THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

MODELLING AND CALCULATION TECHNIQUES FOR ENVIRONMENTAL SYSTEMS

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Abstract

The work presented in this thesis shows how theories from different scientific areas can be successfully applied in the environmental field. The work is divided into two areas: Enhancement of modelling and calculation of LCA-like systems and optimal investment planning for environmentally favourable, but expensive production facilities.

Life Cycle Analysis (LCA) has a lot in common with technical system analysis. In this study similarities and differences between LCA and technical system theory are investigated, followed by suggestions for improvements. As part of an LCA a model of the technical system is built. This model is used for normalisation in accordance with the functional unit. The model is not, however, flexible in terms of the type of calculation it supports. It is found that a computational non-causal representation makes it possible to separate model and problem formulation. One model can then be used for several different types of calculations. The theory is illustrated in the case of cement production where a computational a-causal and object-oriented model is built of a production line for cement. The model can easily be tuned for a specific production site. Not only the usual flow of matter is included, but also monetary units. Some different types of calculations are carried out to show the usability of the concept.

Changes toward more environmentally friendly solutions frequently incorporate large investments in the infrastructure. The cost and uncertainty of changing these facilities are usually considered to be obstacles for the introduction of the new technique. In this study methods for finding optimal investment strategies for such production facilities are investigated. Based on an assumed future development scenario, optimal investment strategies are calculated. The usability of the developed method is exemplified in a study on profitable investment strategies for a hydrogen refuelling station. Taking special considerations like periodic maintenance need into account, optimal control is used to concurrently find a short term equipment variable utilization for one week and a long term strategy. The solution is the minimum hydrogen production cost for the individual gas station. The solution is sensitive to variations in the scenario parameters.

Keywords: LCI modelling, Non-causal modelling, Optimal investment strategies, Hydrogen infrastructure.

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Contents

APPENDED PAPERS

List of publications

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

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

II. 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.

III. Peter Forsberg and Magnus Karlström, On optimal investment strategies for a hydrogen filling station, Submitted to *International Journal of Hydrogen Energy*.

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

IV. 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.

V. 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.

VI. 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.

VII. 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.

Nomenclature

Flow semantics	The connection and use of the general variables intensity and flow.
Functional unit	A reference to which the inputs and outputs of a product systems is related as part of the normalisation.
LCA	Life Cycle Assessment. A systematic method to assess the environmental impact of a product or function produced.
LCI	Life Cycle Inventory. The building of a model of the technical production system as a part of the Life Cycle Assessment. Also includes normalisation of resource use, emissions and waste to the functional unit.
Normalisation	Relating the flows in a product system to the functional unit.
Reference flow	Measure of the needed outputs from processes in a given product system required to fulfil the function expressed by the functional unit.
Unit process	The smallest part of product system for which data is collected when undertaking a LCA.

Tables 1 and 2 show the symbolic conventions and scenario parameters used in the sequel. The letter c, p, x or f indicate the type, which may be further specified using sub and super-scripts. The symbol $c_{hr,w}$ is then interpreted as the weekly capacity of the hydrogen reformer.

Table 1: Symbolic conventions

Type	Name	Description	Unit
Variables, constants	c	Capacity	kg, kg/h
	cn	Nominal capacity	kg, kg/h
	s	Size	kg, kg/h
	p	Purchase price	SEK
	pn	Nominal purchase cost	SEK
	x	Flow vector	kg/h
	f	Factor	-
Subscripts	hr	Hydrogen reformer	
	hs	Hydrogen storage	
	hc	Hydrogen compressor	
	fp	Hydrogen refueling pump	
	hf	Hydrogen refueling	
	fc	Hydrogen fuel cell	
	he	Hydrogen electrolysis	
	eq	Equipment, any part	
	d	Daily, per day	
	w	Weekly, per week	
	ng	Natural gas	
	h_2	Hydrogen	
	el	Electricity	
	inv	Investment	
	m	Maintenance	
Superscripts	i	Input flow	
	o	Output flow	

Table 2: Scenario parameters

Name	Description	Value	Unit
d	Real rate of interest	0.05	1/yr
$V(t)$	Number of vehicles at time t	-	-
V_{tot}	Total nr of vehicles at t_{end}	-	-
b	S-curve slope	0.3	-
t_{ifx}	Inflection point of the S-curve	10	-
P_n	Cost of manufacturing n^{th} unit	-	SEK
P_1	Cost of manufacturing 1^{th} unit	-	SEK
V_n	Cumulative production at n^{th} unit	-	-
R_{pr}	Progress ratio factor	-	-
Hf_m	Mean hydrogen consumption	1000	kg/day
H_{rpd}	Ratio peak-demand to average	1.12	-
H_f	Hydrogen refueling	-	kg/h
f_{cont}	Contingency cost factor	0.1	-
f_{eng}	Engineering permitting cost factor	0.1	-
f_{gen}	Include land cost factor	0.2	-
c_f	Vehicle filling capacity	4	kg/filling
p_{ng}	Natural gas price[7]	3.6	SEK/kg
p_{el}	Electricity price vector	0.3(22-06),0.6(06-22)	SEK/kWh

Chapter 1

Introduction

The environmental awareness in today's society is constantly increasing the requirements of a cleaner production. The requirements may be enforced by law, public opinion or as a concious act by the production company to make a product more appealing to the consumers. At the same time the increasing complexity of the production systems make the environmental analysis harder to perform. Technical analysis of environmental systems is a rather new discipline of science. It is still in the phase of developing new applications and exploring new connections to already existing disciplines. In the 90's more advanced methods were developed to assist environmental analysis of technical systems. One of the methods is Life Cycle Assessment (LCA). In LCA a flow model over the technical production system is made, taking the relevant resources, emissions and product(s) into account. Flows are scaled to give resource use and emission released for one unit produced. Much has been written about LCA. The ISO standards 14040-42 [1] give very general guidelines on how an LCA should be performed. Other texts, e.g. [12, 34, 26, 22, 52, 20], are also very general and does not discuss details on the mathematical treatment. Until 1998 only one text [29] was published giving guidelines on how to perform the actual calculation, the so called normalisation. From 1998 until now a number of articles [31, 30] and one book[32] have dealt with the subject of normalisation in LCA from a mathematical point of view. All of these mathematical methods only consider the state-of-the-art LCA which include a linear and static model representation. For other types of calculations there are only a limited number of texts available. Examples include linear optimisation of LCA systems [8, 55], multi-objective optimization [9] and dynamic LCI modelling [16, 48]. Some cases with integration of economic costs have also been seen [43, 47]. There is still, however, a large potential for improvements in e.g. flexibility of the models. This thesis investigates some applicable techniques, how they can be used and possible improvements. The findings are exemplified on a cement production case [23].

Another method that may be used for technical environmental analysis is investment planning for environmentally good but expensive production facilities. Within economics investment planning is a common topic and some of which make use of optimal control theory [46, 18, 21, 45, 10]. Publications in the area generally analyse return on capital funds and does not, however, address the case of investments in production machinery. This thesis investigates a method for investment planning which can take considerations like periodic maintenance into account. The method make use of optimal control to simultaneously find a short term equipment variable utilization for one week and a long term strategy for the whole investment period. The method is exemplified on hydrogen dispensing infrastructure, which is a major obstacle for the introduction of hydrogen vehicles [37]. Recent studies have been made regarding economical feasibility of hydrogen in regard to the infrastructure needed to be built [4, 5, 2, 44, 38, 51, 50]. None of these studies investigates the implications of investments over time.

1.1 Main contributions

The main contributions of the presented work is summarised below.

- A thorough comparison between LCI and technical system analysis.
- A modelling approach for LCA or LCA-like environmental systems comprising separation of model and problem formulation leading to a more flexible model.
- A method to make concurrent optimisation of investments and run-pattern for lowest production cost.

1.2 Outline of thesis

In Chapter 2 the general purpose and goals of the project is stated. Chapter 3 explains what LCA is and how calculations within LCI are made. It also gives some background on techniques used to improve the capability of these calculations. Chapter 4 starts with an introduction to optimisation and optimal control, which is then used to solve investment planning problems. Chapter 5 gives concluding remarks and suggestions for improvements in further work. Chapter 6 summarises indicated publications made during the project. The first one is a report to draw parallels between LCI modelling & calculation and general technical systems analysis like control theory. The second paper apply the previous findings on a cement production process. The third paper apply the method for investment planning on a hydrogen infrastructure case.

Chapter 2

Purpose and goals

2.1 Purpose

The intentions of this project is to provide practical and functional results that can be used to expand the application area of LCA or LCA-like systems. A mathematically and logically correct structure will make analyses more efficient and decrease the risk of making mistakes. Contributions from the project would be the theoretical basis and practical means for solving problems as exemplified in the following:

- A wider range of problems may be solved using LCA, or LCA-like methods. Examples include dynamic modelling of time-dependant processes such as start-up or shut-down of production processes and optimisation of production networks with long time constants. Another example of a non-linear, time-dependant process that has environmental consequences is the introduction of a new product or a new technology in the market. Such consequences may not be modelled using present LCA-methodology in which neither production volume nor time are variables.

- Existing problems may be solved in a better way. It is sometimes claimed that LCA is used to optimise the life cycle of a product. However, no true optimisation is made. Instead the available tool (present, non-optimising LCA-methodology) is used for comparison between alternatives. Optimisation may of course be done using different objectives, e.g. specific inventory parameters such as energy use or carbon dioxide emissions; or if cost is introduced as a parameter in the analysis, optimisation may be conducted with respect to the ratio between environmental impact and cost. Another example of an existing problem that may be solved in a better way is allocation in open loop recycling of metals. Long-lived products often contain metals.

On the same time the market for many metals expand. Time is clearly a relevant factor here, yet this problem is presently approached using static calculations.

- Increased correctness. The simplifications made in present LCI methodology (e.g. disregarding time and non-linearities) are sometimes justified and sometimes not. Since there is very few choice at present, these simplifications are always made whether justified or not. With calculation methods that allow for time and non-linear relationships, there will be a real choice whether to simplify or not, and thus the resemblance between reality and model may increase.

2.2 Goals

The project goal is to categorise and formulate theoretically based, mathematically expressed calculation methods for LCI supporting more advanced calculations than normalisation. As part thereof, the project goal is to mathematically formulate and solve optimisation problems of dynamic LCA and LCA-like systems. This work intends to develop a methodology to calculate also the cost of the transitions between states. For this purpose the theory of optimal control will be used. Specifically the goal is to develop a methodology to calculate transitions of systems from one present state to another optimal future state from an environmental and economical perspective.

In detail, the goals of the research project are to:

- describe relevant available methods from related engineering, mathematical and system theoretical areas.
- develop new modelling approaches and calculation methods.
- employ mathematical and logical methods to verify the correctness of calculations and simulations.
- formulate the dynamic optimisation problem mathematically.
- investigate the possibility to solve the dynamic optimisation problem or, alternatively possible simplifications which leads to simplified problems which can be solved.
- investigate how sensitive the solution is to changes in the assumptions.
- test the methodology in order to show its usability within on-going, applied LCA projects.

Chapter 3

Modelling of technical environmental systems

This chapter focus on the question how models of LCA like systems can be done more flexible. It starts with an overview of LCA from a system technical perspective. Then some modelling techniques applicable to the LCA technical system description are discussed, after which these techniques are applied to a cement manufacturing production problem.

3.1 Life Cycle Assessment

Life Cycle Assessment (LCA) is a method to evaluate the environmental impact of a product or function over its entire life. The life cycle usually starts with extraction of raw material and continues with transportation, manufacturing, use and possibly re-use. It then ends with waste management, recycling and disposal, see fig. 3.1. There exists a vast literature on the concept of LCA, see e.g. [20, 26, 29, 40, 25, 19, 33].

In 1997 the ISO standard 14040 on Life Cycle Assessment was approved [1]. In this standard LCA is defined as '...the environmental aspects and potential impact throughout a product's life (i.e. crade-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 implication of the production to nature, see fig. 3.2.

The ISO 14040 standard further gives directions on relevant phases in an LCA, see fig. 3.3. These phases are:

- Goal and scope definition. This is a definition of the product or service to be assessed, a functional unit for comparison and the boundaries of the study.

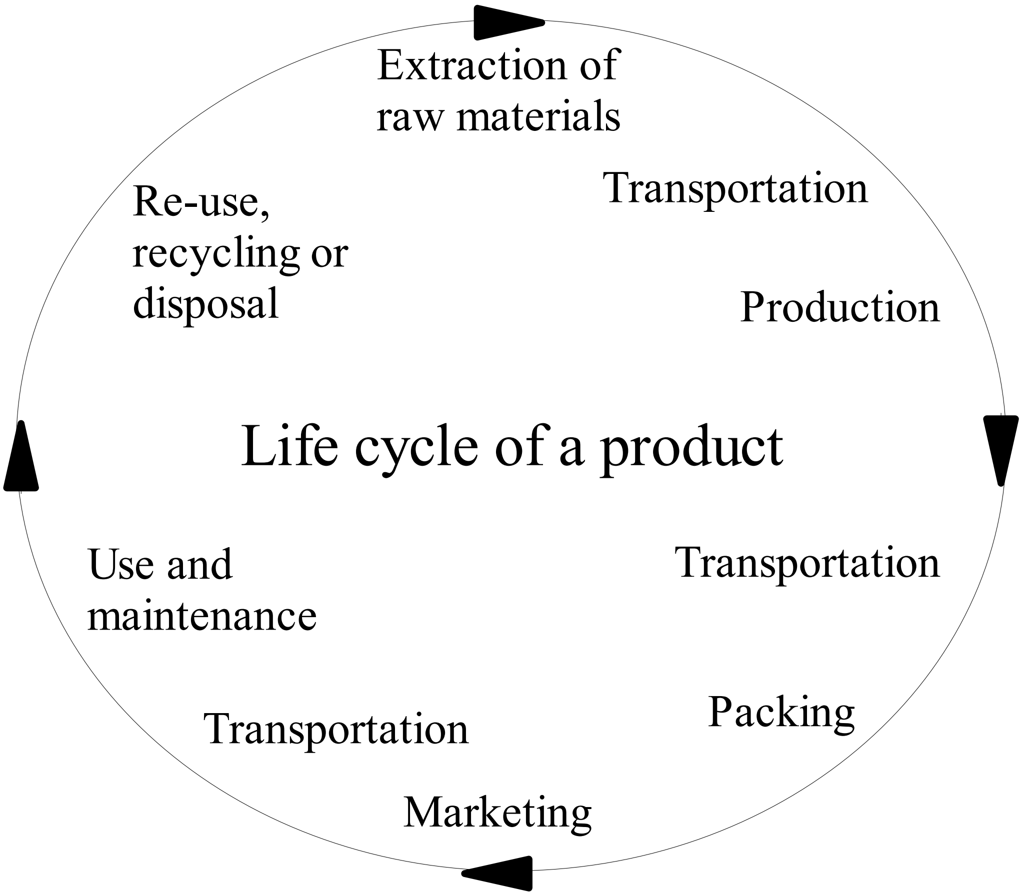

Figure 3.1: The life cycle of products.

It also states why the study is carried out and for whom.

- Inventory analysis (LCI). In this phase the required resource use, emissions released and waste are identified and quantified. Resources include e.g. extractions of raw material, energy carriers and different types of land use. Then this information is gathered in a process flow chart and related to the functional unit from the goal and scope definition.

- Impact assessment. The findings from the inventory analysis are grouped and quantified into a limited number of impact categories. These categories may be further weighted into a single number.

- Interpretation. A report is written on the cumulative results of the study. The report also contains needs and possibilities to reduce the environmental impact.

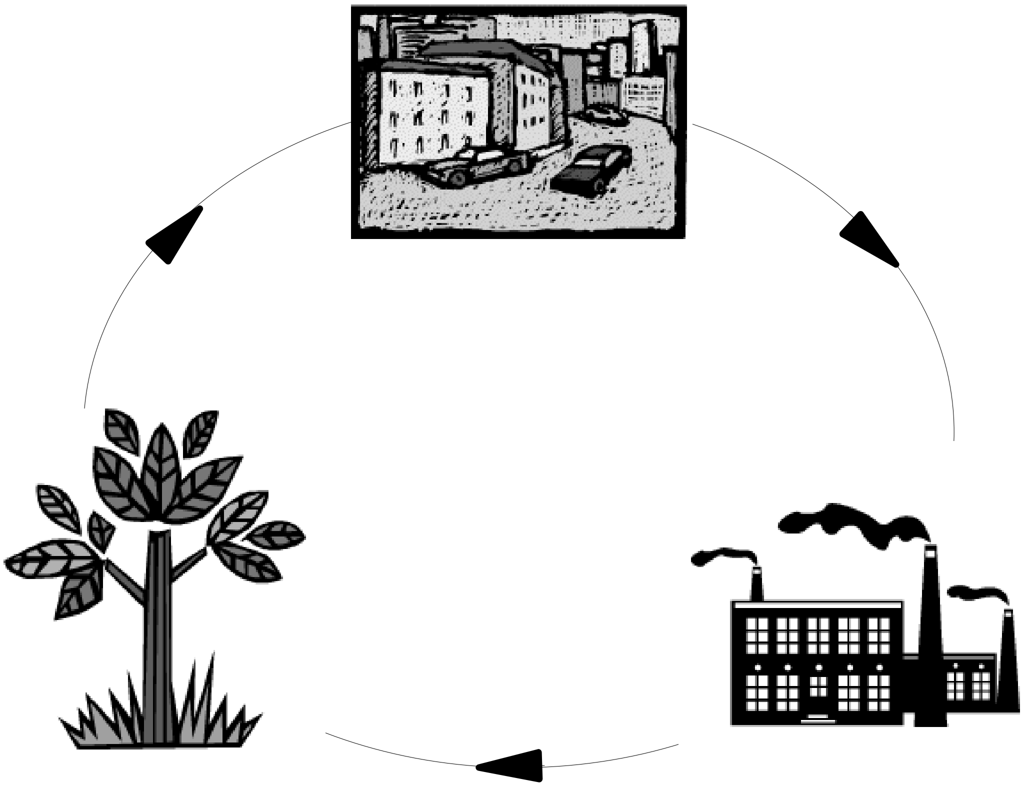

Figure 3.2: The three spheres to consider in an LCA: the social, the technical and the environmental. In the society a demand for a product or service is created. This product is then produced in a factory, which inevitably consumes resources and produce emissions. The emissions ends up in the nature, which we all are part of, hence affecting the society.

As part of the inventory analysis the resources and emissions from the developed flow model of the production system need to be related to the functional unit. This is done by aggregating all unit processes in the product system and scaling the flows of these unit process to match the reference flow of the system. The data used in the inventory is based on time averaged statistics and hence is independent of time. In addition a linear relation between resource use, emissions and production is assumed. The result is that this normalisation step can be mathematically regarded as solving a linear equation system. The equation system is usually well posed, i.e. having equal number of variables and constraints, and hence possible to be solved exactly. Publications on LCA cover handbooks, case studies and theoretical studies on the concept, which do not give any directions on how to rep-

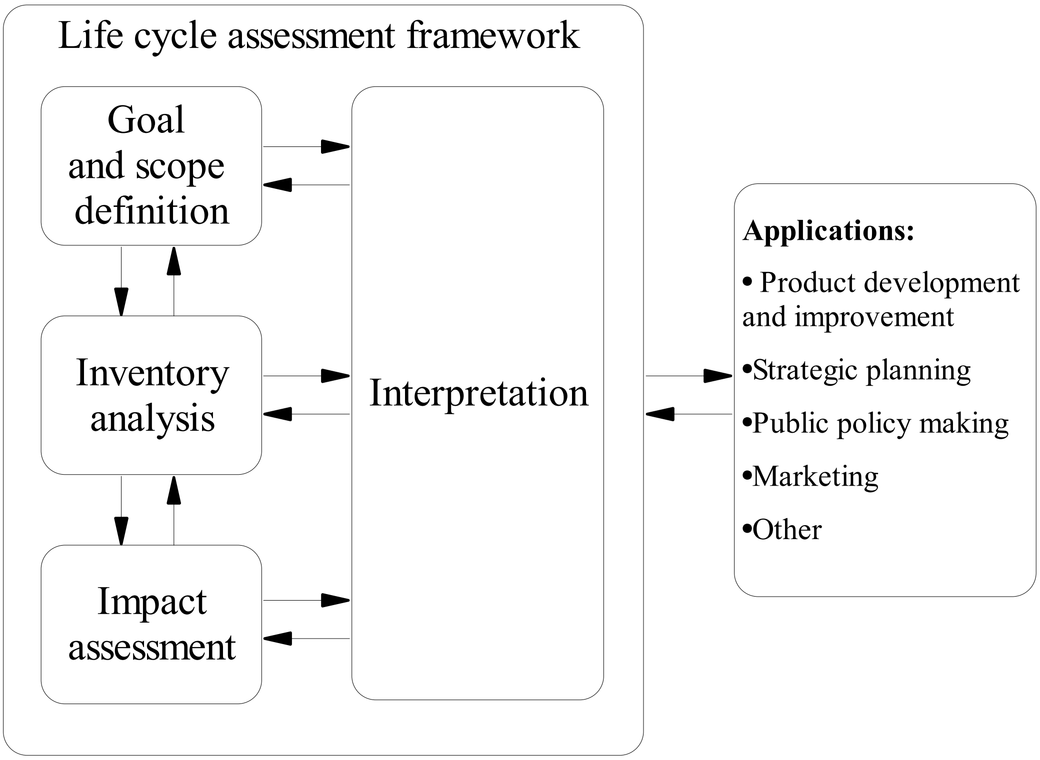

Figure 3.3: The main phases of life cycle assessment according to ISO 14040 [1].

resent the flow model and form the resulting equation system. Recently a rather small number of publications on the computational part have been published, see e.g. [28, 27, 30, 32]. The result of the normalisation to the functional unit in these publications is expressed as

$$g = BA^{-1}f, \tag{3.1}$$

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

When LCI models needs to be stored it is necessary to take both structure and meta data into account. Some examples of published data structures for LCI-data are SPOLD [49], SPINE [15] and ISO/DTS 14048 [3]. None of these make use of the matrix representation discussed above. These data structures can be used to develop e.g. databases for storage, sorting and retrieval of LCI information in a non-redundant way.

3.2 Modelling techniques

This section describes techniques that can be applied to enhance the flexibility of LCI-models. In the next section these techniques are applied to a cement manufacturing case.

When a state-of-the-art LCA is carried out, the linear technology matrix model (A) described in the previous section is sufficient to describe the technical production system. The reason why this matrix is sufficient is not only the linear nature of the created system model, but also that only one type of calculation is made in an LCA, which is the normalisation to the functional unit. The developed mathematical LCI methods are designed to achieve this normalisation only, which affects both system model and calculation. At times it is desirable to make extensions to this matrix type of LCI model. One such occasion is when the inherent physical behaviour of the production system is strongly non-linear seen as a function from resources/emissions to product. A linear LCI model represent in this case a linearisation around a specified point and might lead to unacceptable large deviations in the calculated resource use and emissions released. Another occasion is when dynamic aspects are relevant and hence need to be taken into consideration. One such example is when starting up and closing down a production line for e.g. maintenance is considered. These requirements taken together means that another type of modelling approach is needed. In addition there are other types of calculations that need to be done. Examples include optimisation, simulation over time and other, not yet defined calculations. To be able to fulfil the requirements on calculations, flexibility in the type of problem applicable is needed. It is clear that e.g. a state-space model does not fulfil these requirements.

An important consideration is the amount of knowledge we have about the underlying system, which can be a limiting factor. The extension of the usual LCI modelling approach into a non-linear and dynamic one would require a larger amount and more accurate data.

In paper I and II the nature and effect of some types of causality are discussed. To recapitulate, it was found that by removing the computational causality from the model advantages in flexibility can be achieved. The result is a so called a-causal or non-causal model. In effect, the entity that is normally regarded as the model can be split 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 production system 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 hold constant during this particular calculation and a value to designate each of them.

- A method of calculation. Can also 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 the 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 picture of reality.

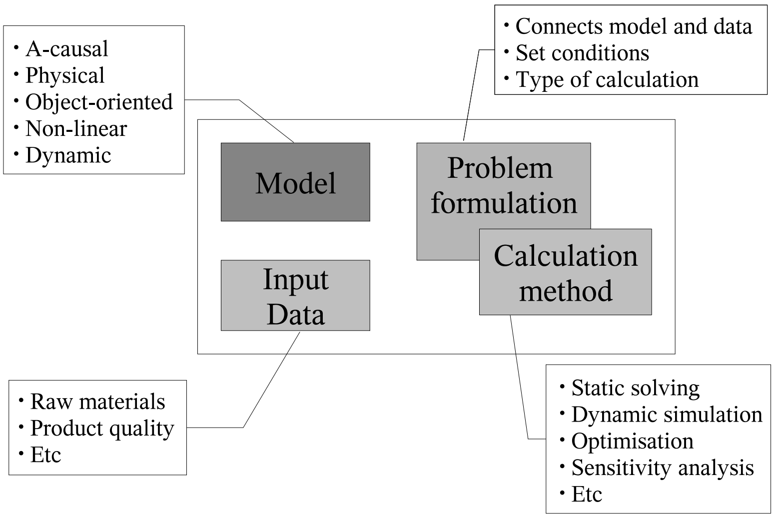

Figure 3.4: The separation of model and problem formulation that can be achieved by the use of a-causal models.

To summarise we have the following requirements:

- A computational a-causal model that contain the structure and constants of the system, but does not contain any information on how to calculate.

- An object oriented modelling language that makes use of inheritance and encapsulation.
- A physical property modelling approach that makes it possible to map the real physical structure to a similar model structure.

However, there are drawbacks with using an a-causal model. Any mathematical model consist of a number of equations. In the computational causal case, e.g. block diagrams and state-space models, these equations are ordered in a specific way to achieve the wanted result. In the computational a-causal 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, which is in general harder to understand. For models based on flow semantics, i.e. correlation between the general variables intensity and flow, the model representation can be based on energy and power flow and is usually relatively easy to do. For the type of flow models used in LCI there are also physical laws applicable, but not in the form of intensity-flow related connections. Under these circumstances a-causal models can be structured in various ways depending on the application, and therefore it is hard to make both consistent and general enough to become flexible.

3.3 The cement production problem

The above discussed enhancements to general LCI models were applied in a test case for a cement production line. The conceptual model consists of a foreground system which defines the at-site production that the company has full control over, and a background system comprising bought services and goods, see fig. 3.5. A more in-depth discussion of the production facility is given in paper II and [23].

The raw materials, i.e. different sorts of sand, are transported to the production site and grinded depending on type. They are then mixed in relevant proportions and burnt to clinker in an Clinker Production System which is in fact a burner. For the burning process fuel is required. The fuel may consist of coal, pet coke or an alternative fuel. All fuels are transported to the site, grinded and mixed in proportions before entering the burner. The produced clinker is then mixed with gypsum and possibly other materials, further grinded 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 tab. 3.1. In addition the approximate monetary costs throughout the production line are to be calculated. Since purchase costs of the raw materials and fuels are known, the production related cost for each equipment in the line can be estimated and added to the product flow. The use of the model is to aid

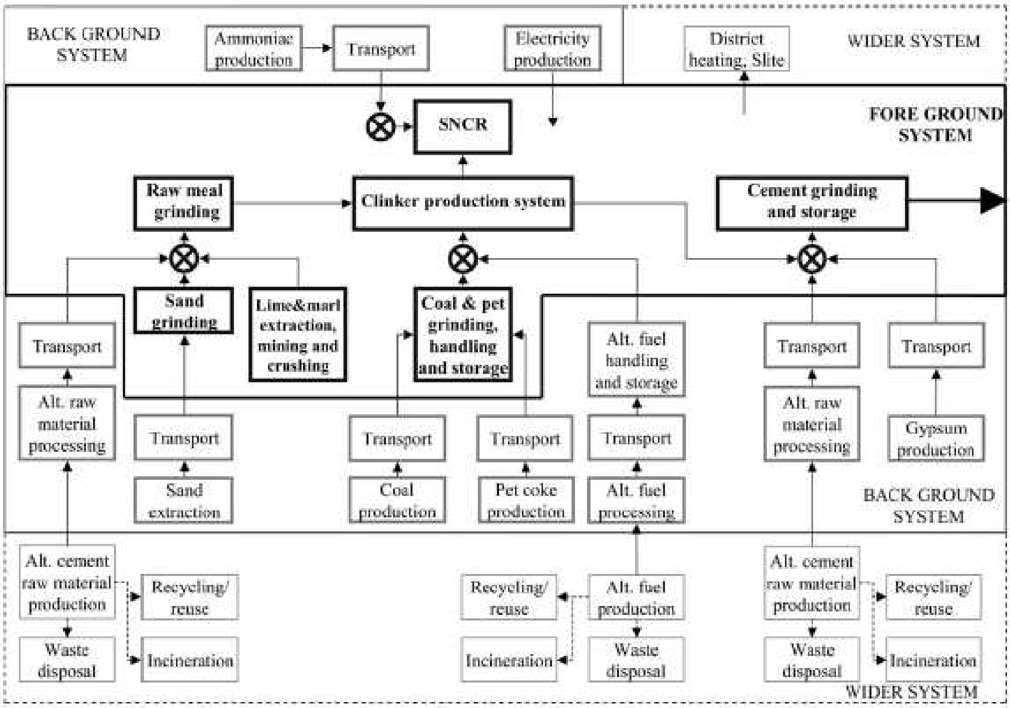

Figure 3.5: The cement production line layout.

in calculations for new types of raw materials, fuels and internal settings and also possible layouts. In addition to static solving, dynamic simulation and optimisation can also be considered. It is therefore a requirement that the model is modular and highly flexible.

Table 3.1: Cement product quality indicators. The notation indicate 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	$AR = \frac{Al_2O_3}{Fe_2O_3}$

At the time of research for the project (fall 1999), only a limited number of modelling languages and calculation software were available and able to fulfil the requirements. Among them there were OmSim (Omola) [42], Dymola (MODELICA) [14] and Ascend [54]. OmSim and Dymola are specially made for modelling of physical system 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 is originally developed for application in chemistry. However, it can be best 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 that it was decided to be used.

The model was built in a bottom-up manner according to paper II. It should be noted that the model is deliberately made redundant. In most cases redundancy is negative, 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 when the model is built and then remain.
- Locked variables. Parameters set to a numerical value throughout a certain calculation in accordance to input data.
- Free variables. Parameters that will be calculated. Some of these are internal variables in the model and others are the ones we want to calculate, i.e. the output.

The number of parameters in each category depends on the specific calculation done. Information on these settings is part of the problem formulation. In the model, information to specify 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 any time, only one of the the ways to specify the parameter is used and the other is redundant. However, it does add to the flexibility to both define variables before calculation and check the result afterwards.

It should also be noted that the entire model on the cement production line was later transferred to MODELICA, which was a much more intricate task than the work described above.

Chapter 4

Investment optimisation techniques

This chapter starts with an overview of unconstrained and constrained non-linear optimisation [41, 36], which will be used in the investment techniques developed later. Then the optimisation is applied to dynamic systems, which leads to a discussion on *Optimal Control* [11, 6]. These two sections are a recapitulation of present technique and may be skipped by initiated readers. Concentrating on investment planning, the optimisation criterion function is next developed in a more general sense than that in paper III. Then some special difficulties which were omitted in paper III regarding the hydrogen infrastructure investment problem are discussed.

4.1 Non-linear optimisation

The general non-linear programming (NLP) problem is to minimise a non-linear functional subject to non-linear constraints[17]. The problem can be defined mathematically

$$\begin{aligned} \min_{x \in \Re^N} \quad & f(x) \\ \text{s.t. } c(x) \quad &= \quad 0 \\ d(x) \quad &\geq \quad 0 \end{aligned} \tag{4.1}$$

where $f(x)$ is the (scalar) criterion function, $c(x)$ the non-linear equality constraints and $d(x)$ the non-linear inequality constraints. The functions $f(x)$, $c(x)$ and $d(x)$ are supposed to be smooth, i.e. at least twice-continuously differentiable. Let $g(x) = \nabla_x f(x)$, being the gradient vector of the objective function $f(x)$, $C(x) = \frac{\partial c}{\partial x}$, being the Jacobian matrix of the constraint vector $c(x)$ and $D(x) = \frac{\partial d}{\partial x}$, the Jacobian matrix of the constraint vector $d(x)$. Now define the

Lagrangian in the classical way

$$\mathcal{L}(x,\lambda) = f(x) - \lambda^T c(x) - \mu^T d(x), \tag{4.2}$$

where λ and μ are Lagrange multiplier vectors. In order to define a local optimal point the first derivative of the Lagrangian with respect to x must be zero, i.e

$$\nabla_x \mathcal{L}(x^*,\lambda^*,\mu^*) = g(x^*) - \lambda^{*T} C(x^*) - \mu^{*T} D(x^*) \;\; = \;\; 0 \tag{4.3}$$

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

$$\begin{array}{rcl} g(x^*) - \lambda^{*T} C(x^*) - \mu^{*T} D(x^*) & = & 0 \\ \mu^{*T} d(x^*) & = & 0 \\ \mu^* & \geq & 0 \end{array} \tag{4.4}$$

and μ is sometimes referred to as the KKT multiplier. In addition the original constraints (4.1), $c(x^*) = 0$ and $d(x^*) \leq 0$ must be satisfied at the optimal point.

In order to solve the KKT for x^*, the active inequality constraints are treated as equality constraints and the inactive ones are ignored, giving

$$\begin{array}{rcl} g(x^*) - \eta^{*T} J(x^*) & = & 0 \\ r(x^*) & = & 0 \\ \eta & \geq & 0, \end{array} \tag{4.5}$$

where $r \in \left\{ x \in \Re^N | c(x) = 0, d_i(x) = 0 \,\forall\, i \in \mathcal{A} \right\}$ and $J(x) = \partial r / \partial x$. Now these re-defined requirements can be solved with Newton's method by doing a Tailor series expansion of (4.5). If $H_L = \nabla^2_{xx}\mathcal{L}$ the expansion becomes

$$\begin{array}{rcl} g(x) - J^T(x)\eta + H_L(x)(\bar{x} - x) - J^T(x)(\bar{\eta} - \eta) & = & 0 \\ r(x) + J(x)(\bar{x} - x) & = & 0 \end{array} \tag{4.6}$$

(4.7)

which can be simplified to

$$\begin{bmatrix} H_L & J^T \\ J & 0 \end{bmatrix} \begin{bmatrix} -p \\ \bar{\eta} \end{bmatrix} = \begin{bmatrix} g \\ r \end{bmatrix} \tag{4.8}$$

where p is the search direction for the step $\bar{x} = x+p$ and $\bar{\eta}$ the Lagrange multiplier at the new point. The equation (4.8) represents the first order optimality conditions for the the optimisation problem

$$\begin{aligned} \min_p \; & g^T p + \frac{1}{2} p^T H_L p \\ \text{s.t. } & Jp = -r, \end{aligned} \tag{4.9}$$

which is a Quadratic Programming (QP) problem.

A widely used algorithm to solve NLP problems is the Sequential Quadratic Programming (SQP), see e.g. [41], [36] or [35]. The SQP is a sequential algorithm that make use of inner and outer iterations. The objective of the inner iteration is to find a search direction p which is used in the outer one to fulfil the first order conditions for optimality. The search direction p is found solving the optimisation problem (4.9). The outer iteration makes use of the the new search direction by taking the step $\bar{x} = x + \alpha p$, where the step magnitude α is determined by a line search method.

In this thesis the optimisation problem is solved with the NPSOL program [24], which is of the above SQP class. First the NPSOL algorithm aims at calculating a point that is feasible, starting from the user initiated point. Then the SQP algorithm described above is used to find the optimal point.

Calculating gradients in the investment problem is not easy. One reason is the objective function $f(x)$ not being differentiable in the whole $\Re^N$. Another reason is the complex structure of summations in $f(x)$. Using NPSOL, no algebraic expressions on 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 away from the solution. The SQL algorithm described above works satisfactory with convex problems. Given such a problem, the solution will be the global optimal point. Since the investment problem is convex (is shown in paper III), we expect the algorithm to find the global optimal point. The objective function and the optimisation problem will be treated in more detail in sec. 4.3 in sec. 4.4 respectively.

4.2 Optimal control

Optimal control theory aims at optimising a given objective function under the constraints of a dynamic system [11, 53, 39]. Common objective functions include energy, fuel and time. The dynamic system can be mechanical, electrical or any type that can be described mathematically. The optimal control problem can be stated generally as

$$\begin{aligned} \min_{u(t)} J &= \Phi(x(t_f)) + \int_{t_0}^{t_f} L(x(t), u(t), t)dt \\ \text{s.t. } \dot{y} &= f(x, u, t) \\ c(x, u, t) &\leq 0 \end{aligned} \tag{4.10}$$

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

$$\begin{aligned} x_l \leq x \leq x_u \\ u_l \leq u \leq u_u. \end{aligned} \tag{4.11}$$

Usually in a optimal control problem one knows the initial state and time, i.e. where to start. The final time t_f and final state $x(t_f)$ can either be prescribed or calculated. The final state can either be given directly or defined to lie on a constraint surface.

The above optimal control problem may be solved using a direct or indirect method[6]. A direct method use 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 sec. 4.1. A indirect method aims at fulfilling the necessary conditions for an optimum according to variational calculus, i.e. the first order condition $J'(x) = 0$, the Euler-Lagrange equations and the adjoint equations. Finding these expressions means calculation of gradients and Hessians, which usually is cumbersome. In addition the indirect method is sensitive to the starting point, i.e. the first estimate. A poor starting point may result in divergence or wild trajectories. The rest of this section will therefore address the direct method.

The integral in the objective function (4.10) can be treated as an additional state $\dot{y}_{n+1} = L(x, u, t)$ with the initial condition $y_{n+1}(t_0) = 0$. It is thus possible to replace the original objective function with one of the type $J = \Phi(x(t_f))$.

Suppose the interval t_0 to t_f is divided into n_s segments and h_k is the time of one segment. Further let $M = n_s + 1$ be the number of point in the interval. The state equations can then be approximated with any numerical integration method, i.e. Euler, Trapetzoid and Runge-Kutta. The theory is here illustrated for the simplest case using the Euler method $\zeta_k = y_{k+1} - y_k - h_k f_k$, which give the NLP problem

$$\begin{aligned} \min_{(u_1, y_1, \ldots u_M, y_M)} J = \Phi(x_M) & & \\ (\zeta_1, \zeta_2, \ldots, \zeta_{M-1}) &= 0 \\ (c_1(x_1, u_1, t_1), c_2(x_2, u_2, t_2), \ldots, c_M(x_M, u_M, t_M)) &\leq 0. \end{aligned} \tag{4.12}$$

This optimisation problem is of the static NLP type and can be solved with the techniques discussed in the previous section. The problem does, on the other hand, have $(1 + n)M$ times more variables than the original dynamic Optimal Control problem. In the case of long interval $t_f - t_0$ and short time constants, the resulting static problem will become hard to solve.

4.3 Production cost

In this section the cost for production is considered. This production cost will later be used as objective function in the optimisation done for the hydrogen refuelling station in sec. 4.4.

The cost we will consider when making investments in equipment or parts of a factory is the total production cost per produced unit or as in the case considered in sec. 4.4, per kg H_2. This production cost will change according to the utilisation of the equipment. It is therefore helpful to calculate a mean production cost over the entire investment period.

First, it is assumed that a loan is taken for the purchase of equipment. This loan is also assumed to be of the annuity type, i.e. giving the yearly instalment

$$p_{eq,yr} = p_{eq}\ anf(d, l_{eq}),\ anf(d, l_{eq}) = \frac{d}{(1 - \frac{1}{(1+d)^{l_{eq}}})}, \tag{4.13}$$

where p_{eq} is the purchase price for one piece of equipment, l_{eq} the expected lifetime of the equipment and d the rate of interest. The above equation gives the yearly cost for a piece of equipment. We would also like to consider a shorter time step than one year, say $1/n$ of a year, where the instalment becomes

$$p_{eq,n} = p_{eq} \frac{d/n}{(1 - \frac{1}{(1+d/n)^{l_{eq} n}})}. \tag{4.14}$$

By setting $n = 52$ the weekly cost $p_{eq,w}$ could be found.

Second, it is assumed that there are costs for running the facility. One of these is maintenance. When operating an equipment there is usually a need for maintenance. The maintenance is in reality dependent on a number of factors, e.g. age of equipment, utilisation and run pattern. Since it is hard to take all these factors into account, the total cost for maintenance in this thesis is estimated with a constant factor ($f_{eq,m}$) of the investment cost $p_{eq,n}$, which gives the equipment cost

$$p_{eq,n,m} = (1 + f_{eq,m}) p_{eq,n}. \tag{4.15}$$

In addition there is also a cost for production. In this case it is electricity and natural gas. In contrast to the cost for equipment these costs are not constant. Instead they vary according to the production. We also have to take the investment cost from all current equipments into consideration. If R_s is the relative utilisation of the full production capacity and $c_{util,n}$ the total production related costs at full capacity, the total cost is

$$c_{prod}(t) = \sum_{\forall eq} p_{eq,n,m} + R_s(t)\ c_{util,n}. \tag{4.16}$$

Note that the number of equipment differs according to timing and extent of investments. The time of purchase might also change the price if technology progress is part of the model. This can be modelled with a factor $R_{pr}(t_{inv})$.

In order to find the cost per produced unit we observe that the number of produced units per $1/n$ year may be written as $x_{prod,n}(t) = R_s(t)\ x_{max,n}$, where $x_{max,n}$ is the number of units produced per $1/n$ year at maximum capacity. The cost per unit thus becomes

$$c_{unit}(t) = \frac{\sum_{\forall eq} p_{eq,n,m} R_{pr}(t_{inv}) + R_s(t)\ c_{util,n}}{x_{max,n} R_s(t)}. \tag{4.17}$$

Note that eq. (4.17) requires the inverted time step n to be the same for $p_{eq,n,m}$, $c_{util,n}$ and $x_{max,n}$. The above calculated $c_{unit}(t)$ gives the momentarily production cost per unit. In order to find the mean cost it has to be integrated over the investment period. If done absolute, i.e. adding the costs at all times without respect to the present day value reduction in accordance to the rate of interest, the result is

$$\bar{c}^1_{unit} = \frac{\sum_{\forall eq} p_{eq,n,m} R_{pr}(t_{inv})}{x_{max} \Delta t} \int_{t_0}^{t_f} \frac{dt}{R_s(t)} + \frac{c_{util}}{x_{max}},\ \Delta t = t_f - t_0. \tag{4.18}$$

Another option is to adjust future costs to present day values using the present value correction

$$pvf(t) = \frac{1}{(1+d)^t}, \tag{4.19}$$

giving

$$\bar{c}^{2}_{unit} = \frac{1}{x_{max}\Delta t}(\sum_{\forall eq} p_{eq,n,m} R_{pr}(t_{inv}) \int_{t_0}^{t_f} \frac{pvf(t)}{R_s(t)} dt + c_{util} \int_{t_0}^{t_f} pvf(t) dt) \quad (4.20)$$

A third option is to use the above present day correlation but distribute the total cost evenly over the whole investment period, i.e

$$\bar{c}^{3}_{unit} = \frac{c_{util} + anf(\Delta t) \sum_{\forall eq} p_{eq} R_{pr}(t_{inv}) pvf(t_{eq})}{x_{max}\Delta t}. \quad (4.21)$$

One must realise that this third option does not reflect the sum of the real cost to the production facility.

The developed mean production cost $\bar{c}^{1}_{unit}$, $\bar{c}^{2}_{unit}$ and $\bar{c}^{3}_{unit}$ represent different ways of calculating the costs for production. They are all candidates for an objective function when doing optimisations. In the next section $\bar{c}^{1}_{unit}$ is used as objective functions in a hydrogen refuelling station test case.

4.4 The hydrogen infrastructure problem

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 be dangerous. Another consideration is the vulnerability to both sabotage and accidents. In this thesis an alternative solution comprising local production of hydrogen using a natural gas to hydrogen re-former is investigated. The input to the re-former can be any type of natural gas that may originate from fossil or renewable resources. One disadvantage is that the re-former 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. A hydrogen production and refueling part can then be added to the already existing natural gas refuelling station. It is also possible to dispense natural gas as an intermediate alternative.

If the refuelling station is equipped with a fuel cell, 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 which can produce hydrogen gas directly from electricity. In this case it is important to keep track of how the electricity is produced. To first produce electricity from coal and then use electrolysis to produce hydrogen is not a good environmental solution.

In addition to the hydrogen re-former, the refuelling station layout that will be considered also has a local fuel cell and an electrolysis plant. Figure 4.1 illustrates all options investigated in this thesis. The result is a refuelling station that is very flexible in terms of resource use and energy production.

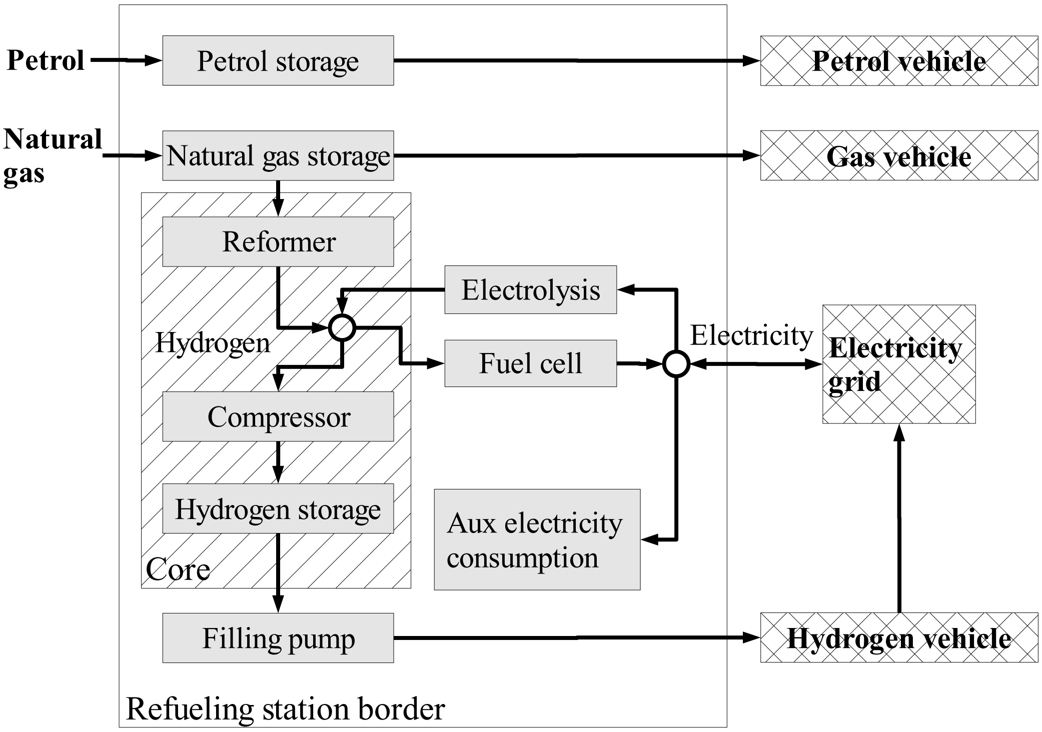

Figure 4.1: Refuelling station layout. Natural gas is re-formed to hydrogen at the site and stored for delivery to vehicles. It is also possible to produce hydrogen from electricity by electrolysis or electricity from hydrogen by using a fuel cell.

The equipment for a hydrogen refuelling 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, estimated number of customers and general technical and economical development. The problem is to find this most profitable configuration. As described in paper III, this problem is equivalent to finding the least expensive mean production cost for hydrogen, which is already developed in sec. 4.3. It is also shown that the original problem can be divided into a number of smaller ones. In this thesis, as was the case in paper III, only the core parts (fig. 4.1) will be considered.

In reality the choice of equipment is limited by supply. Let the set of available equipment, which consists of a finite number of sizes, be denoted by C and the control sequence $u(t)$ be a vector of equipment sizes such that $\delta u(t) \in C$ and $u(t+\delta t) \geq u(t)$. The implication is that u is only allowed to increase and only increase with specific values, namely those in C. Further let $f(u,x,t)$ be the description of the core of the refuelling station in state-space form and x_{eq} the flow through equipment. The problem of finding the most profitable configuration can now be formulated

$$\begin{array}{lcl} \min\limits_{u(t)} & \bar{c}^{n}_{unit}(u(t)) & \\ \text{s.t. } \dot{x} & = & f(u(t),x(t),t) \\ 0 \leq & x_{eq} & \leq u(t). \end{array} \tag{4.22}$$

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 $2 * M = 350402$ variables and $M - 1 = 175200$ extra defect constraints. This would make numerical solving of the resulting NLP hard, if not to say impossible.

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

In order to solve the problem (4.22) it is observed that the first investment has to take place initially, at $t = 0$. Consecutive investments are divided into separate cases according to the total number of investments, i.e. only n_i number of investments are considered for each optimisation problem.

By parametrising set C using a scale function $p_{eq}(s_{eq})$, where s_{eq} is the size of equipment, the problem will become continuous in u.

Since the desired output, the filling curve Hf_w, is given for one week and then scaled using the S-function R_s, it is sufficient enough to consider only one week for each investment. The week to consider is when utilisation is at maximum, namely the week right before the next investment.

The driving signal for the fast dynamics is the filling curve. This curve is given for one week with the time step of one hour. The integral in the objective function x can therefore be approximated with a sum. Also, at the transcription to a NLP a cumulative sum can be used as integration method.

Using the transcription method from sec. 4.2, the resulting NLP problem becomes

$$\begin{aligned}
&\min_{t_{inv},eq} \bar{c}^{n}_{unit}(t_{inv}, eq) \\
&\text{s.t. } \zeta_t = x(t+h_k) - \sum_{s=t_0}^{t} f(s),\ t = t_0 + mh_k,\ m \in Z^+ \leq M \\
&x(t+h_k) \geq 0 \\
&0 \leq x_{eq} \leq c_{eq}.
\end{aligned} \tag{4.23}$$

Considering the dynamics involved is rather simple, the in sec. 4.2 discussed multiple shooting method can be replaced with a single shooting one. The advantage is that we get less variables and constraints, and we would probably make the problem easier to solve numerically. By setting $\zeta = 0$, we obtain

$$\begin{aligned}
&\min_{t_{inv},eq} \bar{c}^{n}_{unit}(t_{inv}, eq) \\
&\text{s.t. } \sum_{s=t_0}^{t} f(s) \geq 0 \\
&0 \leq x_{eq} \leq c_{eq}.
\end{aligned} \tag{4.24}$$

This NLP problem can be solved using the methods in sec. 4.1.

In paper III two cases are considered: variable utilisation as in eq. (4.24) with extra requirements on initial amount of hydrogen stored and periodic maintenance and constant utilisation, which is a special and simpler case of variable utilisation. In the variable utilisation case, the chosen special conditions in this study are 100 kg hydrogen storage initially and at the end, and a weekly stop for maintenance from hour 75 to 87 during the week. Investments are done at 1 and 2 occasions during the investment period. The resulting problem formulation is then

$$\begin{array}{rcl} \min\limits_{t_{inv},s_{hr}} & c_{obj2} & \\ \text{s.t. } \sum\limits_{t_0}^{t}(x_{hs}^{i}-x_{hs}^{o}) & \geq & 0, t_0 \leq t \leq t_f \\ c_{eq} & \geq & x_{eq} \\ x_{hs}(t_0) & = & x_{hs}(t_f) \\ x_{hs}(t_0) & = & 100 \\ \sum\limits_{t=75}^{87} x_{hr}^{o} & = & 0. \end{array} \tag{4.25}$$

The result from the optimization is size of equipment, running pattern of the facility and produced hydrogen price and utilization curve. The figs. 4.2, 4.3 and 4.4 show some of the results in the case of 2 investments. The complete results are given in paper III.

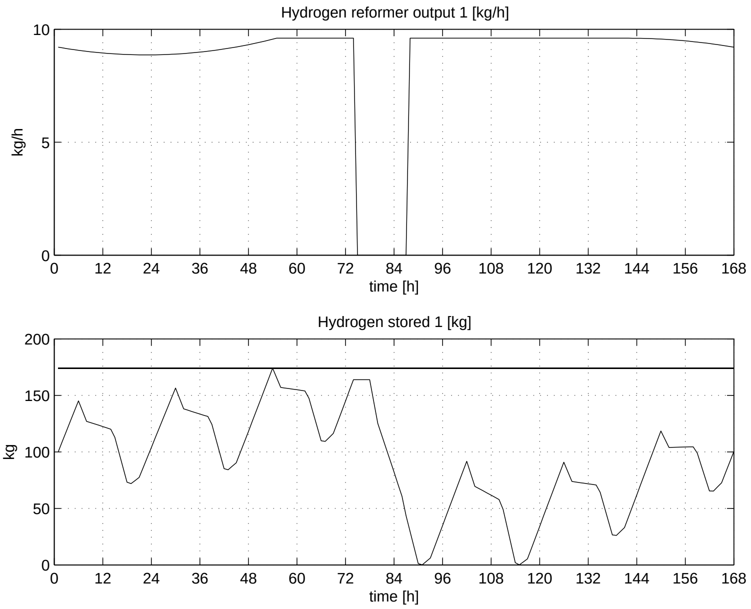

Figure 4.2: Variable utilisation case, 2 investments, throughput and stored hydrogen: Investment 1 at t=0.

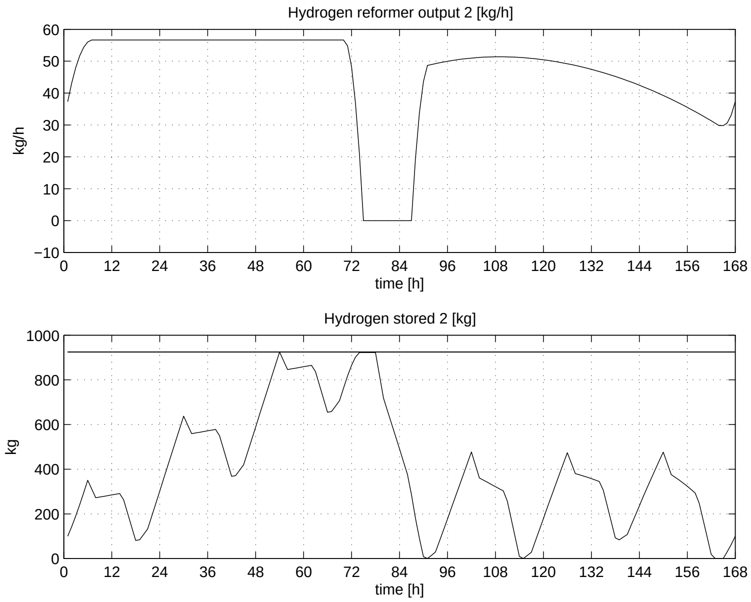

Figure 4.3: Variable utilisation case, 2 investments, throughput and stored hydrogen: Investment 2 at t=5.4.

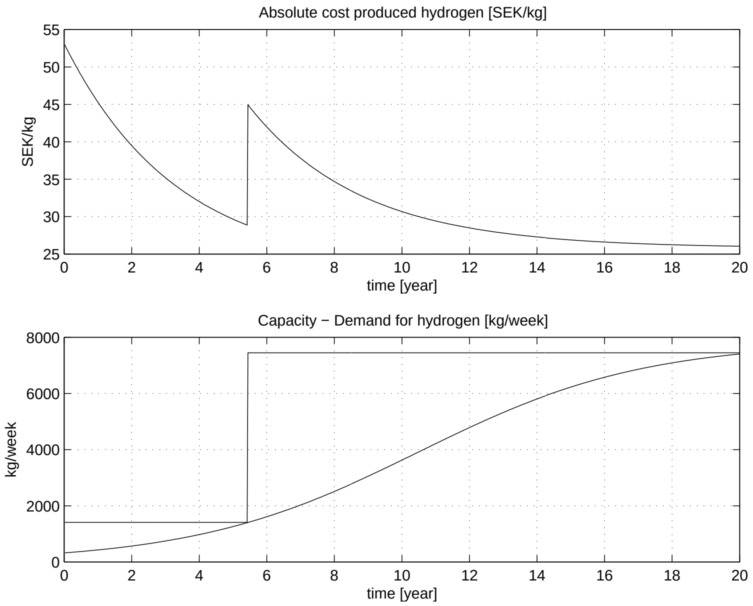

Figure 4.4: Variable utilisation case, 2 investments, hydrogen production cost and capacity-demand.

Chapter 5

Concluding remarks

It has been shown that the flexibility of the model in LCA or LCA-like systems can be enhanced by introducing:

- A-causal models. The removal of computational causality made it possible to separate model and problem description. Hence it was possible to apply several problem descriptions to one model.
- Object oriented models.
- Physical modelling approach.
- Intentional redundancy.

An investment optimisation method based on optimal control has been developed for environmentally favourable, but expensive production facilities comprising simultaneously calculation of long term investment strategy and short term utilisation scheme. The method was successfully tested on a hydrogen refuelling station case. The problem was shown to be convex and hence the resulting optimal solution is global.

5.1 Future work

In the investment optimisation method a number of items can be improved. To be realistic the objective function needs to incorporate e.g. cost of labour for the hydrogen part of the refuelling station. The optimisation method is tested on the hydrogen refuelling station case, which is shown to be convex. In that sense other algorithms for solving the resulting NLP problem could be investigated, e.g. *Interior Point* or *Cutting Plane* [13] 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 can most probably be improved. In case 2 with variable utilisation (see paper III) the computational time is unrealistically high for more than 2 investments. Since the most favourable solution probably lies between 3 and 5 investment, this limitation has to be overcome. Due to the sampled nature of the refuelling curve, the test case investigated contains 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.

It should be emphasised that the investment optimisation method is still in a development stage. Before the method is applied in any real case, there are things to be improved, such as the structure of the notation.

During spring 2003 a co-operation with Physical Resource Theory, Chalmers, started for a Design for Recycling (DfR) project. The case study done aims at finding an economically and ecologically optimal transition to the best design for recycling. In this project more options for optimisation will be explored.

Chapter 6

Summary of appended papers

6.1 Paper I

This technical report is the result of a feasibility study carried out in 1999-2000. The report applies concepts from technical modelling and calculation to Life Cycle Analysis (LCA) in general, and Life Cycle Inventory (LCI) in particular. A mathematical framework for LCI is created and a method to solve for the functional unit is developed. The relation between computational non-causal models and separation of model and problem formulation is investigated. Different model and calculation types are compared to the ones used in LCI. The report also contains a survey and categorisation on calculation methods within the LCA and related areas. The underlying intention of the report is to explain and clarify methods used in LCI from a general technical system perspective and to suggest new methods.

This report defines LCI in the terms and language of a more technical and mathematical system science. It thus relates LCA to present, already established scientific areas, thereby: first it adds credibility to LCA by explaining the method in technical and mathematical terms, giving more people the opportunity to verify the calculations. Second it helps in finding methods and concepts from related areas to develop modelling and calculation in LCA. The difference from previous work, e.g. Heijungs [28], is that the developed methods stem from technical methods (e.g. control theory) and not from management (e.g. economics), which result in a different set of modelling languages are considered.

6.2 Paper II

In cement manufacturing before changes are made to the process, according to the law, the effect needs to be verified. Such changes might include type of sand, fuel or additives. Recently a major cement producer in Sweden started to investigate alternative, more environmentally friendly types of fuel. In addition they also started to improve the understanding of the involved physics and chemistry, which turned out to be complex. Further improvement, which would include dynamic and non-linear elements, should also be possible to include in the verification. 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 fulfils the requirements above. A computational a-causal model made it possible to separate the model describing the cement manufacturing process from the problem formulation. The model was built in ASCEND [54], which is an object oriented, mathematically based modelling language and multi-purpose simulation and calculation environment. 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 chose how to assign the physical property. In addition the model also fully traces the total cost throughout the production line.

6.3 Paper III

Vehicles that run on hydrogen 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 developing. One of the most significant difficulties in the introduction of hydrogen vehicles today is the infrastructure that needs to 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 profiting 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 investeigated 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 re-former need to be taken into account. Both optimisation problems are shown to be convex and hence produce the global optimal point. The result is an hydrogen production cost of 26-40 SEK/kg, which is fully comparable to other studies. The major difference is that this study uses an increasing function to estimate the number of hydrogen vehicles refuelling at the station, which makes the estimated production cost a time average. In other studies, the cost is based on maximum utilization.

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Paper I

Modelling and Simulation in LCA

Technical report

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Paper II

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Paper III

Optimal investment strategies for a hydrogen filling station

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