Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Journal of Cleaner Production 12 (2004) 77–93
Journal of Cleaner Production
www.cleanerproduction.net

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

Karin Gäbel [a,b,*], Peter Forsberg [c], Anne-Marie Tillman [a]

[a] *Environmental Systems Analysis, Chalmers University of Technology, S-412 96 Gothenburg, Sweden*
[b] *Cementa AB, Research & Development, P.O. Box 144, S-182 12 Danderyd, Sweden*
[c] *CPM—Centre for Environmental Assessment of Product and Material System, Chalmers University of Technology, S-412 96 Gothenburg, Sweden*

Received 3 April 2001; received in revised form 26 June 2002; accepted 11 December 2002

Abstract

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

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

1. Introduction

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

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

---

[*] Corresponding author. Tel.: +46-8-625-68-22; fax: +46-8-625-68-98.
E-mail address: karin.gabel@cementa.se (K. Gäbel).

doi:10.1016/S0959-6526(02)00196-8

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

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

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

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

2. Background

2.1. Cement manufacturing and related environmental issues

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

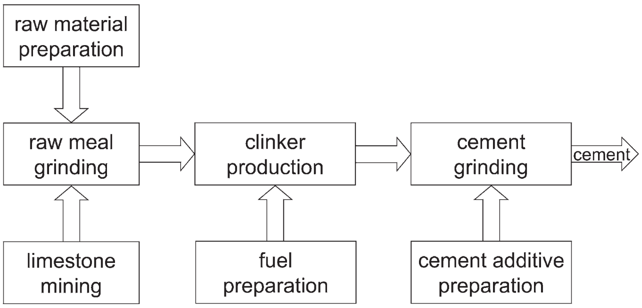

Fig. 1. Cement manufacturing process.

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

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

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

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

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

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

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

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

2.2. Means and work done to minimise negative environmental impact

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4. Conceptual model and system boundary

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

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

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

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

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

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

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

The foreground system was divided into the following processes:

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

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

The background system consists of the following processes:

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

The plant in Slite produces waste heat used for district

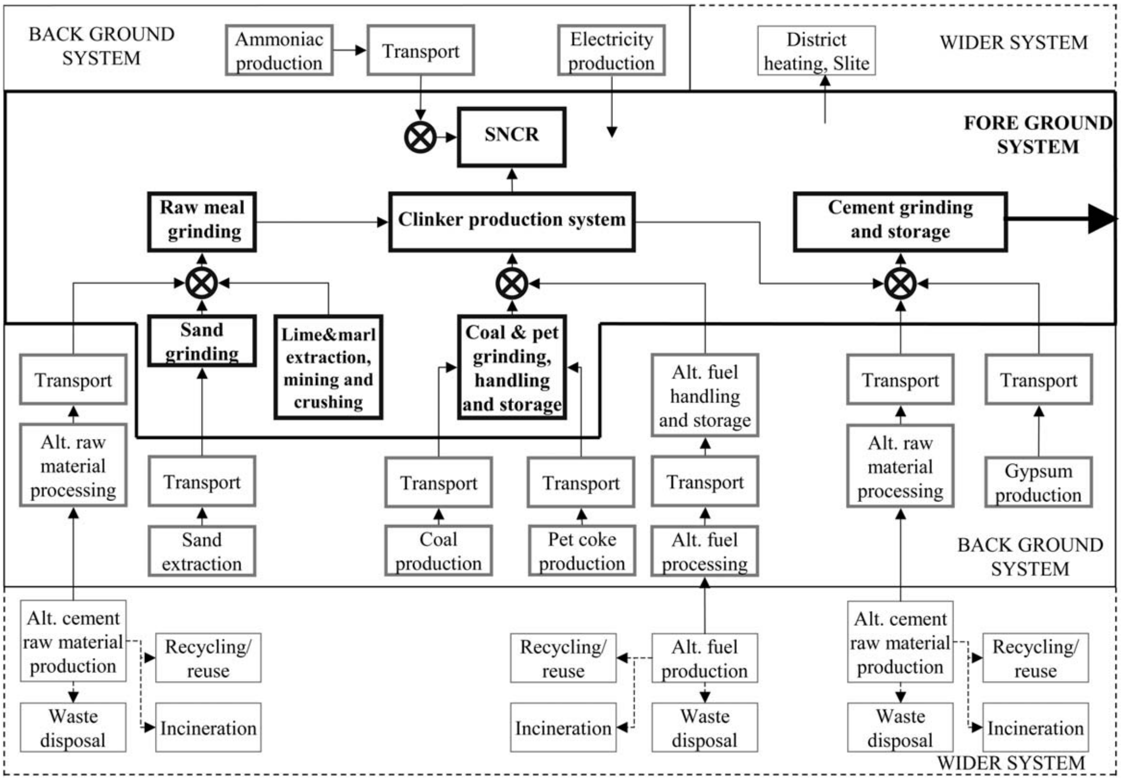

Fig. 2. Conceptual model.

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

Not considered are:

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

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

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

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

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

Table 2
Material and fuel composition

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

5. Modelling and simulation

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

5.1. System technical interpretation

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

In addition, the model needs to support:

- Dynamic elements;
- Non-linear elements.

Simulation types the software tool needs to support:

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

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

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

5.2. Model construction

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

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

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

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

Table 5
Syntax used in declaration of objects

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

5.2.1. Composition

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

Table 4
Total listing of objects in the model

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

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

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

5.2.2. Mass stream

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

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

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

5.2.3. Material–fuel stream

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

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

5.2.4. Kiln exhaust gas stream

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

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

5.2.5. Chemical analyser

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

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

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

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

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

5.2.6. Material–fuel mixer

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

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

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

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

5.2.7. Material–fuel grinder

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

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

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

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

5.2.8. Clinker production

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

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

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

5.2.9. Cement plant

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

5.3. Problem formulations

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

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

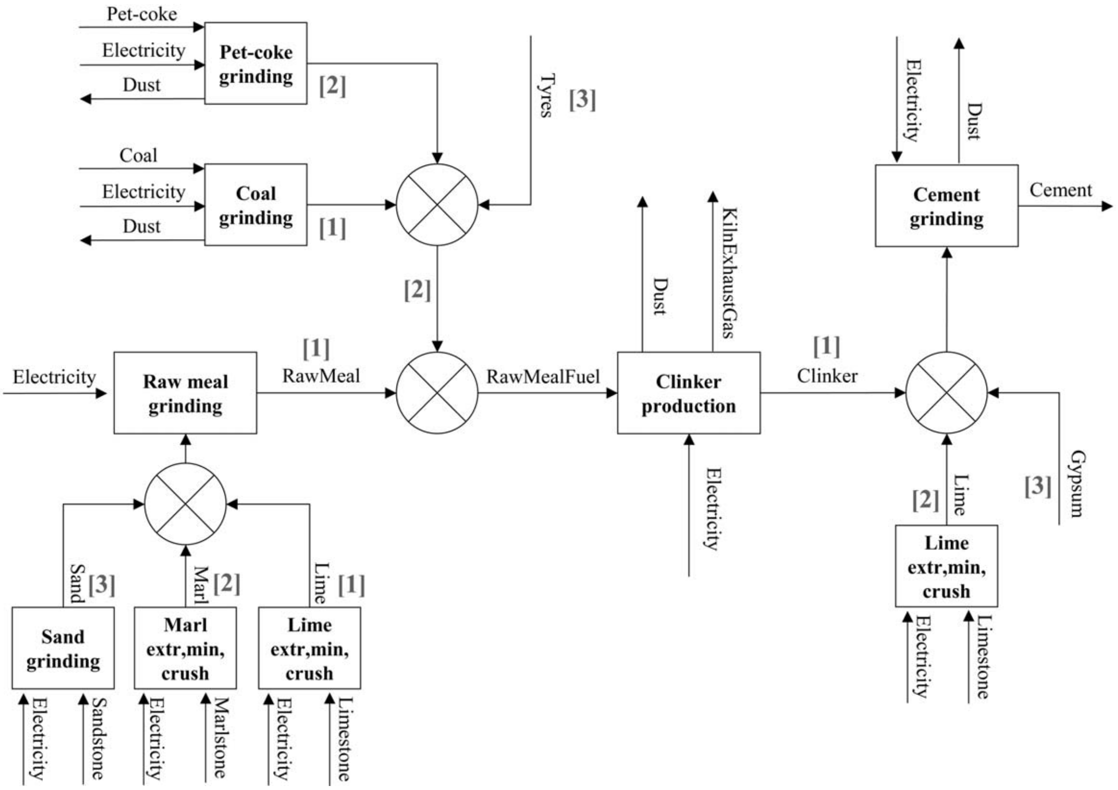

Fig. 3. Foreground system model.

ally locked variables are initiated with suitable input data.

- The calculation method to use, which sorts equations and calculates the result by invoking a mathematical algorithm.

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

5.3.1. Case A

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

5.3.2. Case B

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

5.4. Model validation and simulation

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

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

To validate the foreground-system-model, and in

Table 6
Constants and input data for Case A

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

Table 7
Constants and input data for Case B

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

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

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

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

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

6. Discussion and future research

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

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

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

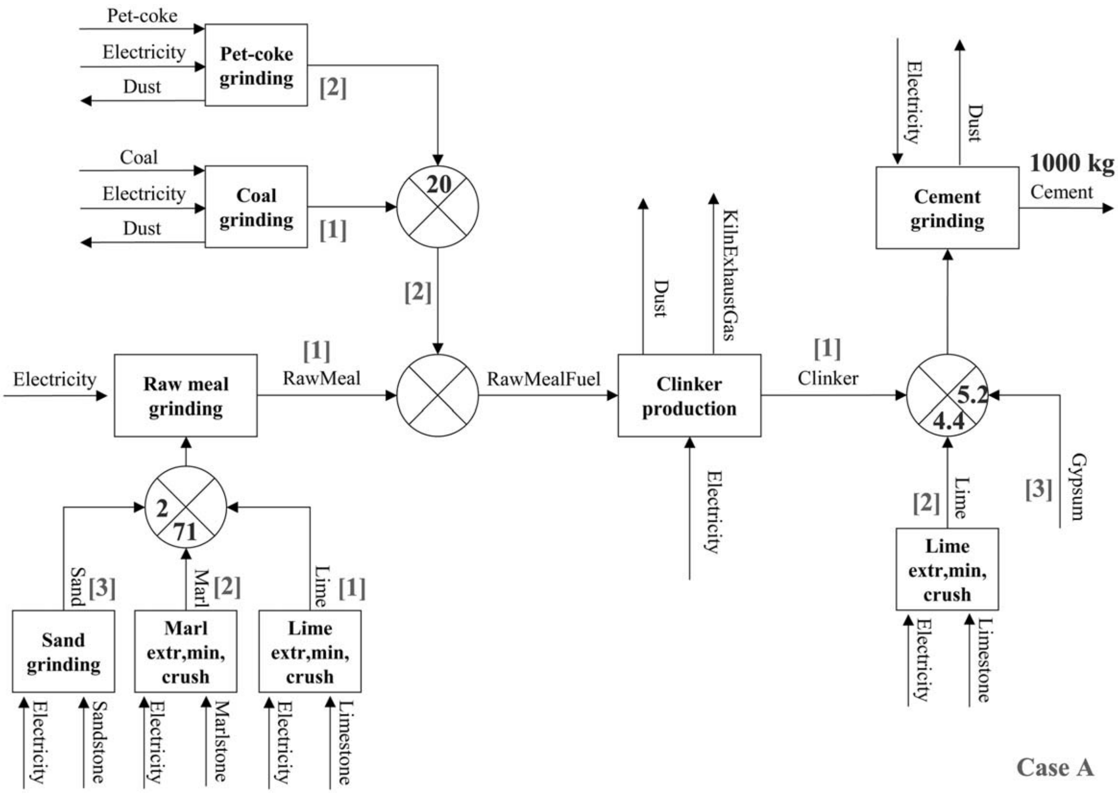

Fig. 4. Real operational alternative A to be simulated.

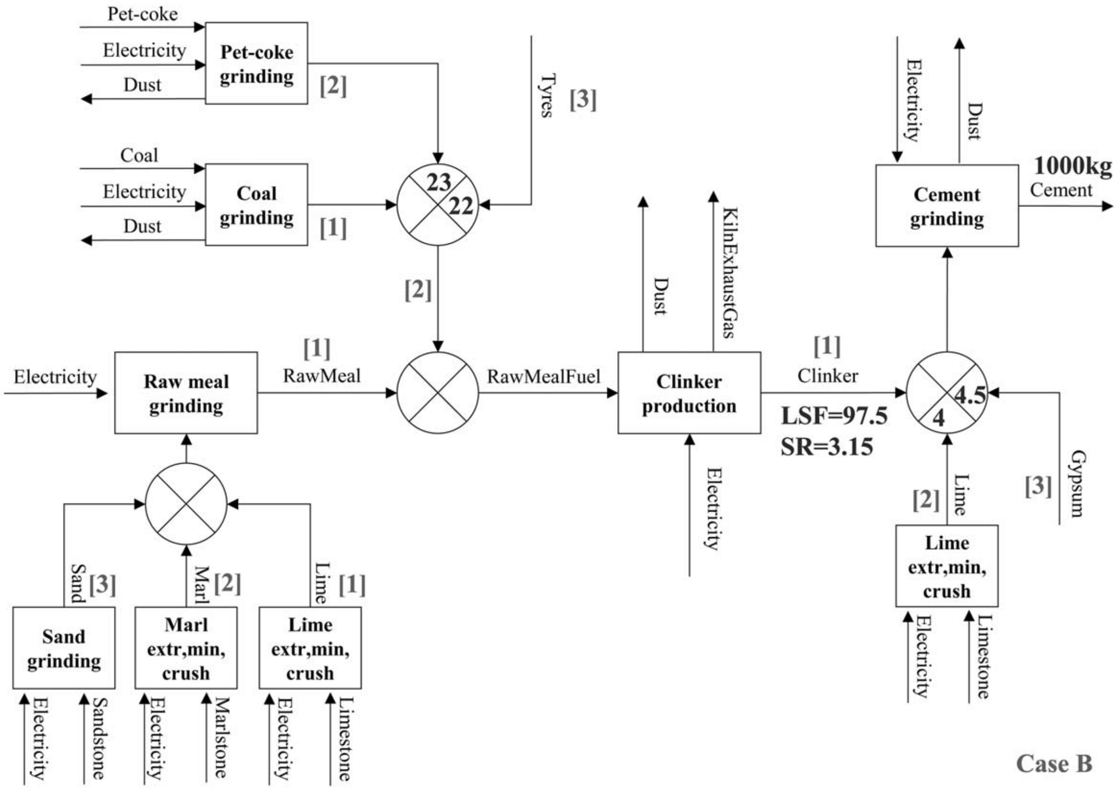

Fig. 5. Real operational alternative B to be simulated.

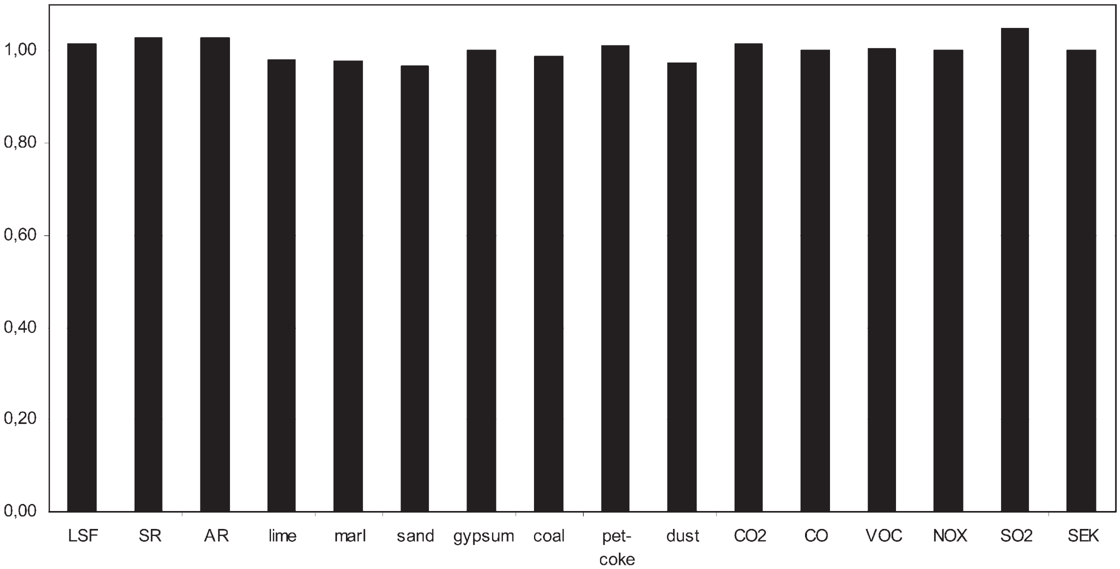

Fig. 6. Simulated values as a percentage of measured values. A selection for operational alternative A.

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

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

Naturally, the validation process of the cement model

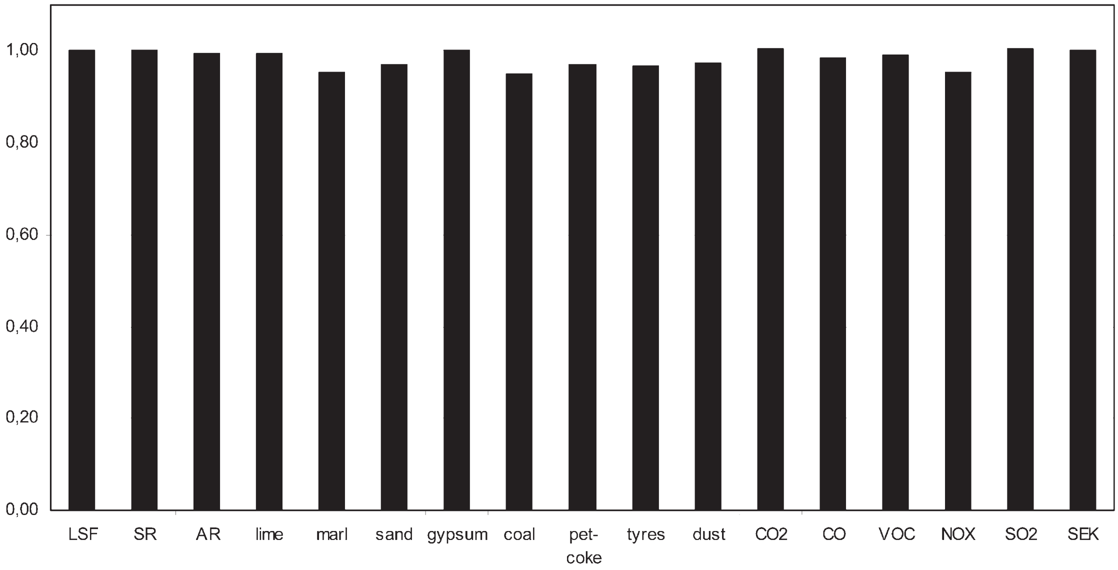

Fig. 7. Simulated values as a percentage of measured values. A selection for operational alternative B.

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

Acknowledgements

We thank Cementa AB for financing Karin Gäbel's industrial doctoral project. The project has been included in the research program at the Centre for Environmental Assessment of Product and Material Systems, CPM. We also thank Bo-Erik Eriksson at Cementa AB for co-ordinating and prioritising the commissioner's needs and requirements and for valuable recommendations on the level of detail in the model.

References

[1] Lundström K. Miljöanpassad betong — Slutrapport (In Swedish). Stockholm, Sweden: Finncement AB, 1997.
[2] Björklund T, Tillman A-M. LCA of building frame structures — environmental impact over the life cycle of wooden and concrete frames. Göteborg, Sweden: Technical Environmental Planning, Chalmers University of Technology; 1997.
[3] Björklund T, Jönsson Å, Tillman A-M. LCA of building frame structures — environmental impact over the life cycle of concrete and steel frames. Göteborg, Sweden: Technical Environmental Planning, Chalmers University of Technology; 1996.
[4] Häkkinen T, Mäkelä K. Environmental adaption of concrete and asphalt pavements. Helsingfors, Finland: VTT, 1996.
[5] Lundström H, Ölind G, Rydberg T. Life cycle assessment of concrete sewage pipe. Göteborg, Sweden: Chalmers Industriteknik, 1996.
[6] Vold M, Rønning A. LCA of cement and concrete — main report. Fredrikstad, Norway: STØ (Stiftelsen Østfoldforskning); 1995.
[7] Lundström H. LCA av betongtakpannor — en analys av miljöbelastning under takpannans livscykel (In Swedish). Göteborg, Sweden: Chalmers Industriteknik, 1997.
[8] Van Geem M. The Portland Cement Association's environmental life cycle assessment of concrete, air & waste management Association's 91st Annual Meeting & Exhibition, San Diego, California, USA, June 14–18, 1998.
[9] Ölund G, Rydberg T. Livscykelanalys av marksten. Göteborg, Sweden: Chalmers Industriteknik, 1998.
[10] Nisbet M, Van Geem M. Environmental life cycle inventory of Portland cement and concrete. World Cement, 1997.
[11] Gäbel K. Cement manufacturing-process and material technology and related environmental aspects. Gothenburg, Sweden: Environmental Systems Analysis, Chalmers University of Technology, 2001.
[12] Best available techniques for the cement industry. Brussels, Belgium: Cembureau, the European Cement Association; 1999.
[13] IPPC — Integrated pollution prevention control — reference document on best available techniques in the cement and lime manufacturing industries. Seville, Spain: European Commission, Technologies for Sustainable Development European IPPC Bureau; 2000.
[14] Cementa och miljön (In swedish). Stockholm, Sweden: Cementa AB; 2001.
[15] Byggcement- Teknisk beskrivning (In Swedish). Stockholm, Sweden: Cementa AB; 2000.
[16] Tillman AM. Significance of decision-making for LCA methodology. Environmental Impact Assessment Review 2000;20(2000):113–23.
[17] Environmental management — life cycle assessment — goal and scope definition and inventory analysis. ISO 14041:1998. Geneva, Switzerland: International Organization for Standardization; 1998.
[18] Strömberg JE. A mode switching modelling philosophy. In: Electrical Engineering. Linköping: Linköping University; 1994. p. 24-9.
[19] Heijungs R. Environmental life cycle assessment of products; 1992.
[20] Eborn J. OmSim. Lund, Sweden: Department of Automatic Control, Lund Institute of Technology, Box 118, SE-221 00; 1998.
[21] Dymola. Dynasim AB, Research Park Ideon, SE-223 70 Lund, Sweden; 2001.
[22] ASCEND IV. Engineering Design Research Center, Carnegie

Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213-3890, USA; 2000.

[23] Westerberg A. A modified least squares algorithm for solving sparse N×N sets of nonlinear equations. Engineering Design Research Center, Carnegie Mellon University EDRC TECH REPORT 06-5-79; 1979.

[24] Carlson R, Tillman AM, Steen B, Löfgren G. LCI data modelling and a database design. International Journal of LCA 1998;3(2):106–13.