THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

A Life Cycle Process Model

Simulation of Environmental, Product and Economic Performance in Cement Production

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Abstract

This thesis presents a modelling approach, which produces more flexible models in terms of types of simulations possible to perform. Designing and building a model of the cement manufacturing process illustrates the approach. The purpose of the model is to provide a flexible tool for supporting decisions made on potential product, as well as process development, options. The model simulates different development options and generates information on potential environmental, product and economic performance. Interesting future development options, such as an increase in the use of recovered material and alternative fuels is explored using the model. The results, the environmental, product and economic performance of the potential development options are discussed.

The research presented in this thesis not only has its roots in systems analysis, in general, but also in life cycle assessment (LCA), in particular. The life cycle, the cradle to gate perspective, is seen as important, although limitations on the LCA methodology have been recognised. The modelling approach has its point of departure in the commissioner's, in this case Cementa AB's, requirements on a flexible model that can perform different types of simulations and generate information on environmental, product and economic performance.

Making use of a calculational non-causal, physical and object-oriented modelling approach satisfied the commissioner's requirements for flexibility. The result is a model that can be used for a number of purposes.

The model has been used to explore the potential for reducing the negative environmental impact of cement manufacturing through an increase in the use of recovered material and alternative fuel. It has been shown that the model can simulate the different desired development options. The desired information is generated and assessed in relation to current requirements on product performance. The generated information can be used to give indications of development options for further investigation and study. The nine simulations show that the use of recovered material and alternative fuel can be increased with no negative effect on product performance. The use of resources and the studied emission to air can be substantially reduced.

Key words: life cycle assessment, LCA, life cycle inventory, model, flexible, simulation, cement manufacturing process, decision support tool

List of Papers

The Licentiate of Engineering thesis is based on the following appended papers:

I. **The Design and Building of a Life Cycle-based Process Model for Simulating Environmental Performance, Product Performance and Cost in Cement Manufacturing.**
Gäbel, K., Forsberg, P. & Tillman, A-M.
Submitted to Journal of Cleaner Production April 2001

II. **Simulating Operational Alternatives for Future Cement Production.**
Gäbel, K.
Submitted to Journal of Cleaner Production July 2001

Preface

After finishing my Master of Science degree in civil engineering at Lund Institute of Technology I was employed by Scancem's Trainee Program. During the year and a half long program I followed the process from cement manufacturing via research and development and sales to market development. The trainee program gave me experience of the whole operation, from "cradle to grave".

I have for a long time carried an interest in and devoted much time to environmental issues. I believe they will be, if they not already are, as important as technical and economical factors in the development and selection of products and processes. Ever since I first heard of the concept of Sustainable Development and its definition (WCED 1987); "development that meets the needs of present generations without compromising the ability of future generations to meet their own needs"; I have wondered and speculated about it's implications and how it applies to industry.

Three years ago I was given the opportunity to become one of 15 industrial doctoral students in the Scancem Doctors of Engineering Program. The possibility to combine applied research in the field of environmental studies at Chalmers University of Technology with my work at Cementa AB was very attractive.

The industrial challenge, as I perceive it, is to develop and offer, at competitive prices, products and product systems of good quality, with a minimum of negative impact on the environment, from production, via use and reuse, to final disposal of our products. The immediate question that pops up is "How do we meet this challenge?". Due to the large complexity of environmental issues, I don't think there is one and only one answer to this question. Maybe it is this understanding of environmental issues that interests and fascinates me.

Another aspect of working with my PhD project that I find especially interesting is that I am standing with one leg in industry and the other in the academic world. When in the cement world, I strive to identify and make "concrete" the most urgent and important requirements for sustainable production, the use and final disposal of cement and concrete. As a scientist, I interpret these requirements and their implications and base my research on these requirements. Back in the cement world, the research findings will be implemented and made use of. This is what applied research really is.

Cementa AB is gratefully acknowledged for financing my industrial doctoral project.

My research has been carried out in the context of CPM, the Centre for Environmental Assessment of Products and Material Systems, a national competence centre that involves Chalmers, NUTEK (the Swedish National Board for Industrial and Technical Development) and a group of Swedish industrial companies.

During these three years working with my research project many colleagues, both at Cementa and Chalmers, relatives and friends have shared their knowledge and experience, as well as assisted me. Thanks to your support and encouragement I have now completed the licentiate thesis.

I would like to thank my two supervisors, Professor Anne-Marie Tillman at Environmental Systems Analysis, and Mr Bo-Erik Eriksson at Cementa AB. Anne-Marie for introducing me to, and guiding me in my research and for spending so much time and effort reading and discussing my drafts. Bo-Erik for always believing in me and supporting me in my research, and for the help to co-ordinate and prioritise Cementa’s needs and requirements.

Many thanks to Peter Forsberg, my co-worker in the design and building of the cement life cycle process model and co-author of paper I.

I would also like to thank my fellow PhD students and colleges at the Department of Environmental Systems Analysis, especially Magnus Karlström, my “office mate”. You have been a great support.

Table of Contents

1. Introduction

The interest in environmental issues is constantly increasing. At the same time, environmental issues have gradually been broadened with concepts, such as sustainable development[1], which implies not only ecological, but also economic and social responsibilities. The growing environmental awareness and demands of customers and society increase the pressure on industries to develop more environmentally adapted products and processes. Environmental issues have become an additional impetus for product and process development in the industry.

On a global level, cement industry leaders have realised the opportunities as well as the need to properly address sustainable development issues in order to continue their "license to operate" (WBCSD 2000). A group of cement companies have initiated a project on sustainable cement. The project lead by the World Business Council for Sustainable Development (WBCSD) aims at defining how the cement industry can become more sustainable. The "Kyoto Protocol" to the UN's Framework Convention on Climate Change has set the agenda for global CO_2 emission reductions. The European Union has agreed how its Member States will share the burden. The cement industry in Europe, through the European Cementa Association (Cembureau), has recognised its role and will continue to play a strong part in the global effort to fight climate change (Cembureau 1998a).

Cementa AB, the sole cement manufacturer in Sweden, aims to contribute to the development of a sustainable society and has committed itself to set environmental goals annually to achieve continual improvement (Cementa 2000).

Cementa AB has previous experience of life cycle assessment (LCA) through a Nordic project on Sustainable Concrete Technology (Lundström, K. 1997). One conclusion drawn from the project was that life cycle assessment is a tool, with improvement potential, to be used in the development of more environmentally adapted cement and concrete products and manufacturing processes (Lundstöm, K. 1997).

The need to integrate life cycle thinking into process evaluation, design and optimisation is well recognised (e.g. Azapagic (1996), Azapagic & Clift (1999a) with references therein). Kniel et al. (1996) with references therein, suggest the unexplored potential of LCA for the design of processes. In addition, Kniel et al. (1996) have identified the need to accommodate both economic and environmental constraints in the design and operation of processes. The researchers propose that life cycle assessment (LCA) may prove valuable to establish a link between the environmental impact, operation and economics of a process.

There are limitations with the current LCA. One important limitation, from an industrial perspective, is that traditionally LCI models do not address the economic

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[1] The Brundtland Report "Our Common Future" (WCED 1987), defines sustainable development as "..development that meets the needs of the present without compromising the ability of future generations to meet their own needs".

aspect of a product (ISO 14040 1997). Barriers to wider use in industry are the high cost and time necessary for carrying out the study (Azapagic 1999).

State of the art life cycle inventory models are typically used to relate resource use and emissions to a product, or rather the function of a product. Corresponding software tools are generally specialised to perform normalisation of the flows to the functional unit. Current LCI modelling has a limited capability to perform other 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.

To support decisions on product and process development options, knowledge and information on the consequences of planned changes are needed. There is a need for models that simulate different development options and generate information on potential environmental, product and economic performance. The purpose of the model and the problem to be solved using the model may vary from one time to the next. Thus, there is a need for more flexible models, and that each simulation assesses the environmental, product and economic performance, from a life cycle perspective.

1.1. Aim of the Thesis

The aim of the research presented in this Licentiate of Engineering thesis is to explore the potential for building more flexible life cycle inventory models, in terms of the types of simulations possible to perform.

The potential to generate information on environmental, economic and product performance in the same mathematical model of a manufacturing process are also explored.

An additional aim is to provide the commissioner with a model that fulfils their needs and requirements and that can be used for its intended purpose. The commissioner wants to be able to simulate different development options and generate information on the consequences. The model is to support decisions on product and process development options. The potential of future development options, such as an increase in the use of recovered raw material and alternative fuel are to be explored using the model.

The design of a model of the cement manufacturing process is described in Paper I. The modelling approach has taken its point of departure in the commissioner's, Cementa AB's, requirements for a flexible model that can perform different types of simulations and generate information on product performance, economic cost and environmental performance.

In Paper II the potential of the modelling approach is demonstrated by using the model to explore the possibility of minimising the negative environmental impact of cement manufacturing through an increase in the use of recovered material and alternative fuel.

1.2. Disposition of the Thesis

In Chapter 2, the cement manufacturing process and related environmental issues are briefly described. This is followed by a literature review of related work in Chapter 3.

The research method and choice of modelling and simulation techniques are presented in Chapter 4. In Section 4.1 systems analysis, in general, and life cycle assessment, in particular are described. In Section 4.2 the commissioner's needs and requirements on the model resulting in the choice of modelling and simulation techniques are presented. A more detailed description of the commissioner's needs and requirements, the interpretation of them and the choice of mathematical modelling and simulation techniques are found in Paper I.

Chapter 5 presents the life cycle process mode. Section 5.1 briefly outlines design and building and 5.2 briefly describes the validation of the foreground system model, describing the "gate-to-gate" part of the manufacturing process. A more detailed description is found in Paper I.

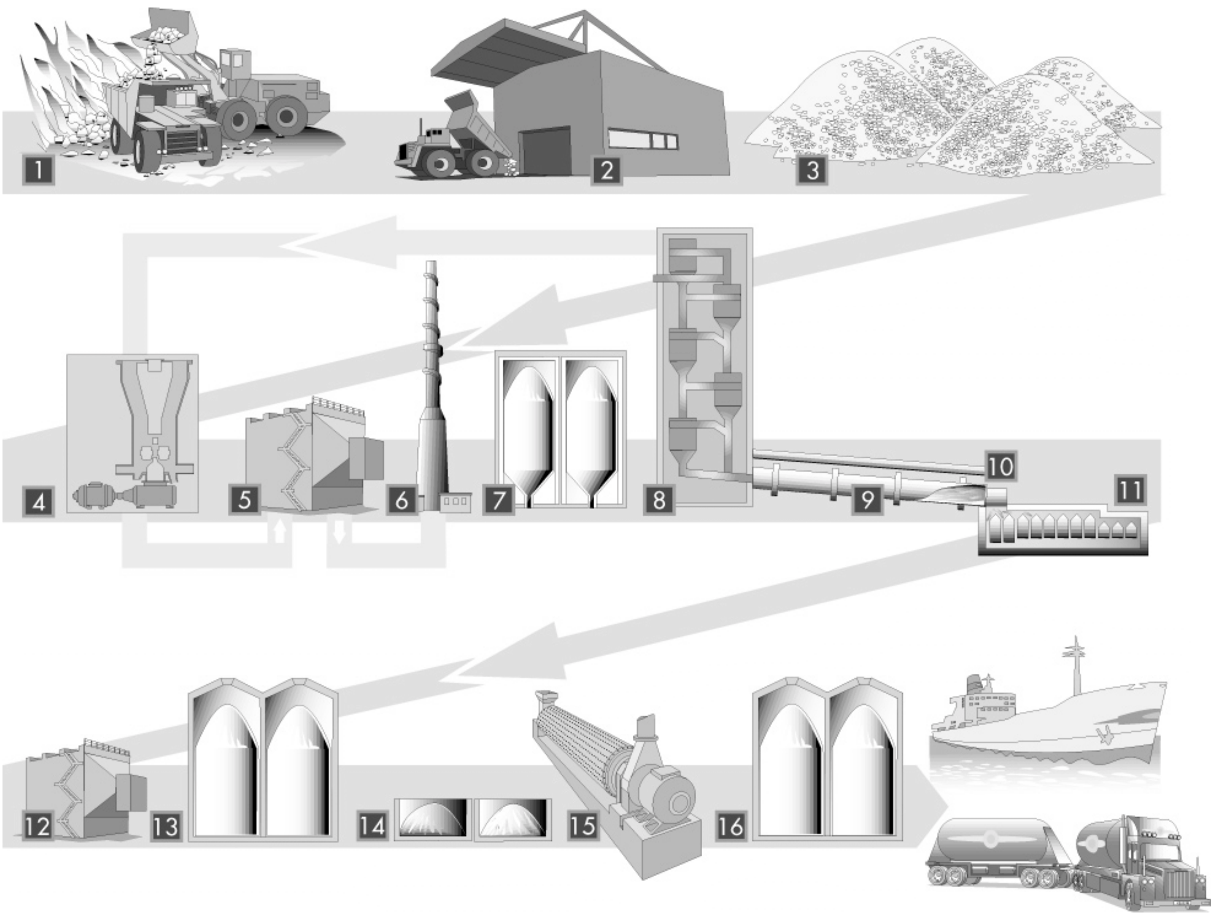
The life cycle process model has been used to explore the potential for minimising negative environmental impact through an increase in the use of recovered material and alternative fuel in cement manufacturing. The explored scenarios and the main results are presented in Chapter 6. Paper II gives a more detailed description of the study, the results and the conclusions drawn.

In Chapter 7 the conclusions of this thesis are presented and discussed. Future research needs are presented in Chapter 8.

2. Cement Manufacturing and Related Environmental Issues

This section briefly describes the cement manufacturing process and related environmental issues. The description is based on the manufacturing process at Cementa’s Slite plant. The process and related environmental issues are described in more detail in a report (Gäbel 2001).

The cement manufacturing process, shown in Figure 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.



1. **Mining.** Limestone is needed to produce cement.
2. **Crushing.** The rock is crushed to a maximum of 80 mm.
3. **Storage piles.** Serves two purposes (i) as a buffer for the raw mill (ii) as a mixing station, where the raw material is mixed to achieve best possible uniform quality.
4. **Raw mill.** The rock is ground into a fine powder of which 90 percent consists of particles smaller than 0.09 mm.
5. **Electrostatic precipitator.** Dust from the production of the raw meal, as well as dust-laden flue gas from the rotary kiln, is removed in a highly efficient electrostatic precipitator.
6. **Flu gas de-sulpharisation system**
7. **Raw meal silos.** The raw meal is stored here before being introduced to the clinker production system.
8. **Cyclone tower with precalcination.** The raw meal is precalcined, the calcium carbonate is split into calcium oxide and carbon dioxide.
9. **Rotary kiln.** The kiln is an 80-meterlong iron pipe that rotates. The material travels slowly through the kiln to the burner and is transformed into clinker.
10. **By-pass filter.** If the alkali content is too high, it will negatively affect the durability of the cement. After the cyclone tower, the material passes through a filter to remove the alkalis in a condensation process.
11. **Clinker cooler.** The clinker is air-cooled.
12. **Electrostatic precipitator.** Clinker is removed in a highly efficient electrostatic precipitator.
13. **Clinker silos.**
14. **Gypsum and additives storage.**
15. **Cement mill.** The clinker is ground with a small amount of gypsum to produce cement.
16. **Cement storage silo**

Figure 1 *Cement manufacturing process (Cementa 1999)*

Limestone, the main raw material is mined and crushed. Other raw materials, which may be used, are sand, iron oxide, bauxite, slag and fly ash. The raw materials are prepared, proportioned to give the required chemical composition and then 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 (Cembureau 1999). 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 clinker, through heating, calcining and sintering the finely ground raw meal into glass-hard spherically shaped minerals, clinker. 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, where the carbon dioxide bound in the limestone is released, i.e., calcination takes place. The calcined raw meal then enters the rotary kiln and moves slowly towards the main burner where the other half of the fuel is introduced. The hot clinker leaving the rotary kiln falls into the clinker cooler and is quickly cooled down.

Raw materials and fuels contain organic and inorganic matter in various concentrations. Normal operation of the kiln provides a high temperature, a long retention time and oxidising conditions adequate to destroy almost all organic substances. Essentially all mineral input, including combustion ashes, is converted into clinker. The way metals entering the kiln behave depends largely on their volatility. Most metals are fully incorporated into the product, some precipitate with 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 pass through a dust reduction device before being released 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, water vapour from the combustion process and raw materials, and nitrogen oxide from the combustion process. 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.

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 by a slurry consisting of limestone and water. The separated product is used as gypsum in cement grinding.

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 (Gäbel 2001). 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 materials and fuel. The metal content largely varies over time and, consequently, so does metal emission.

In one of the studies (Vold & Rönning 1995), in the Nordic project on Sustainable Concrete Technology, emissions of carbon dioxide, nitrogen oxides, sulphur dioxide and mercury, and the consumption of fossil fuel are identified as the main environmental loads of cement production. According to the European Commission, the main environmental issues associated with cement production are emissions to air and energy use (IPPC 2000). The key emissions are reported to be nitrogen oxides, sulphur dioxide, carbon dioxide and dust.

3. Related Work

The literature review covers life cycle assessment studies and experience of the cement industry, presented in Section 3.1. The review also covers life cycle assessment and similar approaches, with application to process design, selection and development, in which environmental aspects are combined with economic and product performance aspects. Here I have found some review articles, presented in Section 3.2, and a large number of articles that describe different optimisation approaches, presented in Section 3.3. These methods focus on production processes. Finally, I have found a number of models, more or less related to LCA, developed to simulate and test different process choices and operational alternatives, presented in Section 3.4. These models focus on waste processes.

3.1. The cement industry's previous life cycle assessment experience

Several life cycle assessment studies (LCAs) of cement, concrete and concrete products have been carried out (Lundström, H. 1997, Geem Van 1998, Ölund & Rydberg 1998, Nisbeth & Geem Van 1997).

Cementa AB has previous experience of LCA through a Nordic project on Sustainable Concrete Technology (Lundström, K. 1997). In the project, several LCA studies were carried out on cement, concrete and concrete products (Björklund & Tillman 1997, Björklund et al. 1996, Häkkinen & Mäkelä 1996, Lundström et al. 1996, Vold & Rönning 1995). One conclusion drawn in the project was that life cycle assessment is a tool, with improvement potential, to be used in the development of more environmentally adapted cement and concrete products and manufacturing processes (Lundstöm, K. 1997).

Cembureau, the European Cement Association, suggests that life cycle inventories (LCI) are increasingly more important for industries, which realise that their survival, in the long run, is dependent on the environmental image of their products (Cembureau 1998b). As a consequence, Cembureau has developed an LCI format for cement. The Cembureau LCI format for cement identifies the parameters relevant to cement and concrete, describes the basis for the selection of the parameters and provides information and guidance on the acquisition of LCI data for the cement industry.

3.2. Reviews of incorporation of environmental issues into process selection, design and development

Cano-Ruiz & McRae (1998) have reviewed approaches for incorporating environmental issues into the design of new processes and manufacturing facilities in the chemical industry. The design process itself, including framing the problem, generating design alternatives, analysing alternatives, evaluating alternatives, and sensitivity analysis form the framework of the review. The focus of the review is on identifying the issues, information sources, and approaches to process design that have the potential to lead to improvements in both economic performance and environmental quality.

Another researcher has reviewed the application of LCA to process selection, design and optimisation (Azapagic 1999). The procedures for incorporating environmental criteria, along with economic and technical criteria, into the systems optimisation framework are also reviewed and discussed. Moreover, the review covers the state-of-the art of the methodological development and uses of LCA.

The integration of environmental impact minimisation into conceptual chemical process design has been reviewed by Yang & Shi (2000). The review focuses on two aspects of conceptual design, the synthesis of reaction paths, and the generation of process flowsheet alternatives. The review is limited to two main aspects of the process flowsheet alternative; the environmental impact assessment system, and the process synthesis methods integrated with environmental impact minimization.

3.3. Integrating environmental criteria into process optimisation

Many researchers (e.g., Kniel et al. 1996, Stefanis et al. 1995, Azapagic 1996, Azapagic & Clift 1995, Alexander et al. 2000, Spengler et al. 1998, Carnahan & Thurston 1998, Marano & Rogers 1999) have developed procedures and methodologies in which environmental issues and / or life cycle assessment are combined with multiobjective optimisation. These approaches have similarities with my work in the sense that processes are in focus and both environmental and economical and quality aspects are addressed. My own work, however, is not limited to optimisation, but allows for different types of simulations.

Azapagic & Clift (e.g., Azapagic & Clift 1995, Azapagic & Clift 1998, Azapagic & Clift 1999b) have developed an approach for incorporating LCA into systems optimisation. The approach establishes a link between the environmental and economic performance of a process from “cradle to grave” by combining multi-objective optimisation (MO) and LCA.

The approach for incorporating LCA into system optimisation is comprised of the following three main steps (Azapagic 1999).
1. Carrying out a life cycle assessment study,
2. Formulating the multi-objective optimisation problem in the context of LCA,
3. Multi-objective optimisation of environmental and economic criteria and choice of best compromise solution.

Azapagic & Clift have illustrated and demonstrated the value of the approach in a case study of the borate product system (e.g. Azapagic & Clift 1998, Azapagic & Clift 1999a), and by a simplified analysis of a system for producing thermoplastics (Azapagic & Clift 1995).

In a study of a nitric acid plant, Kniel et al. (1996) demonstrate a methodology in which LCA is combined with an economic analysis as the basis for multi-objective optimisation. LCA was used to quantify and compare the environmental performance of a number of alternative process designs aimed at waste reduction. Economic models for assessing economic performance were linked to the environmental model. The aim was to maximise the economic return and minimise the environmental impact. The plant model was implemented in the process simulator HYSIM.

Drawing on Kniel et al. (1996), Alexander et al. (2000) uses life cycle assessment to assist in developing environmental objectives for process design and analysis. They restrict the analysis to the multi-objective optimisation of environmental and economic aspects. Their approach is demonstrated in a case study of a nitric acid plant. The nitric acid process was modelled in HYSYS, a process simulation software, to obtain mass and energy information. The mass and energy data provide the basis for a life cycle inventory from which the environmental impact profile is developed. Goal programming, a multi-objective optimisation technique was used to solve the multi-objective problem to identify the Pareto surface for this situation.

A methodology for environmental impact minimization (MEIM) has been developed by Stefanis et al. (e.g Stefanis et al. 1995, Pistikopoulos & Stefanis 1998). The methodology embeds LCA principles within a process optimisation framework. This is, according to the authors, achieved by (i) expanding the conventional process boundary to include all processes associated with raw material manufacture and energy generation, (ii) defining the emissions inventory as a vector of gaseous, liquid and solid wastes disposed to the environment from the process system, (iii) transforming the emissions inventory into an impact vector of low dimensionality, (iv) incorporating environmental impact criteria into a multi-objective optimisation setting. In the last step, which constitutes the heart of the methodology, the environmental impact criteria are incorporated into an overall process optimisation strategy.

The applicability of the approach has been illustrated, e.g., on the process optimisation of the production of vinyl chloride monomer (VCM) (Stefanis et al.1995), and on the optimal design and scheduling of batch processes (Stefanis et al. 1997).

Carnahan & Thurston (1998) have developed a Trade-off Modelling method for the design of products and manufacturing processes. Unavoidable trade-offs among pollution, manufacturing cost and quality are the central issues. The method integrates statistical process control and LCA into a multi-objective design optimisation formulation. The authors propose this integration to be performed according to the following procedure. First, both product quality and the environmental impact are explored from a life cycle perspective. The gathered information is used to formulate constraints on the multi-attribute objectivity function. These constraints quantify the relationship between decisions made about the design and manufacturing process, and the resulting effects on product quality, environmental impact and cost. Then a multi-attribute function is employed to determine the raw material and manufacturing settings that result in the optimal trade-offs. The modelling method has been applied to a floor tile manufacturer.

Another similar method has been developed by Marano & Rogers (1999). Their methodology incorporates process performance, economics and life cycle inventory data to synthesize process systems. The method relies on a systematic description of the product life cycle and utilises successive Linear Programming to formulate and optimise the non-linear constrained problem. The practicality and power of the approach have been demonstrated by examining options for the reduction of the emission of CO_2 from petroleum-based fuel.

Spengler et al. (1998) have tried a different approach. They present a decision support system KOSIMEU, to integrate the assessment of production processes with ecological, technical and economic aspects. The methodological approach combines process models simulated with a flowsheeting program and a multi-criteria decision support system. The approach is illustrated with an example from iron and steel making. A process model was developed using ASPEN PLUS, a commercially available flowsheeting program, to generate mass and energy balances. The valuation of mass and energy balances takes place in the multi-criteria decision support part in which the user defines the weights according to their preferences.

3.4. Waste process models

Much of the effort to integrate environmental issues and to provide more general models has been concentrated on waste treatment processes. Work in this field started early and much has been accomplished. Only a few of these models are described in the following.

Sundberg and co-workers (Sundberg 1993, Sundberg & Wene 1994) have developed a model for the description and optimisation of integrated material flows and energy systems, MIMES/Waste. The model is intended for systems that can be described by material and energy balances, but in which the details of phase transitions and chemical reactions can be omitted. MIMES focuses on the linkage between different process units, rather than the detailed properties of individual devices. The joint optimisation of energy and material flows is, according to Sundberg (1993), the outstanding feature of MIMES. MIMES is a nonlinear programming model, which optimises a defined objectivity function. The objectivity function is usually a cost function, which describes the total system cost.

The MIMES/Waste model has been improved by using life cycle assessment methodology for describing and comparing environmental impact (Sundberg & Ljunggren 1997).

A simulation model for the handling of organic waste in urban areas, ORWARE, has been developed and designed by Dalemo et al. (1997). The model calculates energy flows, plant nutrient flows and emission to air, water and soil for various alternatives to organic waste handling and municipal wastewater treatment within the municipality. For evaluation, the results are translated into environmental effects using life cycle assessment methodology.

In ORWARE, a modular approach was used and each process was modelled separately to facilitate the design of several types of scenarios. For all process parts the consumption of energy and resources, the production of energy, emission to air and water, and residual effluent were related to the quantity and composition of the material flow to the model. All physical flows between the sub-models were described with the same 43-elemets vector. Energy flows were handled separately. The ORWARE model was designed using MATLAB/SIMULINK.

Mellor et al. (2001) have developed a mathematical model and decision support framework for material recovery, recycling and cascade use. The flow of material is modelled through a succession of uses with different performance requirements. The cost and environmental impact of activities are included in the modelling framework and are assessed on a life cycle basis. The methodology includes acceptance criteria, which determine whether a material is suitable for specific uses or activities.

4. Research Method and Modelling Techniques

To support decisions on product and process development options in cement production, information on the consequences of planned changes are needed. For this purpose, a mathematical model was designed and built. The model describes the cement manufacturing process from "cradle to gate". The model simulates different operational alternatives for producing cement. For each operational alternative simulated, the model calculates the potential product performance, the economic cost and the environmental performance, from a life cycle perspective.

The development of the cement life cycle process model follows the established procedures in systems analysis (e.g., Gustafsson et al. 1992) in general, and life cycle assessment (e.g. ISO 14040 1997), in particular. The mathematical model was designed using known and established modelling and simulation techniques. A calculational non-causal (Strömberg 1994), physical and object-oriented modelling approach was used. For this application the model was implemented in the software tool ASCEND IV (CMU 2000). ASCEND IV supports steady state, dynamic solving and optimisation.

The life cycle process model has been developed in the cement industry. However, the modelling approach used is also applicable to manufacturing processes in general. The approach could, thus, provide the basis for decision support models in other process industries.

In the following I will briefly present systems analysis and life cycle assessment. The commissioner's needs and requirements resulting in the choice of mathematical modelling techniques are also presented.

4.1. Systems analysis and life cycle assessment

All human activities interact with and have impact on the environment. We use and consume products and services. To provide the products and services, we build and control technical systems. The technical systems use resources from the natural system, emit pollutants and dispose waste into the natural system. The resource use, emission of pollutants and disposal of waste have an impact on the natural system. We, individuals in the social system, value the impact and the potential impact and decide to what extent it is regarded an environmental problem (Bauman & Tillman 2001). Using the cement industry as an example, Figure 2 illustrates the interaction between the social system, the technical system and the natural system.

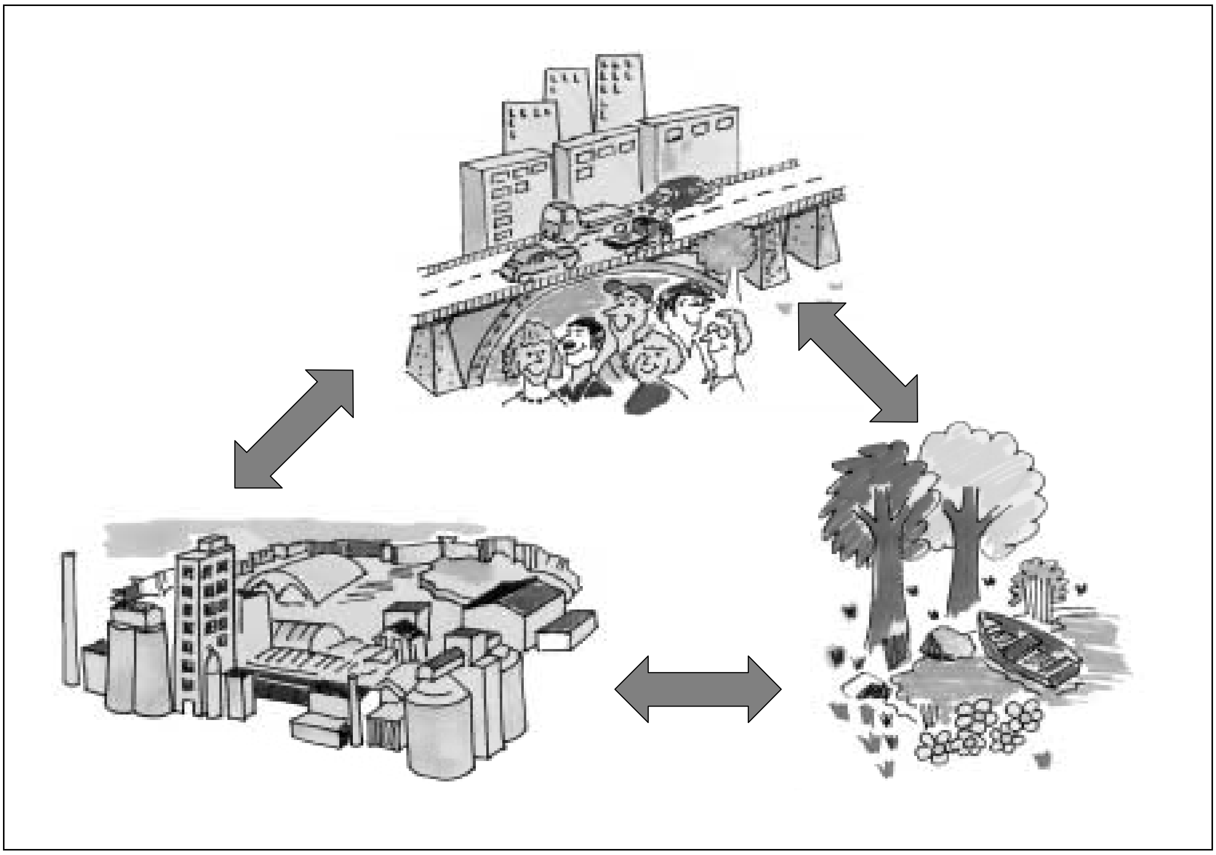


Figure 2 *The social system, the technical system and the natural system*

When analysing large and multidisciplinary issues, which environmental issues are, a systems approach is necessary. From a system approach, the focus is on the entire structure and the relationships between the components of a complex system, rather than on the separate components and their characteristics. A system is defined by a number of components, as well as the relationships between them. This approach has led to the development of systems analysis, a general and interdisciplinary problem solving methodology (Gustafsson et al. 1992).

The main phases in the systems analysis project are, according to Gustavsson et al. (1992); (i) problem briefing, (ii) problem formulation, (iii) modelling, (iv) validating of the model, (v) problem solving, (vi) evaluation of the results, (vii) presentation of the results and (viii) implementation of the results. Most of the steps include data and information collection.

The purpose of the modelling phase is to construct a model of the studied system suitable for solving the problem defined in the problem formulation. The purpose of building the model and its intended use naturally determine the design of the model. The model is then used to analyse and solve the problem. A model can be more or less formal depending on the nature of the problem. The model may be mathematically formulated, but may as well be, e.g., verbally, mentally, physically formulated. A mathematical model is an assembly of mathematical relations that approximate the behaviour of the studied system. The model is one result of the systems analysis project.

The research presented in this thesis not only has its roots in systems analysis, in general, but in life cycle assessment (LCA), in particular. The life cycle, the cradle to gate perspective is seen as important, although limitations in the LCA methodology are recognised. Life cycle assessment (LCA) is a systematic method developed for assessing the potential environmental impact related to a product or a service during its entire life cycle. The system, or systems, which provide a given function are studied. All processes, from the extraction of raw material via use to final disposal, associated with the function are included in the system. All environmental loads associated with the function are taken into account and assessed.

The main procedural phases in LCA are, according to the ISO standard (ISO 14040 1997); (i) goal and scope definition, (ii) inventory analysis, (iii) impact assessment and (iv) interpretation. A study excluding the impact assessment phase is called life cycle inventory, LCI, study (ISO 14040 1997).

In the first phase, the goal and purpose of the study and the intended use and user of the results are stated. The system boundaries and assumptions are defined based on the goal. In the inventory analysis phase, a life cycle inventory model (LCI model) is developed based on the goal and scope. The LCI model is a flow model of the product system describing the mass and energy balance to quantify the material and energy inputs and emissions and wastes from the system, i.e., environmental load. The third phase, impact assessment, is aimed at evaluating the significance of potential impacts using the results of the life cycle inventory analysis. The impact assessment phase involves subjectivity, such as the choice, modelling and evaluation of impact categories. In the interpretation phase, the fourth phase, the findings in either the inventory analysis or impact assessment, or both, are combined in order to reach conclusions and recommendations consistent with the defined goal and scope.

The cement life cycle process model does not include the impact assessment phase. Instead, the inventory results, the environmental load, are interpreted.

4.2. Model requirements and choice of modelling and simulation techniques

It has already been mentioned but deserves to be mentioned again; a model is always designed and built based on the purpose and its intended use. I will now summarise the commissioner’s, Cementa AB’s, needs and requirements, as interpreted from discussions with representatives from different departments. I will also present the choice of mathematical modelling techniques made based on the requirements on the model. A more detailed description of the commissioner’s needs and requirements, the interpretation of them and the choice of mathematical modelling and simulation techniques can be found in Paper I.

Cementa AB needs a model for predicting the consequences of planned changes. The model is to be used to support company internal decisions on product and process development and strategic planning.

Cementa intends to learn about the system and the system's properties regarding product performance, economic cost and environmental performance and how these properties relate to one another. 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 each combination tested, information should be generated on potential product performance, economic cost and environmental performance from a life cycle perspective. The generated information should enable the assessment of these factors in relation to feasibility criteria, such as product performance, emission limits and economic cost. Product performance is regarded as the most important feasibility criterion.

Product performance is directly related to the chemical composition of the cement. The model should calculate the chemical composition of the cement and all intermediate products. Product performance is described with three ratios (Gäbel 2001); the lime saturation factor (LSF), the silica ratio (SR), and the alumina ratio (AR). The ratios describe the relation between the four main components and are shown in Table 1.

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.

Environmental performance described as environmental load, i.e., as resource use, emissions to air and water, and waste should be calculated. The composition of the kiln exhaust gas from clinker production should be calculated separately. The total material and production cost in "SEK" per kilogram cement produced should be calculated.

The purpose of building the model and the problem to be solved is not exactly and unambiguously defined. Instead, the model should enable solving many different problems. Besides, all problems to be solved may not yet be clearly formulated. In this respect, this modelling approach differs from the main procedure for systems analysis described by Gustafsson et al. (1992). The cement life cycle process model must be flexible in terms of being able to be used to analyse and solve many different problems.

The following two examples illustrate how the model should be used to simulated different combinations of raw materials, fuels and cement additives.

A. The amount of cement produced is given. The percentage of each raw material in the raw meal mix, each fuel in the fuel mix and each cement additive in the cement mix are given. The model should then calculate the potential chemical composition and the performance of the raw meal, clinker and cement.

B. The amount of cement produced is given. The available raw materials in the raw meal mix are given together with the requirements on clinker performance. The percentage of each fuel in the fuel mix and each cement additive in the cement mix are also given. The model should then calculate the percentage of each raw material in the raw meal mix, as well as the potential chemical composition and performance of the raw meal, clinker and cement.

The model should describe the current manufacturing process at the Slite plant. However, it must be easy to modify the model to simulate process developments and future end-of pipe solutions, e.g., for enhancing energy efficiency and more efficient dedusting devices. This is another type of flexibility.

Cementa produces cement at three plants in Sweden. The different plants use the same main production process. However, there are variations between the plants, especially in the design of the clinker production system. These variations are mainly due to the nature of the available raw material, when the plant was built, modifications made and the installation of different emission reduction systems. It should be easy to adapt the model to represent any of the commissioner’s cement manufacturing plants. This is yet another type of flexibility.

The cement manufacturing process is, by nature, non-linear and dynamic. The model should describe stable and steady state conditions, and the static and linear transforming of the raw material and fuel into clinker. However, in the future it should be possible to include the non-linear transformations in the manufacturing process. In addition, in the future it should be possible to simulate dynamic behaviour, e.g., during start-up and shut down of production.

To build a model fulfilling the commissioner’s needs and requirements we have chosen the following mathematical modelling techniques.

- A calculational non-causal model (Strömberg 1994) to separate the model from 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 software used must support dynamic and non-linear elements.

5. The Life Cycle Process Model

The cement manufacturing process, “from cradle to gate” was divided into a background system and a foreground system (Tillman 2000). In addition, there is a wider system, which was not modelled. The conceptual model, in Figure 3, shows the foreground and background system along with the wider system.

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 products from the background system. Alternative raw materials, fuels and cement additives are by-products or waste from other technical systems. The production of these alternative products is not included in the model. However, the additional preparation, handling and transport to make them fit the cement industry are included. Depending on whether the additional preparation, handling and transport is done by Cementa or someone else, the processes are either in the foreground system or the background system. The wider system shows the consequences of actions taken at the cement plant, which exist but are not modelled.

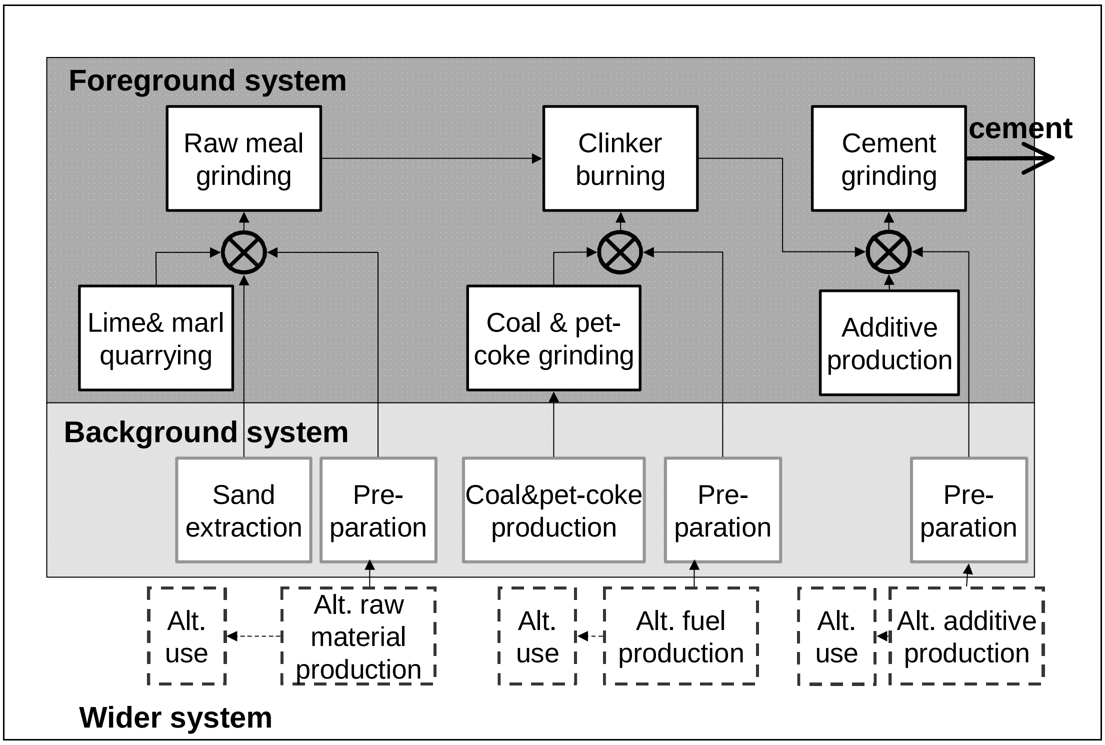


Figure 3 *The conceptual model*

The two sub-systems were modelled with different techniques and levels of detail. The background system was modelled with normal LCI technique (ISO 14041 1998) and stored in SPINE format (Carlsson et al. 1998).

The foreground system model was built using calculational non-causal (Strömberg 1994), physical and object-oriented modelling techniques. For this application, the model was implemented into the software tool ASCEND IV (CMU 2000). ASCEND IV supports steady state solving, dynamic solving and optimisation. In the following I will briefly describe how the foreground system model was built. A more detailed description can be found in Paper I.

The foreground system and background system models were connected to complete the in the life cycle aspect of the model. Product performance and economic cost in the background system were taken into account by assigning the products entering the foreground system a chemical composition and a cost.

5.1. The designing and building of the foreground system model

The model, or what normally is thought of as a model, was separated into three main parts, namely:

1. A neutral model. A neutral model is a number of equilibrium equations connected to each other. A neutral model does not say anything about the order in which the equations should be calculated, nor does it include any specific problem to be solved.
2. A problem formulation. The problem formulation is a list of the parameters to be locked, and also the values to lock them with. The problem formulation decides the order in which the equations in the neutral model are to be calculated.
3. A simulation method (could also be considered as part of the problem formulation). To perform the calculations and solve the problem, a calculation method must be used.

The neutral model of the foreground system is "graphically" illustrated in Figure 4.

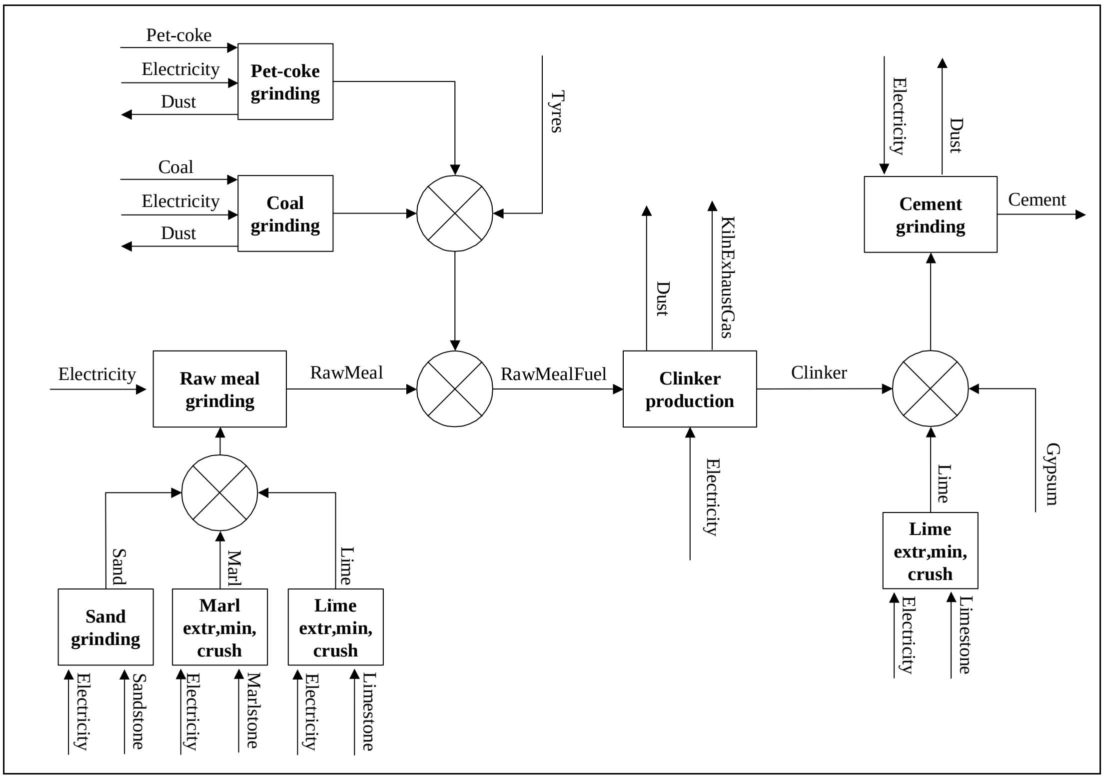


Figure 4 *The neutral model of the foreground system*

5.2. Validation of the foreground system model

In this section, I will present two simulations we performed to validate the model. For each simulation, the problem was formulated and added to the neutral model.

To use the foreground system and to validate it, we performed simulations on two real operational alternatives. The operational alternatives have actually been used at the plant, and hence, there were measurements to validate against. The two simulations were the ones used in Section 4.2 to illustrate how the model should be used. In the following, I will describe the problem formulation that must be added to the neutral model in order to perform the simulations. The problem formulation states which parameters to lock and the value the parameters are locked with. The problem formulation, added to the neutral model for case A and case B, is graphically illustrated in Figures 5 and 6, respectively.

A. To simulate the production of 1 000 kg cement. The raw meal mix should be comprised of 71 % marlstone, 2 % sand and the rest limestone. The fuel mix should consist of 20% petroleum coke and the rest coal. The cement mix should consist of clinker, 5.2% gypsum and 4.4% limestone.

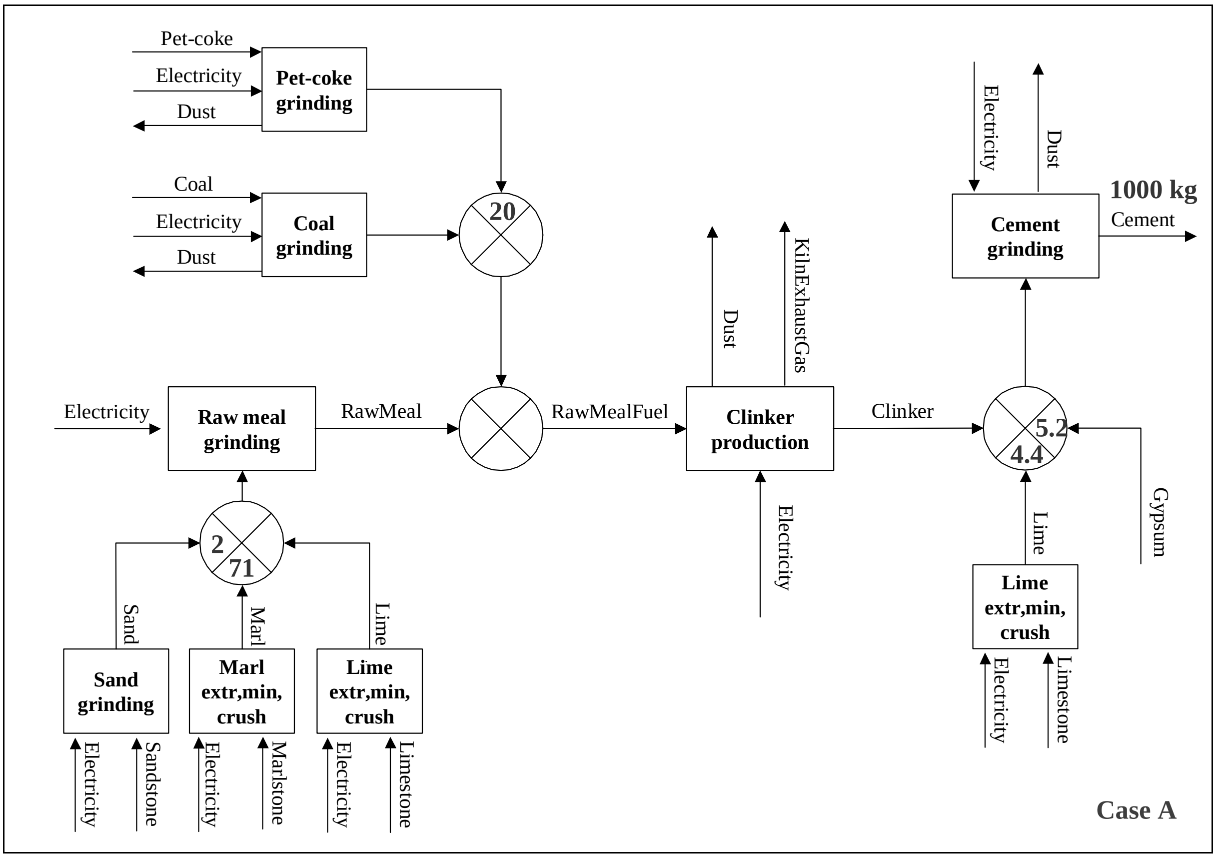


Figure 5 *Problem formulation added to the neutral model, case A*

B. To simulate the production of 1 000 kg cement. The available raw meal materials are limestone, marlstone and sand, and the clinker should have the following performance, LSF= 97.5 and SR=3.15. The fuel mix should consist of 20% petroleum coke and the rest coal. And the cement mix should consist of clinker, 5.2% gypsum, and 4.4% limestone.

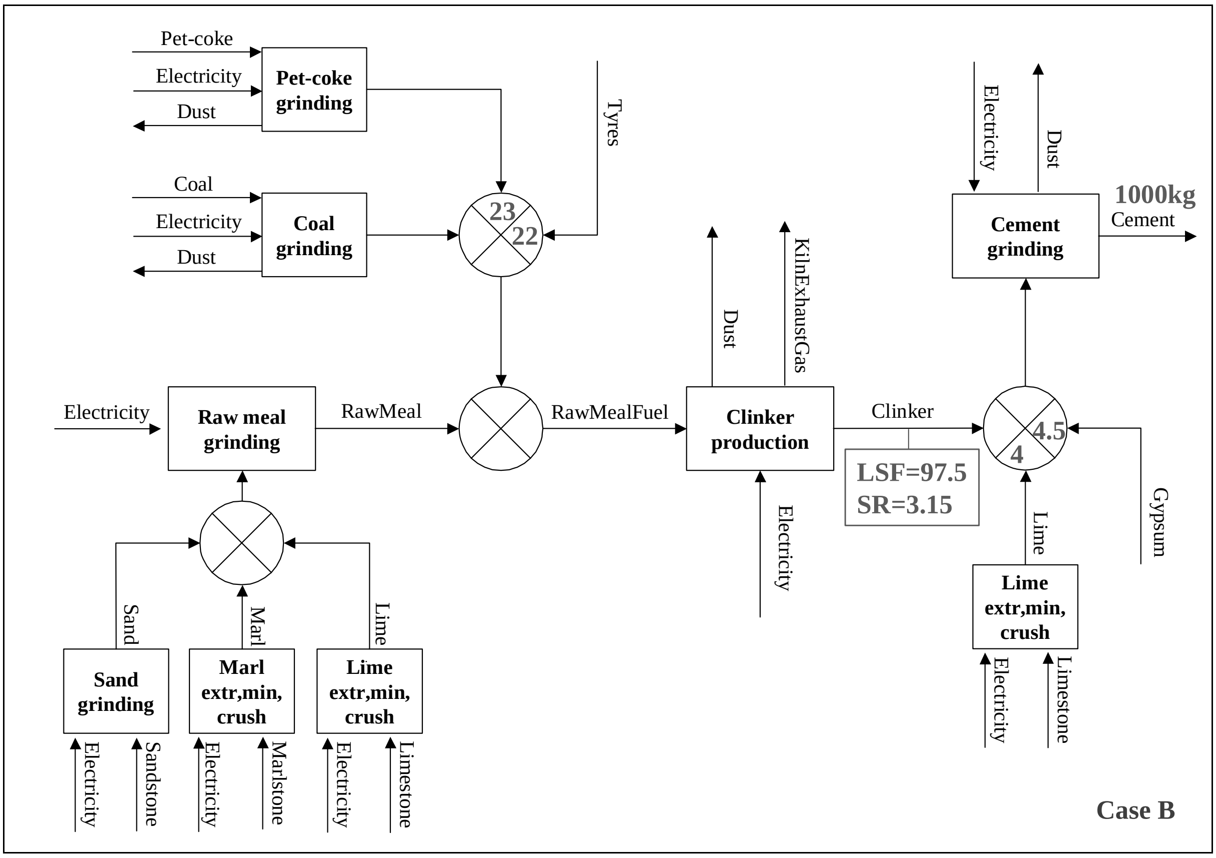


Figure 6 *Problem formulation added to the neutral model, case B*

For each of the two operational alternatives, data generated with the model was compared with observations and measurements from 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 Figures 7 and 8 for the two real operational alternatives, respectively.

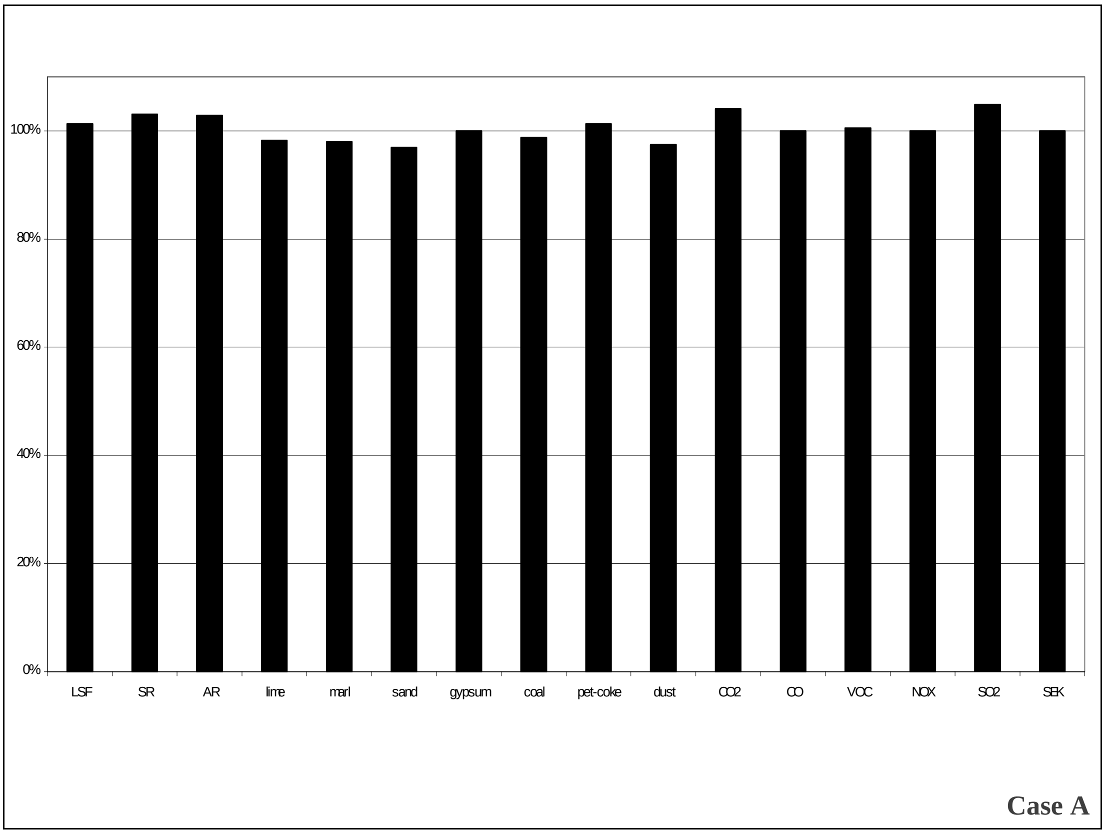


Figure 7 *Simulated values as a percentage of measured values. A selection from operational alternative A*

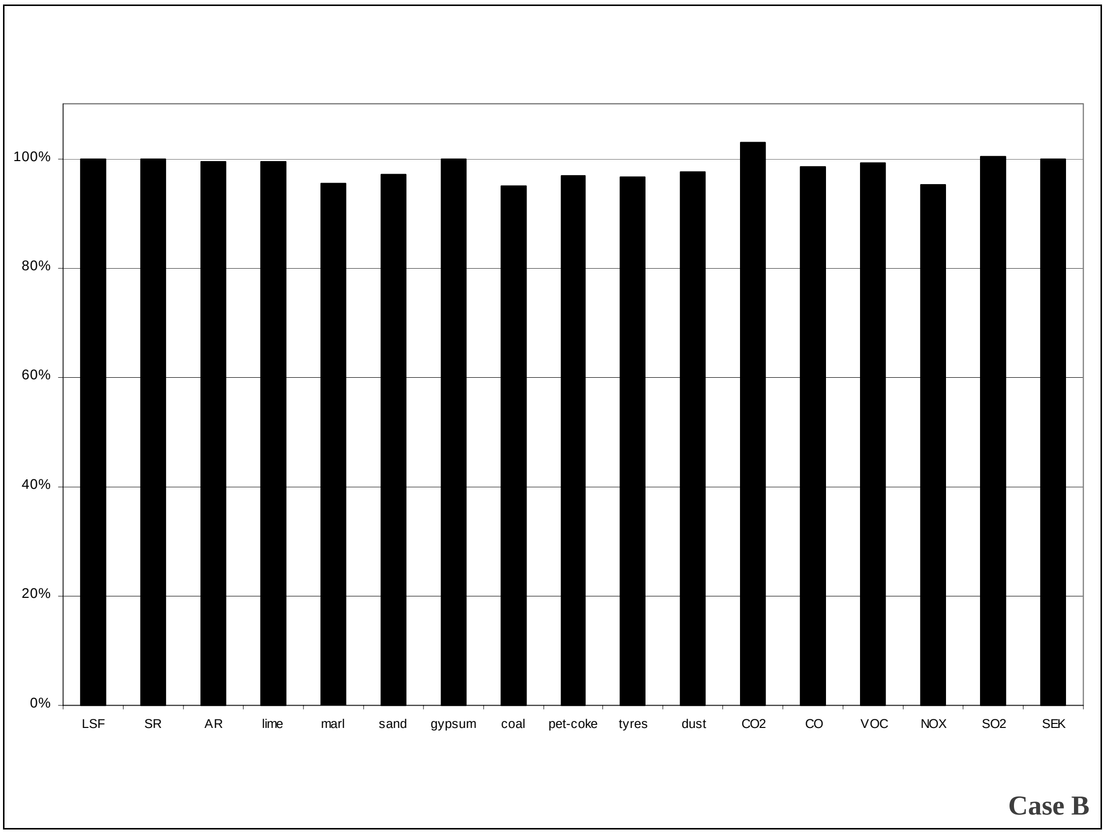


Figure 8 *Simulated values as a percentage of measured values. A selection from operational alternative B*

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

The model has been technically validated for metals. However, 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.

In the next section I will present how the life cycle model is used to explore the potential for minimising negative environmental impact through an increase in the use of industrial by-products and defined waste in cement manufacturing.

6. Simulating Operational Alternative for Future Cement Production

With the life cycle process model the potential for minimising negative environmental impact through an increase in the of industrial by-products and defined waste in cement manufacturing has been explored. I will present the main results and conclusions drawn in this section. However, first I will begin by explaining the nine different scenarios simulated. A more detailed description of the study and the results and conclusions can be found in Paper II.

6.1. Scenarios simulated

Industrial by-products can be used either in the raw meal mix or in the cement mix, and defined waste can be used in the fuel mix. In discussions with representatives from different departments at Cementa AB, it was agreed that it would be interesting to explore two raw meal mixes, two cement mixes and three fuel mixes. A raw meal mix, a fuel mix and a cement mix were then combined into an operational alternative, a scenario, to be simulated. This section briefly describes the different mixes and how they were combined into nine scenarios.

Industrial by-products (e.g., slag, fly ash, industrial gypsum, industrial sand) can be used as substitutes for traditional natural raw materials. The recovered materials can either be used as raw material in the raw meal, or in the cement grinding as substitutes for clinker or cement additives. According to the European standard “Cement – Composition, Specifications and Conformity Criteria” (EN 197-1 2000), a Type I cement must contain at least 95% clinker, a Type II cement 80% clinker, and a Type III cement at least 60% clinker. Different types of defined waste (e.g., used tyres, used plastics, spent solvents, waste oils) that cannot be recycled can instead be used as substitutes for traditional fossil fuel in cement manufacturing.

Cementa currently produces a Type II/A cement in which recovered material is used as cement additives and limestone replaces part of the clinker. The raw meal mix used today consists of limestone, industrial sand and a small amount of iron oxide. And, currently, about 25% of the fossil fuel is replaced with used tyres. These current mixes were combined to give an O-scenario.

Cementa’s environmental goal for 2003 is to replace at least 40% of the fossil fuel (by thermal energy content) used at Cementa’s three plants in Sweden, with alternative fuel (Cementa 2001). One future fuel mix to study, subsequently, is the substitution of 40% of the fossil fuel. Another interesting fuel mix is the substitution of 80% of the fossil fuel. An interesting raw meal mix to study is the substitution of part of the limestone with recovered material. Furthermore, an interesting cement mix to study is a Type III cement in which additional clinker is replaced by limestone and recovered material.

The current mixes and future mixes were combined into nine operational alternatives to be simulated, as shown in Table 2.

Table 2 *Operational alternatives to be simulated*

Scenario	**Raw meal mix**	**Fuel mix**	**Cement mix**
0	Current; 93.5% limestone and 6.5% recovered material	Current; 25% alternative fuels	Current type II; 84% clinker, 10% limestone, 6% recovered material
A	Current; 93.5% limestone and 6.5% recovered material	**Replace 40% fossil fuel**	Current type II; 84% clinker, 10% limestone, 6% recovered material
B	Current; 93.5% limestone and 6.5% recovered material	**Replace 80% fossil fuel**	Current type II; 84% clinker, 10% limestone, 6% recovered material
C	**80% limestone, 20% recovered material**	**Replace 40% fossil fuel**	Current type II; 84% clinker, 10% limestone, 6% recovered material
D	**80% limestone, 20% recovered material**	**Replace 80% fossil fuel**	Current type II; 84% clinker, 10% limestone, 6% recovered material
E	Current; 93.5% limestone and 6.5% recovered material	**Replace 40% fossil fuel**	**A type III; 60% clinker, 15% limestone, 25% recovered material**
F	Current; 93.5% limestone and 6.5% recovered material	**Replace 80% fossil fuel**	**A type III; 60% clinker, 15% limestone, 25% recovered material**
G	**80% limestone, 20% recovered material**	**Replace 40% fossil fuel**	**A type III; 60% clinker, 15% limestone, 25% recovered material**
H	**80% limestone, 20% recovered material**	**Replace 80% fossil fuel**	**A type III; 60% clinker, 15% limestone, 25% recovered material**

6.2. Main results

The nine simulations performed show that the use of recovered material and alternative fuel can be increased with no negative impact on cement performance. All nine scenarios are feasible in relation to current requirements on product performance.

All development options A to H result in improvements in the studied parameters. The foreground system is the dominant contributor to most of the parameters.

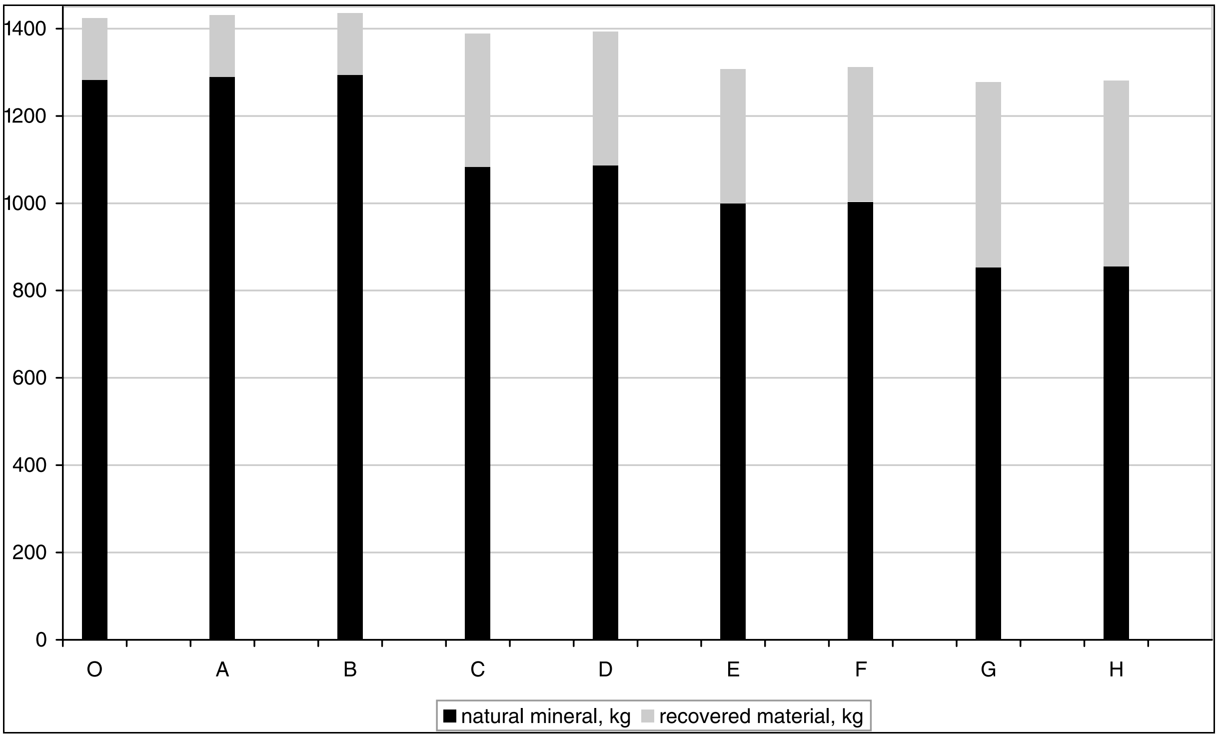


Figure 9 *Use of natural mineral and recovered material, kg per 1 000 kg cement, in the foreground system, scenarios O to H.*

Natural mineral resources are only used in the foreground system (Fig. 9). An increase in the use of recovered material replaces the use of natural mineral resources. An increase in use of recovered material also reduces the total use of natural mineral resources.

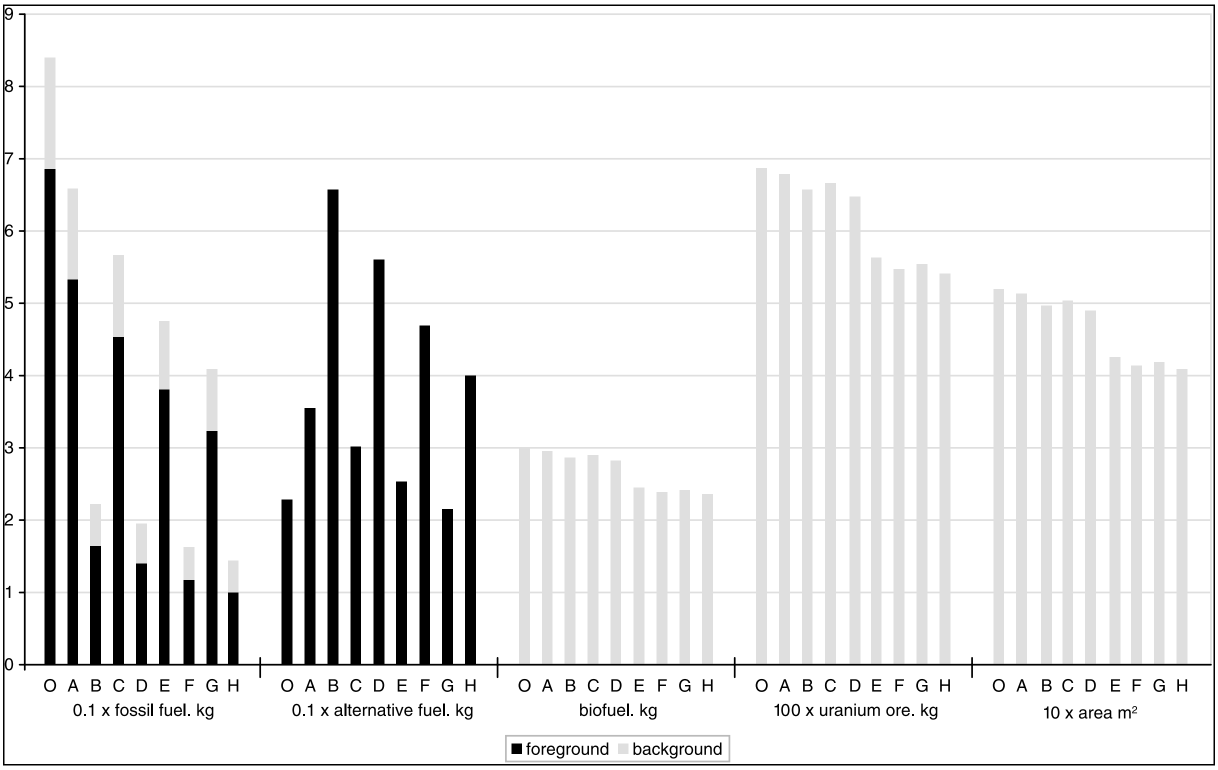


Figure 10 *Resource use, per 1 000 kg cement, in the background and foreground systems, scenarios O to H. For each category, the bar for each scenario is divided into the use in the foreground system and the use in the background system. Note that different units are used.*

The use of other natural resources is reduced with an increase in the use of recovered material and alternative fuel (Fig. 10). An increase in the use of alternative fuel replaces the use of fossil fuel.

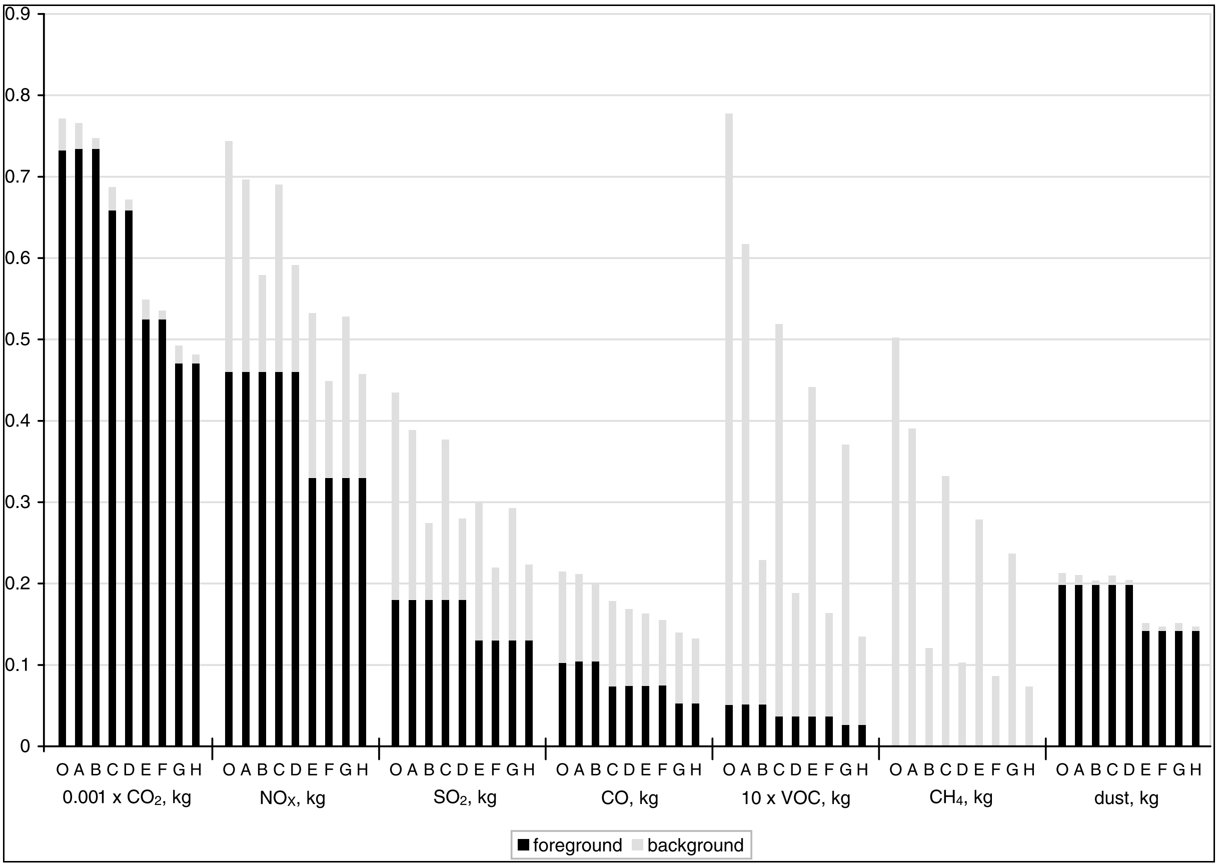


Figure 11 *Emission to air, per 1 000 kg cement, from background and foreground systems, scenarios O to H. The bar for each scenario is divided into the emission from the foreground system and the emission from the background system. Note that different units are used.*

The simulations show that emissions of CO_2, NO_X, SO_2, CO, VOC CH_4 and dust can be reduced with an increase in the use of recovered material and alternative fuel (Fig. 11). Even if the emission of CO_2 from alternative fuel is valued the same as the CO_2 emission from fossil fuel, the total CO_2 emission can be reduced from about 780 to about 480 kg per ton cement.

The emission of small amounts of toxic substances, such as metals, dioxins and furans has not been modelled. These emissions depend, to a large degree, on minor variations in the raw material and fuel chemical composition.

7. Discussion and Conclusion

Based on the needs and requirements of the cement industry, a life cycle process model has been designed and built. The purpose of the model is to provide a tool for supporting decisions made on product and process development options. The requirements on a flexible model that generates information on product performance, economic cost and environmental performance, from a life cycle perspective, were seen as important.

The chosen approach, which entailed dividing the cement manufacturing process into a foreground and a background system and modelling the two sub-systems with different techniques and levels of detail proved to be successful.

The modelling approach used to build the foreground system model, a calculational non-causal model, physical modelling and an object-oriented modelling language, can enhance the flexibility, modularity and comprehensiveness of the model. Together with an appropriate simulation tool (for this application, ASCEND IV was used) the approach provided a flexible and general purpose model. The chosen software also supports non-linear and dynamic elements for future use.

By separating a neutral model from the problem formulation and simulation technique, the model can be used to perform different types of simulations and to solve different problems. By making use of physical and object-oriented modelling all physical entities in the manufacturing process are kept together and described independently of each other. This satisfies the requirement for flexibility, in terms of future modifications to represent and simulate process development options and other manufacturing plants.

The foreground system model has been validated and shows satisfactory agreement with the real system’s properties, with the exception of metals.

The result is a flexible and valid life cycle model of the current manufacturing process at the Slite plant. The model can be used to solve many different problems. Different development options can be simulated and information on potential environmental, product and economic performance is generated. Thus, the same model can be used for a number of different purposes.

The model has been used to explore the potential for reducing the negative environmental impact of cement manufacturing through an increase in the use of recovered material and alternative fuel. It has been shown that the model can simulate the desired development options differently. The desired information is generated and assessed in relation to current requirements on product performance. The generated information can be used to give indications of development options for further investigation and study. The nine simulations show that the use of recovered material and alternative fuel can be increased with no negative effect on product performance. The use of resources and the studied emission to air can be substantially reduced.

8. Future Research Needs

As a result of the chosen modelling approach and simulation tool, the model, as such, has potential for development. One area for future research is to develop the model and the problem formulations so as to enable performing optimisation with the model. The library of re-usable problem formulations and model parts can be developed and extended. Additional modelling developments to be studied would be non-linear and dynamic interaction, which transforms input into output, and increases the level of detail in the model, where applicable.

Detailed knowledge about the formation of, e.g., metal, dioxin and furan emissions and how these emissions depend on variations in raw material and fuel composition are needed. The life cycle process model should be complemented to include these.

The valuation of CO_2 from different sources can be further explored. This includes both enlarging the model to include alternative waste treatment, as well as studies of the carbonisation rate of concrete.

The model was designed and built based on the commissioner's needs and requirements. Thus, the model is to be used to support decisions made on product and process development options. Another interesting area for future research is to study in what ways and how the model supports decisions made on product and process development options.

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