the success of the transition to a hydrogen infrastructure.

The topic of this paper is the problem of finding the optimal investment strategy for a single hydrogen and hythane refueling station giving minimum production cost, while matching the hythane and hydrogen capacity to a demand generated from three stochastic scenarios over a 20-year period.

A minimal resulting production cost between USD 2-6/kg for hydrogen and USD 1-1.5/kg for hythane (depending on preferences concerning unsatisfied demand, flexibility etc.) was found. It was also found that the production cost and the amount of unsatisfied demand constitute conflicting objectives so that, for example, if the total hydrogen and hythane demand is to be satisfied, the production cost of hydrogen will be unrealistically high. The effect of uncertainties for the constructed scenarios is minimized by the use of stochastic optimization techniques.

Keywords: Hydrogen; Hythane; Infrastructure; Investment; Optimization; Refueling station

1 Introduction

Hydrogen is a promising fuel for vehicles. Four main arguments support this assertion: (1) The potential of reducing greenhouse gases from the transport sector; (2) An increase in energy supply security, since hydrogen can be produced from many energy sources so that the risk of a shortage of supply may be reduced; (3) Hydrogen has higher energy efficiency than do other fuels; (4) The use of hydrogen leads to the possibility of zero local emissions with the use of fuel cells [1, 2, 3]. The magnitude of the benefits of hydrogen fuel cell vehicles has been assessed by Karlström [4] and Sanden and Karlström [5].

However, these benefits can only be exploited if several barriers to a large-scale introduction of hydrogen fuel cell vehicles are reduced. One of the major barriers is the lack of a hydrogen infrastructure [6]. The construction of a full-scale hydrogen infrastructure with production facilities, a distribution network, and refueling stations is likely to be very costly. The venture of constructing a hydrogen refueling infrastructure constitutes a long-term, capital intensive investment with great market uncertainties for fuel cell vehicles. Therefore, reducing the financial risk is a major objective of any long-term goal to build a hydrogen infrastructure [7].

Ogden [8] has described several hydrogen supply options. Investigations have also been made for large scale production of hydrogen [9, 10, 11]. Many studies of cost and technology for a hydrogen infrastructure and for individual stations have also been carried out [12, 13, 14, 15, 16, 17, 18, 19]. The H2A analysis group at the US department of energy (DOE) has recently developed two H2A delivery models: the H2A Delivery Components Model and the H2A Delivery Scenario Model [20].

The above studies mainly consider hydrogen as a fuel from an environmental and economic standpoint in a large scale perspective. By contrast, Forsberg and Karlström [21] investigated the most profitable investment strategy for the individual hydrogen refueling station featuring on-site small-scale reforming of methane [21]. The question was when, and to what extent, to build the parts of the station, satisfying an increasing demand of hydrogen. The result was a minimum hydrogen production cost of 4-6 USD/kg, depending on the number of re-investments during the 20-year-period considered. This paper is a continuation and an improvement of [21]. The improvements explored are mainly:

1. The earlier study relied on single-objective optimization of the production cost and hence produced one optimal investment strategy. In this study, multi-objective optimization is used for finding Pareto optimal fronts for contradictory objectives. For decision-making it is more favourable to have a set of solutions, each representing different possible investment alternatives. Preferably

these should lie on the pareto-optimal front of important objectives.

2. The sensitivity analysis in the previous study showed that the results were quite sensitive to variations in the strategic parameters and in particular to the estimated number of refueling vehicles (represnted by the S-curve, i.e. a curve indicating the estimated technology adaptation, see below). In this study we present three scenarios with considerably different future developments. For each scenario we generate a large number of samples and make use of stochastic optimization to find the best solutions.

3. Hythane, i.e. natural gas mixed with a small fraction of hydrogen, is a viable intermediate alternative fuel for vehicles. Whereas the earlier study only considered hydrogen, in this study both hydrogen and hythane are taken into account.

4. In reality equipment is available in a (finite) number of sizes. For simplicity, the earlier study made use of continuously sized equipment. By contrast, this study applies presently available sizes of equipment, thus achieving a higher degree of realism. In addition, the costs of equipment, electricity, and natural gas have been updated to current (2006) values.

The most important issues in this study are to reduce the effect of uncertainties for scenario parameters and to identify connections between production cost and other results. The calculations cover 20 years, from 2010 until 2030. If an investment is made, it takes place at the very beginning of the year, i.e. an investment is in year 1 occurs on the 1st of January 2010.

2 Strategic parameters

The strategic parameters influence how the generated future scenarios are calculated and are therefore crucial to the results. These parameters and their respective values are given in Table 1.

The number of produced units of reformers, electrolysis etc. is considered to equal the number of hydrogen refueling stations, which is estimated to reach 5,000 in the year 2010 and 50,000 in the year 2030, and to follow the S-curve

$$R(t) = \frac{1}{1 + \mathrm{e}^{-B(t-T_x)}}, \tag{1}$$

in between. t is the time from year 2010, T_x the S-curve inflection point and B the slope. The estimation concerning the growth of hydrogen fuel cell vehicles is assumed. The growth of number of stations is based upon the estimated growth of hydrogen fuel cell vehicles and their hydrogen demand. A report presented by E4tech [14] and funded by the UK Department of Trade and Industry and the Carbon Trust predicts that ”if the hurdles are overcome, the mainstream propulsion market is expected to open up after 2010”. Melaina [24] made a preliminary investigation concerning the sufficient number of initial hydrogen stations in the US, and concluded that between 4,500 and 17,700 hydrogen stations would be required to initiate a hydrogen infrastructure for fuel cell vehicles. The estimate of 50,000 hydrogen stations in 2030 used here is motivated by the fact that this investigation takes the whole world into account. Also, in this study, the market reaches a high level of maturity, further motivating the estimate for the number of stations in 2030.

Table 1: Strategic parameters. The electricity price is assumed to be higher during daytime (6 am-10 pm) than at night (10 pm-6 am). All parameter values are estimates except natural gas price, which is from [22] and electricity price, which is from [23]

Name	Description	Value	Unit
B	S-curve slope	0.3	-
D	Real rate of interest	0.1	1/year
F_{cont}	Contingency cost factor	0.1	-
F_{eng}	Engineering permitting cost factor	0.1	-
F_{gen}	Include land cost factor	0.2	-
F_{h2y}	Mass ratio hydrogen in hythane	0.03	
N	Number of time steps	175 200	-
P_e	Electricity price vector (6am-10pm)	0.10 USD/kWh	
	Electricity price vector (10pm-6am)	0.08	USD/kWh
P_{ng}	Natural gas price	0.97	USD/kg
t_0	Start time of calculations (2010)	0	
t_f	End time of calculations (2030)	175 200	
T_x	Inflection point of the S-curve	10	year
W	Scenario sample	-	-
X_{hf}	Hydrogen demand (from scenario)	-	kg/h
X_{yf}	hythane demand (from scenario)	-	kg/h

The decrease in purchase price, in relation to the present-day purchase price, owing to increased production and technology development (f_t) for a given type of equipment eq is approximated as

$$\begin{aligned} f_{t,eq}(t) &= \frac{(50000R(t))^{(\log f_{p,eq}/\log 2)}}{5000^{(\log f_{p,eq}/\log 2)}} \\ &= (10R(t))^{(\log(f_{p,eq})/\log(2))}. \end{aligned} \tag{2}$$

Here, $f_{p,eq}$ is a progress factor for the equipment in question, i.e. a factor that determines the purchase cost decay rate for the specified equipment. Equation (2) is used for all equipment parts of the refueling station, regardless of size. It should be kept in mind that the function $f_{t,eq}$ is purely exogenous and therefore uncertain. This uncertainty will influence the results, as is discussed in Section 6.

Using the *present day value correction factor*, (C_p), future costs can be discounted to present day value as

$$C_p(t) = \frac{1}{(1+D)^{t/8760}}, \tag{3}$$

where t is the number of hours from the start of calculation, t_0, and D is the real interest rate. Furthermore, the *consecutive present day value correction vector* is defined as

$$\mathbf{C} = [C_p(1)\ C_p(2)\ \ldots\ C_p(N)]\,. \tag{4}$$

The average of the components of this column vector, i.e.

$$C(t) = \frac{1}{N}\sum_{t=1}^{N} C_p(t) \tag{5}$$

can be used to calculate the present value of evenly distributed costs. For $D = 0.1$, $C(t) = 0.4466$.

2.1 Scenario generation

The number of vehicles visiting the single refueling station is a stochastic variable which is estimated in three scenarios. In these scenarios, the following vehicles are considered:

1. Ordinary combustion engine powered buses running on hythane.
2. Ordinary combustion engine powered cars running on hythane.
3. Ordinary combustion engine powered buses running on hydrogen.
4. Ordinary combustion engine powered cars running on hydrogen.
5. Fuel cell driven buses running on hydrogen.
6. Fuel cell driven cars running on hydrogen.
7. Fuel cell driven scooters running on hydrogen.

The first four vehicles represent intermediate solutions, used until the fuel cell driven alternatives have become dominant. The above vehicles are considered to have filling data and statistics in accordance with Table 2.

Using these data, three possible future scenarios are given in Table 3. The first scenario emphasizes hythane and hydrogen powered buses as an intermediate alternative. The second scenario focuses on hydrogen cars, primarily with combustion engines early on, and fuel cells toward the end of the period considered. In the third scenario hydrogen fuel cell powered scooters are in focus. In all three scenarios hydrogen fuel cell cars are used in the longer perspective.

For interpolation between the three time periods specified in Table 3, the S-curve has been used, giving the smooth curve shown in Figure 1. The smoothness obtained through the interpolation is likely to be valid for the car purchases of groups of individuals, but may, of course, be violated e.g. in the case of large corporations that may acquire several vehicles (such as buses) at the same time.

For each scenario a set of samples (W) is generated using Poisson distributions with parameters from Tables 2 and 3. With a time step length of one hour, the total number of steps is $N = 24 \times 365 \times 20 = 175,200$ for each sample. For the scenario generation, hydrogen filling is separated from hythane filling. The resulting hydrogen and hythane demand is denoted X_{hf} and X_{yf}, respectively.

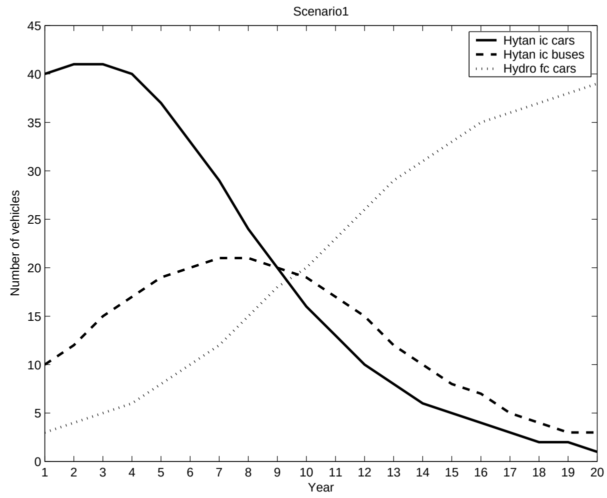

Figure 1: Number of vehicles in scenario 1 as a function of time. Data based on S-function-smoothened values from Table 3.

3 The refueling station

The task of the refueling station is to provide fuel for hydrogen and hythane vehicles. As the main energy carrier, natural gas is chosen. One reason is the already present natural gas refueling network. Moreover, natural gas is one of the cheapest production sources for hydrogen in the short term. The hythane dispenser part of the refueling station is an intermediate alternative on the path to hydrogen vehicles.

After reforming, the produced hydrogen gas is compressed and stored. The high storage pressure then makes it possible to refuel hydrogen without further compression. Some of the hydrogen can be used for mixing with natural gas to form hythane, which is refueled using a special hythane dispenser. The mixture of hydrogen in hythane is here set to 3% by weight. When electricity prices are low (i.e. at night), it might be more profitable to produce hydrogen by electrolysis than through the reformer. For this option an electrolyser can be added. All in all, this is a flexible layout capable of simulating many types of possible future hythane and hydrogen refueling stations, see Figure 2. The model is also flexible with respect to refueling station types, e.g. car, truck, or bus, and refueling station locations e.g. central, suburban, or countryside, by changing the strategic parameters.

The model developed and the optimisations made involve the components within the refueling station. Components outside the station are considered to be already present.

3.1 The parts of the refueling station

Table 4 gives data on the parts of the refueling station from Figure 2. Data are taken from actual produced equipment in the year 2000 [25].

The reformer, electrolysis, and compressor are chosen from a finite set of available sizes, while the H_2 store as well as the hythane and H_2 dispensers are purchased on a piece-wise basis depending on the required capacity. Some equipment cannot be used below a certain minimum level, which is indicated by the minimum usage rate (f_u) and given as a fraction of maximum capacity. For the reformer, the minimum usage rate equals the minimum capacity. For the H_2 store, the minimum usage rate indicates the minimum storage level. Below this minimum storage level the pressure drops too low to be dispensed to vehicles. For sizes different from the nominal capacity (c_n), the purchase price is calculated using the scale

Table 2: Filling statistics for vehicles visiting the single refueling station. ic denotes *internal combustion engine* and fc denotes *fuel cell powered engine*. ΔT denotes the time between fillings, and T_d denotes the time of day at which filling takes place. The numbers are estimates.

Vehicle type	hythane [kg/filling]	H_2 [kg/filling]	ΔT [days]	T_d [h]
hythane ic bus	61	0	1	5-8
hythane ic car	6	0	3	1-24
Hydrogen ic bus	0	60	1	5-8
Hydrogen ic car	0	6	3	1-24
Hydrogen fc scooter	0	2	5	1-24
Hydrogen fc bus	0	40	1	5-8
Hydrogen fc car	0	5	5	1-24

Table 3: Number of vehicles visiting the single refueling station for each scenario. ic denotes *internal combustion engine* and fc denotes *fuel cell powered engine*. Figures are based on assumptions of different future scenarios for the introduction of hydrogen vehicles.

Time span	Scenario 1	Scenario 2	Scenario 3
Year 1-5	10 hythane ic buses, 40 hythane ic cars	10 H_2 ic cars, 2 H_2 ic buses	30 hydro fc scooters
Year 5-10	20 hythane ic buses, 10 H_2 fc cars	10 H_2 ic cars, 2 H_2 ic buses, 20 H_2 fc cars	30 H_2 fc scooters, 20 H_2 fc cars
Year 10-20	40 H_2 fc cars	40 H_2 fc cars	40 H_2 fc cars

Table 4: Data on the refueling station parts. Electricity use is the amount of electrical energy consumed for each kg of output for the piece of equipment in question. ng denotes natural gas and pc number of pieces. Data on the hythane dispenser are estimated from data on the hydrogen dispenser. Figures are from [25].

Part	Reformer	Electrolysis	Compressor	H_2 store	Hythane dispenser	H_2 dispenser
Life time (l)	10 year	20 year	10 year	20 year	10 year	10 year
Nom. capacity (c_n)	4.2 kg/h	62.5 kg/h	4.2 kg/h	21 kg	96 kg/h	48 kg/h
Nom. purchase cost (p_n)	100,000 USD h/kg	34,632 USD h/kg	12,143 USD h/kg	22,500 USD/pc	120,000 USD/pc	60,000 USD/pc
Scale factor (f_s)	0.75	0.72	0.8	-	-	-
Available sizes	4.2, 12.5, 62.5 kg/h	4.20, 12.5, 62.5 kg/h	5, 15, 75 kg/h	21 kg	96 kg/h	48 kg/h
Maintenance cost (f_m)	0.07	0.07	0.05	0.01	0.035	0.035
Efficiency (η)	0.26 kg H_2/kg NG	0.02 kg H_2/kWh	1.0	1.0	1.0	1.0
Electricity use (f_e)	1.5 kWh/kg	-	2.2 kWh/kg	0.0 kWh/kg	0.0 kWh/kg	0.0 kWh/kg
Progress ratio (f_p)	0.9	0.9	0.9	0.9	0.9	0.90
Min. usage rate (f_u)	0.25	0.0	0.0	0.56	0.0	0.0

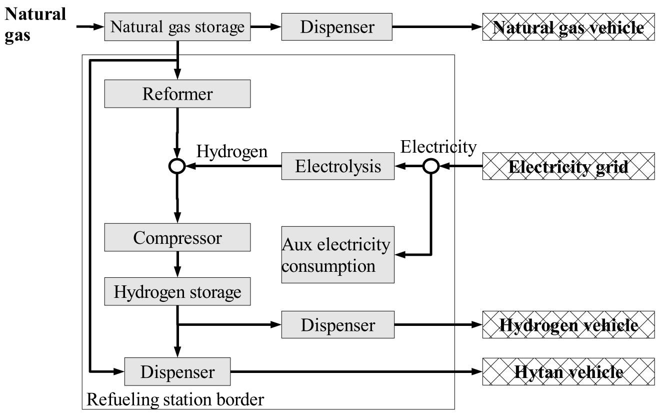

Figure 2: Hythane and hydrogen refueling station layout. Natural gas is reformed to hydrogen on-site and stored for delivery to vehicles. It is also possible to produce hydrogen from electricity by electrolysis. In this study, only the parts within the refueling station are considered.

function

$$p_{eq}(s) = p_n s \left(\frac{c_n}{s}\right)^{1-f_s} = p_n\, c_n^{1-f_s} s^{f_s}. \qquad (6)$$

Here f_s is a scale factor (see Section 2). Using this function an estimated purchase price is obtained for a piece of equipment of arbitrary size (s [kg/h]), using the purchase price p_n for an existing piece of equipment, with capacity c_n. The function (6) applies to the reformer, electrolysis, and compressor. The expected life time l is used to reduce the investment cost, should the investment period (2010-2030) end before the end of life of the piece of equipment in question. The reduction in purchase cost is approximated by a linear function (in time). The efficiencies in Table 4 indicate the relation between the mass entering and leaving the equipment. In the case of the reformer, the substance entering is methane and that leaving is hydrogen.

3.2 Initial considerations

The hydrogen/hythane refueling station is assumed to be built in conjunction with an existing natural gas refueling station. The supply of natural gas can be delivered by truck or, more commonly, by pipeline. In any case, the supply is considered to be already established and only the cost for the purchase of natural gas is taken into account. All costs for the hythane/hydrogen part of the station, i.e. land use and wages, are accounted for. In reality some resources can probably be shared between the natural gas and hythane/hydrogen parts of the refueling station. Initially, the hydrogen storage is considered to be empty.

3.3 The model

The model for the refueling station in Figure 2 only has one state variable, i.e. a variable to be integrated, which is the amount of stored hydrogen, x_{hs}. Once the stored amount of hydrogen is known, all other relevant quantities can be calculated directly. Letting k denote the time step, one can express x_{hs} in the form of the difference equation $x_{hs}(k+1) = x_{hs}(k) + x^o_{hc} - x^o_{hs}$, where x^o_{hc} is the amount leaving the compressor (see Figure 2), which equals the amount entering the storage, and x^o_{hs} the amount leaving the storage. The compressor output comes from the reformer x^o_{hr} and electrolysis x^o_{he} and taking the compressor efficiency η_{hc} into account one can write $x^o_{hc} = (x^o_{hr} + x^o_{he})\eta_{hc}$. In order to determine the natural gas consumption of the reformer x^i_{hr}, the equation $x^o_{hr} = x^i_{hr}\eta_{hr}$ is added, where η_{hr} is the efficiency of the reformer. The amount leaving the hydrogen storage is the sum of dispensed hydrogen x^o_{hd} and the hydrogen part F_{h2y} of dispensed hythane x_{yd}. Taking the dispenser's efficiencies η_{hd} and η_{yd} into account, this amount is obtained as $x^o_{hs} = x^o_{hd}/\eta_{hd} + x^o_{yd}F_{h2ng}/\eta_{yd}$. Now the total natural gas consumption x_{ng} from both the hydrogen x^i_{hr} and hythane $x^o_{yd}(1 - F_{h2y})$ part can be calculated as $x_{ng} = x^i_{hr} + x^o_{yd}(1 - F_{h2y})/\eta_{yd}$. Thus, in summary, the following equation system is obtained

$$\begin{aligned} x_{hs}(k+1) &= x_{hs}(k) + x^o_{hc} - x^o_{hs}, \\ x^o_{hc} &= (x^o_{hr} + x^o_{he})\eta_{hc}, \\ x^o_{hr} &= x^i_{hr}\eta_{hr}, \\ x^o_{hs} &= \frac{x^o_{hd}}{\eta_{hd}} + \frac{x^o_{yd}F_{h2ng}}{\eta_{yd}}, \\ x_{ng} &= x^i_{hr} + \frac{x^o_{yd}(1 - F_{h2y})}{\eta_{yd}}. \end{aligned} \qquad (7)$$

However, these equations are subject to some constraints. First of all, there are minimum and maximum levels both for the flow and for the amount stored. Second, the amount of dispensed hydrogen and hythane, x^o_{hd} and x^o_{yd}, must be non-negative and are limited from above by the scenario sample demand (X_{hf} and X_{yf}, respectively). Note that the demand is not necessarily totally satisfied. All in all, the following constraint equations are obtained

$$\begin{aligned} f_{u,hr}\, s_{hr} &\leq x^o_{hr} \leq c_{hr}, \\ 0 &\leq x^o_{he} \leq c_{he}, \\ 0 &\leq x^o_{hc} \leq c_{hc}, \\ f_{u,hs}\, s_{hs} &\leq x_{hs} \leq c_{hs}, \\ 0 &\leq x^o_{hd} \leq c_{hd}, \\ 0 &\leq x^o_{yd} \leq c_{yd}, \\ 0 &\leq x^o_{hd} \leq X_{hf}, \\ 0 &\leq x^o_{yd} \leq X_{yf}, \end{aligned} \qquad (8)$$

where c_he denotes the hydrogen electrolysis capacity, c_{hc} the compressor capacity, c_{hs} the storage total capacity, c_{hd} and c_{yd} the hydrogen and hythane dispenser capacity, respectively. Note that, for the reformer and storage, the minimum utilization level is higher than zero. This is due to the fact that the hydrogen dispenser cannot be run below a certain minimum flow rate, given as a ratio $f_{u,hr}$ of the maximum capacity s_{hr}, giving $f_{u,hr}\, s_{hr}$ as the minimum allowed flow rate. For the storage, the hydrogen gas pressure falls below acceptable limits for the dispenser if the stored amount is less than the ratio $f_{u,hs}$ of the total capacity s_{hs}, thus making $f_{u,hs}\, s_{hs}$ the minimum amount to be stored.

For the optimization, the state variable is the hydrogen storage (x_{hs}), the control variables are the outputs of reformer and electrolysis (x^o_{hr} and x^o_{he}, respectively), and the disturbances are the stochastic variables hydrogen and hythane demand (X_{hf} and X_{yf}, respectively).

4 The optimization problem

The optimization problem under consideration can be formulated as a discrete-time stochastic optimal-control problem [26, 27, 28]. In this type of problem the aim is to find the control U that minimises an objective function $J(U)$ for a dynamical system $f(X, U, W)$ during a specified time, in the discrete case indexed by the time step variable k. The system is also influenced by an independent random disturbance W. The general formulation is

$$\begin{aligned} \min_U \; J(U) &= \sum_{k=0}^{N-1} \gamma(k, X_k, U_k, W_k) + \Gamma(X_N, W_N) \\ \text{s.t. } X_{k+1} &= f(k, X_k, U_k, W_k) \\ c_k(X, U) &\leq 0 \; \forall k = 1, \ldots N, \end{aligned} \tag{9}$$

where $\gamma(k, X_k, U_k, W_k)$ is the cost associated with each time step k, $\Gamma(X_N, W_N)$ is the terminal cost and $c_k(X, U)$ represents simple limits of the state and control variables. The controller makes use of the information set ξ_k, the contents of which depend on the type of control system. For an *open-loop* system, $\xi_k = \{X_0\}\ \forall k$, whereas for a *feedback* system, $\xi_k = \{X_0, X_k\}, k = 0, 1, \ldots, N-1$. For a *closed-loop* system, $\xi_k = \{X_0, X_1, \ldots, X_k, U_0, U_1, \ldots, U_{k-1}\}$. In this study, the investment strategy is set prior to t_0 and then followed until t_f, thus defining an open-loop control system as described above.

The problem is to find the optimal investment strategy π^* that will subsequently minimise two objective functions, further discussed in Section 4.1. An inner control loop is used to keep the hydrogen storage level at a given amount. In this loop, a control algorithm is implemented to keep the hydrogen storage at a specified level. Since the time constants of both reformer and electrolysis are very short (of the order of minutes) compared to the time step (one hour), the desired control action will be considered to take effect immediately. Due to the rapid dynamics of both reformer and electrolysis, these devices can be shut down fast and, therefore, there is no need to keep the storage below 100% as a precaution to avoid overflow due to slow production adaptability for unexpectedly low levels of demand. The control algorithm first calculates the deviation in hydrogen storage from the set point (the error), then fills up the storage with available hydrogen, which is the sum of reformer maximum capacity and electrolysis during the period when electricity is cheaper, i.e. 10pm - 6am. No electrolysis is used during the remaining expensive hours. The calculated amount is then added to the storage. Depending on the demand priority policy υ, either an attempt is made to satisfy first the hydrogen refueling demand and then the hydrogen part of hythane, or vice versa. Tuning this policy will have a significant influence on the amount of unsatisfied demand. The total control vector is then

$$U = [\upsilon\ \pi]. \tag{10}$$

The inner control loop does not have any tunable parameters and is thus not part of the optimal control problem. It is implemented as an obvious optimal solution to keep the size of the variable space at a minimum.

Direct control parameter mapping methods, i.e. methods that will need dedicated control parameters for each step, are not used. Such techniques are intractable due to the large number ($N = 175, 200$) of steps involved.

No terminal cost $\Gamma(X_N, W_N)$ is used. Instead the total investment cost (for the entire life time) is scaled linearly, in accordance to the usage time of the piece of equipment, see Eq. (13) below. The system equation and the simple constraints have been given in Eqs. (7) and (8). The random disturbance W is the hythane and hydrogen demand, further described in Section 2.1 above.

4.1 Objective functions

In this study, the following performance measures are used

1. Production cost per kg for hydrogen p_{hf}. This is the production cost for hydrogen at the hydrogen dispenser and is calculated as the sum of all hydrogen related costs divided by the total amount of sold hydrogen x^o_{hd}.

2. Unsatisfied demand for hydrogen $x_{h,u}$. This is the demand that cannot be satisfied at the hydrogen dispenser and is a negative measure, i.e. a low amount of unsatisfied demand is desirable.

3. Production cost per kg for hythane p_{yf}. This is the production cost for hythane at the hydrogen dispenser and is calculated as the sum of all hythane-related costs divided by the total amount of sold hythane x^o_{yd}.

4. Unsatisfied demand for hythane $x_{y,u}$. This is the demand that cannot be satisfied at the hythane dispenser and is a negative measure, i.e. a low amount of unsatisfied demand is desirable.

5. Unsatisfied demand for all hydrogen $x_{ht,u}$. The total amount of hydrogen demand that cannot be satisfied, i.e. the sum of unsatisfied demand at the hydrogen dispenser $x_{h,u}$ and as part of hythane F_{h2y} at the hythane dispenser $x_{y,u}$.

6. Flexibility $p_{h\Delta}$. A measure used for quantifying the difference between the cost for the active scenario, i.e. the scenario for which the present solutions have been optimized, and the passive ones, i.e. the scenarios that are not part of the optimization.

For the optimization, the production cost per kg for hydrogen $x_{h,u}$ and the unsatisfied demand for all hydrogen $x_{ht,u}$ are used in the objective function J which then takes the form

$$J(U) = [p_{hf}\ x_{ht,u}]. \tag{11}$$

In order to compute the above performance measures, a number of costs and flows need to be calculated. Before carrying out the calculation, however, an assumption is made (and applied to all calculations below) that each part of the refueling stations takes on its own expenses. This implies that expenses from the hythane part will be added to the hythane production cost and the same for the hydrogen part. Parts used in both hythane and hydrogen production, such as storage, are charged according to the usage ratio

$$f_{hpc} = \frac{\sum x_{hf}}{\sum(x_{hf} + F_{h2y} x_{yf})}. \tag{12}$$

For each part (eq) of the refueling station where the purchase cost is scaled to the used size, i.e. reformer, electrolysis and compressor, the cost is computed as

$$p_{eq}(t_i, s_{eq}) = f_{t,eq}(t_i)\, p_{eq}(s_{eq}) \max(\frac{20 - t_i}{l_{eq}}, 1), \tag{13}$$

where l_{eq} is the estimated lifetime of the part in question, see Table 4. For those items purchased on a piece-wise basis, i.e. storage tanks and dispensers, the cost is computed as

$$p_{eq}(t_i, n_{eq}) = f_{t,eq}(t_i)\, p_n n_{eq} \max(\frac{20 - t_i}{l_{eq}}, 1). \tag{14}$$

This implies a linear scaling of the total investment cost for the entire estimated life time to the time it is actually used.

The total cost consists of costs for purchase of equipment, resources, maintenance and a factor to cover for construction, land use and general expenses. It is estimated that the cost for loans for equipment will cancel the effect of the present value correction for the sum of instalments. This is exactly the case of annuity loans. All other costs are discounted to present day using equation (3).

The cost for equipment shared by the hythane and hydrogen parts is then

$$\begin{aligned} p_{c,eq} = \sum_{\forall i} (p_{hr}(t_i, s_{hr,i}) + p_{he}(t_i, s_{he,i}) + \\ p_{hc}(t_i, s_{hc,i}) + p_{hs}(t_i, n_{hs,i})). \end{aligned} \tag{15}$$

The cost for maintenance is estimated to a specified fraction (f_m) of the equipment cost, that is

$$\begin{aligned} p_{c,m} &= \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \sum_{\forall i} \left\{ \frac{f_{m,hr} p_{hr}(t_i, s_{hr})}{8760\, l_{hr}} + \frac{f_{m,he} p_{he}(t_i, s_{he})}{8760\, l_{he}} \right. \\ &+ \left. \frac{f_{m,hc} p_{hc}(t_i, s_{hc})}{8760\, l_{hc}} + \frac{f_{m,hs} p_{hs}(t_i, n_{hs})}{8760\, l_{hs}} \right\}, \end{aligned} \tag{16}$$

which is an $N \times 1$ column vector. The factor 8760 is used to convert the equipment life time from years to hours. The electricity cost is calculated from equipment flows as

$$p_{c,e} = P_e \otimes (f_{e,hr} x^o_{hr} + f_{e,he} x^o_{he} + f_{e,hc} x^o_{hc} + f_{e,hs} x_{hs}) \tag{17}$$

where $\otimes$ is the element-wise multiplication operator. The natural gas cost is

$$p_{c,mg} = P_{ng} x^i_{hr}. \tag{18}$$

The total cost for the shared parts is then

$$\begin{aligned} p_c = (1 + F_{cont} + F_{eng} + F_{gen})\, p_{c,eq} + \\ pds \times (p_{c,m} + p_{c,e} + p_{c,mg}). \end{aligned} \tag{19}$$

For the hydrogen and hythane specific parts, calculation of costs follows the same pattern as in Eqs. (15)-(19) above, and is therefore not listed here.

The resulting production cost per kg of hydrogen p_{hf} and hythane p_{yf} is now

$$p_{hf} = \frac{p_c f_{hpc} + p_h}{\sum x_{hf}} \tag{20}$$

and

$$p_{yf} = \frac{p_c(1 - f_{hpc}) + p_y}{\sum x_{yf}}, \tag{21}$$

respectively.

It is clear from Eq. (8) that not all the demand from the scenario samples need be satisfied. The difference between the demand and the actual sold amount is called unsatisfied demand. Three measures of unsatisfied demand are used, namely (1) hydrogen dispenser unsatisfied demand

$$x_{h,u} = X_{hf} - x^o_{hd}, \tag{22}$$

(2) hythane dispenser unsatisfied demand

$$x_{y,u} = X_{yf} - x^o_{yd}, \tag{23}$$

and (3) total unsatisfied hydrogen demand from both the hydrogen dispenser and the hydrogen part of the hythane at the hythane dispenser

$$x_{ht,u} = x_{h,u} + F_{h2y}\, x_{y,u}. \tag{24}$$

The variance of the above objectives p_{hf}, p_{yf}, $x_{h,u}$ and $x_{y,u}$ between samples is used as a measure of sensitivity, which can also be interpreted as risk. A high variance would imply a higher risk. Flexibility is a complex measure that can be defined in a number of ways [29]. Here, it has been defined as

$$p_{h\Delta} = p^a_h - \frac{p^{p1}_h + p^{p2}_h}{2}, \tag{25}$$

i.e. as the mean difference between the hydrogen production cost for the active scenario and the passive ones. A positive value indicates a lower cost for the passive scenarios and vice versa.

4.2 Optimization strategy

The stochastic control problem (9) is solved with a simulation-based optimization technique [30]. For each candidate solution U to the problem, the refueling station is evaluated in a number of discrete simulations under the stochastic influences from samples generated from scenarios. When all samples have been evaluated, the performance measures are estimated and the solutions are tuned accordingly. In this study a genetic algorithm (GA) has been used to optimise the

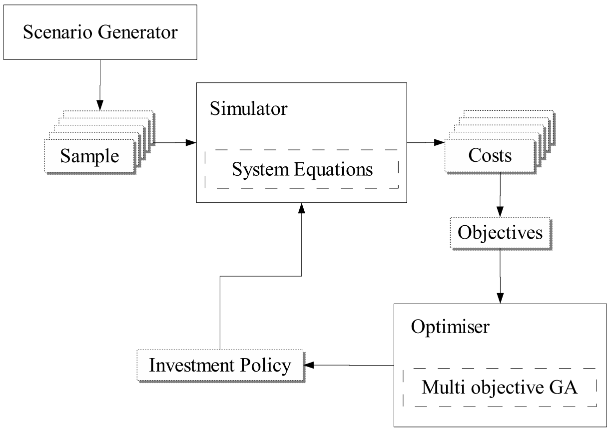

Figure 3: A schematic illustration of the optimization framework.

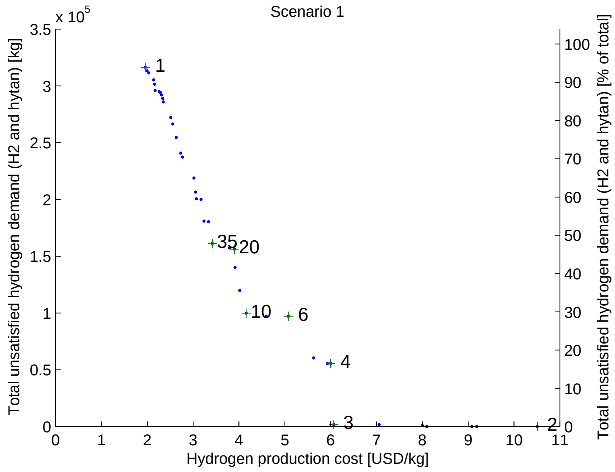

Figure 4: The resulting Pareto-front when optimising U for scenario 1.

solutions. GAs are optimization algorithms inspired by biological evolution. Such algorithms can easily be adapted to a wide range of optimization problems [31], including multi-dimensional problems [32]. The optimization algorithm used in this study is an elitist non-dominated sorting GA, called NSGA-II [33], which uses an explicit diversity-preserving mechanism. For each Pareto-optimal front, this algorithm will remove solutions lying close to each other, while preserving those far from each other. The result is a good spread of solutions along the front. However, the longer the front, the more solutions are needed to get a good picture of the details of the curve. Since each solution corresponds to one individual in the GA, more solutions means a larger population which takes longer time to evolve.

The major parts in the optimization framework is the *scenario generator*, *simulator* and *optimiser*, see Figure 3. The steps of the evaluation are

1. A sequence of samples are generated for each scenario in the scenario generator. The probability distributions used are discussed in Section 2.1.
2. A number of initial individuals (candidate solutions, U) are randomly generated.
3. For each individual (candidate solution, U), the simulator simulates the refueling station (Section 3.3) over the entire investment period. The simulator also contains a control algorithm for proportional control of the amount of hydrogen stored.
4. When all samples for all scenarios have been simulated, the simulator estimates the performance measures and objectives for the individual.
5. When all individuals in the population have been evaluated, the front and objective distance (crowding) sorting is carried out, followed by a generational replacement with crossover and mutation.
6. Steps 3-5 are repeated until convergence.

5 Results

This section presents the results from the optimization for the three scenarios discussed in Section 2.1. For each scenario the optimization has been carried out using the objective function defined in Eq. (11).

5.1 Scenario 1: hythane combustion engine buses

Scenario 1 emphasizes hythane and hydrogen powered buses as an intermediate alternative, after which fuel cell powered cars take over. The hydrogen cost versus total hydrogen unsatisfied demand from both hydrogen and hythane dispenser can be seen in Figure 4, in which several interesting solutions (discussed below) are marked with their respective numbers. It is evident that as the cost decreases, the unsatisfied demand increases and therefore that these objectives are in conflict with each other. The discontinuities represent stepwise increases of capacity to the next available size as defined in Table 4.

As can be seen in Figure 4, Solutions 1 and 2 represent extreme points regarding the two optimization objectives. For Solution 1, the production cost is at a minimum, 1.96 USD/kg. In this strategy, an investment in a small electrolysis equipment is made in year 18. The strategy results in a large amount of unsatisfied demand, 1.4×10^5 kg (87% of the total) and 6.0×10^6 (100% of the total) for hydrogen and hythane, respectively. By contrast, in Solution 2 where the production cost is at its maximum (10.5 USD/kg), investments are made in years 0, 5, and 10. With this strategy, the unsatisfied demand is negligible for both hydrogen and hythane. Furthermore, the strategy exhibits a preference for reformer use in the beginning of the period, and electrolysis towards the end.

Intermediate solutions include number 3, 10 and 35 in Figure 4. These solutions represent extreme points before the next possible equipment size is used. If unsatisfied demand is to be kept at minimum, Solution 3 may be a good alternative. If hydrogen production cost is to be kept low, while still not

Table 5: Investment strategy for solution 3 for scenario 1.

Investment no	1 at year 1	2 at year 11
Reformer	4.2 kg/h	0.0 kg/h
Electrolysis	0.0 kg/h	12.5 kg/h
Compressor	5.0 kg/h	15.0 kg/h
H_2 store	84 kg	147 kg
H_2 dispenser	48 kg/h	48 kg/h
Hythane dispenser	864 kg/h	864 kg/h
Investment cost	1.5×10^6 USD	9.5×10^5 USD
Prio. strategy	Hydrogen	
Total inv. cost	2.4×10^6 USD	
Maint. cost	5.1×10^4 USD	

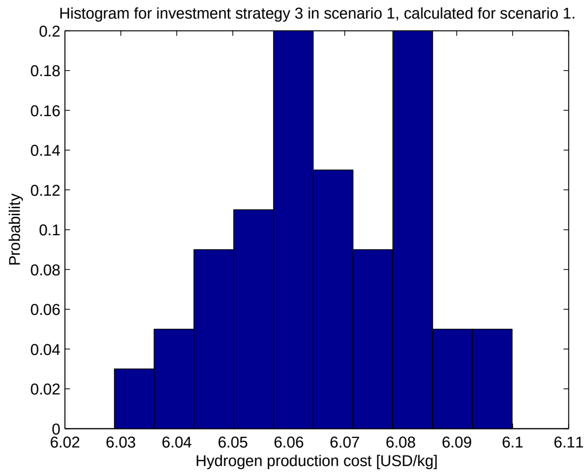

Figure 5: Histogram for hydrogen production cost for solution 3.

allowing a large amount of unsatisfied amount of hydrogen, Solution 10 may be considered. The details of the investment strategy, including the investment cost, can be seen in Table 5.

If the hydrogen production cost is calculated for all samples, a cost distribution is generated. Figure 5 shows a histogram of the cost distribution for solution 3. The distribution shows only a relatively small variance. A calculation of the cost for all solutions indicates a decrease in relative variance (details omitted), i.e. $\mathrm{var}(x)/x$, for lower production cost. Since a high variance indicates a high uncertainty, the variance does not conflict with the hydrogen production cost. This dependence is typical for all scenarios.

In Figure 6, which shows hydrogen versus hythane production cost, a strong non-linear correlation with a minimum for Solution 35 can be noticed. The non-linearity is most evident for the region left of this minimum. These points correspond to solutions to the left of Solution 35 in Figure 4. The lowest hydrogen production cost, represented by Solution 1, utilizes no hythane and is therefore not shown in Figure 6.

Each solution and sample corresponds to one trajectory of the state variable x_{hs}. Given the state variable and the refueling flows X_{hf} and X_{hf}, all other flows can be calculated from Eqs. (7). When these flows are calculated for Solution 3, a good utilisation of equipment is found for most of the 100 samples, and this is verified by the small variance in production cost in Figure 5.

If the optimal solutions for Scenario 1 are calculated using

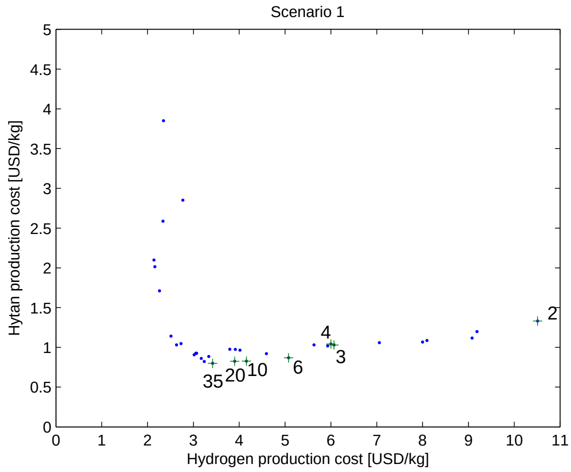

Figure 6: Hydrogen cost versus hythane cost, Scenario 1.

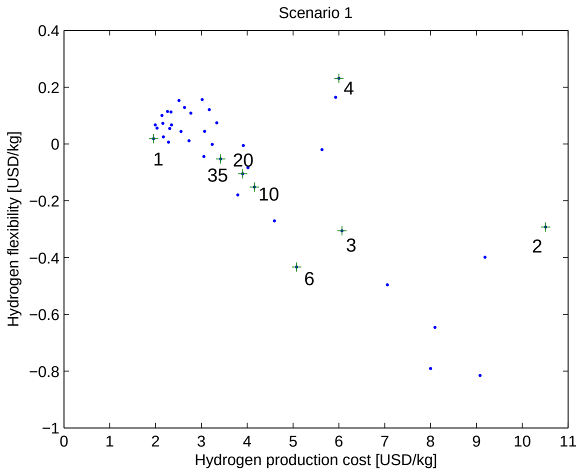

Figure 7: Hydrogen cost versus hydrogen flexibility for Scenario 1.

Scenarios 2 and 3, it is found that hydrogen production cost will most likely increase. The flexibility index in Figure 7 shows that some solutions result in considerably higher hydrogen production cost, e.g. Solution 6, while others do not, e.g. Solution 1. Note that a positive value indicates a lower cost for the passive scenarios and vice versa. The solutions are no longer part of the Pareto-optimal front since they originate from the solution for Scenario 1. However, the original extreme Solutions 1 and 2 will still be the extreme ones.

5.2 Scenario 2: Hydrogen combustion engine cars

The second scenario focuses on hydrogen cars, with primarily combustion engines in the beginning and fuel cells towards the end of the 20-year time period. No hythane is used in this scenario.

In essence, the production cost versus hydrogen unsatisfied demand curve resembles that of Scenario 1. Figure 8 shows that almost zero unsatisfied demand can be maintained down to a production cost of around \$6/kg, below which the amount

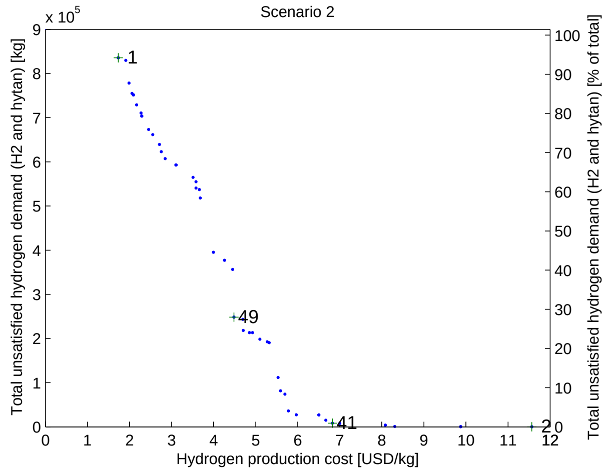

Figure 8: The resulting Pareto-front when optimising U for Scenario 2.

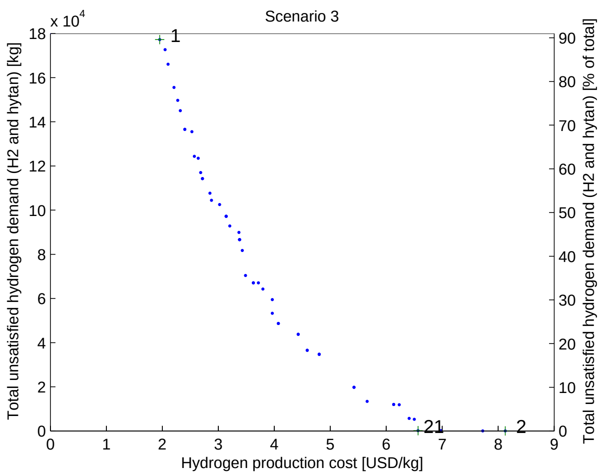

Figure 9: The resulting Pareto-front when optimising U for Scenario 3.

of unsatisfied demand starts to rise.

The flexibility of the solutions for scenario 2 is in general lower than for other solutions, which is evident when the passive Scenarios 1 and 3 are used. The production cost for these passive scenarios is at least double that obtained when the active Scenario 2 is used.

5.3 Scenario 3: Hydrogen fuel cell cars

In the third scenario, hydrogen fuel cell powered scooters are in focus in the beginning, and later fuel cell driven cars. No hythane is used in this scenario.

The production cost versus unsatisfied demand curve in Figure 9 reveals a slightly more expensive production than in the previous cases. This is even more obvious when the solutions for Scenario 3 are applied to Scenario 1 and 2.

6 Discussion and conclusion

In this paper, it has been demonstrated that it is possible to use stochastic optimization in order to find investment strategies for a combined hydrogen and hythane on-site reformer refueling station. The resulting cost of hydrogen and hythane are 2-6 USD/kg and 1-1.5 USD/kg respectively, depending on the preferences concerning unsatisfied demand, flexibility etc.

The results from this study can be used as decision support when planning combined hydrogen and hythane refueling stations. Not only the production cost and unsatisfied demand for the present scenario are important, but also the flexibility of the solution to unforeseen events and developments. In addition, there are other performance measures such as variance and the comparison between hydrogen and hythane that should be taken into account. The selected solution is a matter of preference.

The problem of finding investment strategies involves a considerable amount of information, and therefore aggregate measures have been defined for flexibility.

As observed from the connection between production cost and unsatisfied demand for all scenarios, these two measures are in conflict. One reason for this is the stochastic demand curve which makes it unrealistic to achieve zero unsatisfied demand. This is so since, occasionally, a larger amount of vehicles will come to the station than it can serve, which is probably close to what would be observed in reality. Other reasons for this conflict in measures are the technology development reduction in purchase price (see Eq. (2)) and the discounted costs (see Eq. (3)). Since it is likely that it will be cheaper to build and run the refueling station in the future, the optimization tends to prefer future solutions to present ones. An evenly distributed cost will be discounted to 0.4466 of the original value, so the discount effect is not negligible.

Improvements can be made to the scenario data in Section 2.1. It may be unrealistic having all buses refuelling in the morning. Instead, a slow filling during night time might be considered. Also the 24-hour car refueling curve, which assumes a constant filling frequency throughout the day, may be adjusted to a more realistic setting.

A key to successful investment planning is the minimization of the uncertainty of future developments. For this reason, three different future scenarios, with 100 samples each, have been used. Within each scenario the uncertainties are kept at minimum given the strategic parameters, by taking all samples into account. The strategic parameters can easily be changed for other cases. For each solution, the effects are easy to quantify should another scenario become reality. However, the S-curve (Eq. (1)) has still been used for estimating the (uncertain) number of produced units. These numbers are taken in a global perspective, which may make them less sensitive.

In this study, linear scaling of equipment cost to usage time is used. Another option, often used in the literature [26], would be to use salvage value or terminal cost. Given that the salvage value can be defined arbitrarily, these two approaches can be considered identical.

In the optimisations presented here, the investment strategy is set prior to the calculations. Another option would be to define control policies that use system information for decisions, i.e. a fully closed-loop. Such a strategy would be able to incorporate not only investments but also a quantitative demand satisfaction calculation. At present, the only real feedback loop has been implemented for the hydrogen storage level.

An increase in the number of solutions will give better resolution for the Pareto curve. On the other hand, a larger population will be needed in the GA, which in turn will increase the calculation time. At present, simulation of one scenario sample takes about 0.25 s, giving a total of 75 s per individual and hence 1 h 40 min. for a population of 80 individuals. By aggregating calculated measures and coding more of the algorithm in a low-level language, the simulation time can probably be shortened considerably. If this is done, the resolution can be enhanced.

It should also be noted that, as for all heuristic methods, convergence cannot be guaranteed. Instead, one has to settle for a solution which is good enough and preferably better than any other known solution.

To conclude, it has been found that it is possible to optimise the hydrogen production cost for a combined hydrogen and hythane refueling station, and that the resulting costs lies between 2-6 USD/kg for hydrogen and 1-1.5 USD/kg for hythane. The production cost and the amount of unsatisfied demand constitute conflicting objectives so that, for example, if the total hydrogen and hythane demand is to be satisfied, the production cost of hydrogen will be unrealistically high. However, an intermediate realistic solution can be found along the curve of cost versus unsatisfied demand. In all cases, the lowest production cost for hydrogen and hythane is achieved by satisfying the hydrogen demand first and then the hythane demand.

Acknowledgments

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