Chemitecs Concept Model

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ChEmiTecs
ChEmiTecs is a research program funded by the Swedish EPA. The program's goal is to improve the understanding of emissions of organic substances from articles and to clarify and determine the magnitude of this problem. The program aims to support development of Swedish and EU management programs to minimise risks from harmful substances. The program started in December 2007 and will proceed until December 2012. Participating organisations and organisation representatives are:

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1 Introduction

1.1 Purpose and Scope

A concept model is a collection of named and described concepts including descriptions of their relations. The main purpose of a concept model is to facilitate communication and to structure information so that it can be unambiguously understood from different stakeholder perspectives within a given scope.

The scope in Chemitecs is extraordinary wide and encompasses the release of substances into the environment due to combined use of products in society and how these emissions alter the state of the environment. In short this scope is referred to as the "product use system". Human/societal activities are part of this system and therefore the analysis of the system covers both chemicals, goods, its production in values-chains, final use and to some extent waste handling.

This scope can be viewed from numerous different perspectives, for example research and development of chemical compounds and materials, product development, product manufacturing, product user scenarios, user perceptions of risk, media coverage, marketing strategy, emission processes, direct exposure assessment, chemical risk management, environmental impact assessment, eco-toxicology and human toxicology, control by authorities, macro economics in terms of national statistics on sector production, import and export activity, etc. Within each perspective a collection of concepts are being used to describe the relevant parts of the system. Often the same words are used by practitioners from different perspectives; however, the exact meaning of the concepts may differ. Also, the exact same concept may have different names (synonyms) depending on what perspective is applied. Indeed, the terminologies, models and approaches related to the scope are easily perceived as a complex web hampering an efficient discourse between different stakeholders. The Chemitecs concept model is intended to relate the different perspectives to a model which serves as a commonly understood language platform that with a required accuracy describes the relevant parts of the product use system.

The purpose of the work performed in Chemitecs is to gain a better understanding of the processes that governs emissions of chemical substances from products in general and of organic (carbon-based) substances in particular. This will be further studied in case studies on a selected set of organic chemical compounds existing in products. Further, an overall estimation of the total emissions and environmental effects from the combined use of all products in Sweden will be performed predominantly through a model of the product use system.

The concept model provides an initial platform for the quantitative modelling process. The different concepts can be used as definitions of dimensions need to be precisely defined in terms of what is included in and what is excluded. E.g. it must be decided what types of products, materials, use types, and emission processes are considered in the total emissions assessment. Any quantitative results from such a broadly scoped model is foreseen to be relatively crude as every aspect cannot be accounted for in detail due to the vast data requirement and lack of full knowledge of actual material content of products, of product use, of emission mechanisms, and of environmental cause-effect chains. They would rather provide an indication of the magnitude and nature of the dominating causes of the environmental impact of the product use system. In order to understand what the model actually does and what real world phenomenon it represents the concept model will again serve as a crucial communication platform and a starting point for further development.

The Chemitecs concept model has been developed based on previous concept models on related subjects. These models are presented in the next chapter on state of the art. From the ongoing continuous communication within the research programme key concepts emerge. Focussed concept modelling sessions have been performed in order to choose relevant concepts and describe how they relate to each other. A key question for the choice of included concepts is "What information is needed to quantify emissions of chemical substances from using products?". The model presented in this report is considered as version 1 and may be adjusted if inconsistencies, crucial omissions or redundancies are discovered when using the model.

1.2 State of the art – related approaches

Based on a thorough literature research (Fuhrman et al. 2010) concept models covering the issue of total emissions and environmental impact of the product use system has not been developed earlier. There are however some related scientific work that has been undertaken. One important approach is life-cycle assessment. However the LCA methodology has in practice omitted much of these emissions as the focus has been on more directly quantifiable flows such as discharges to water, process exhausts, and final disposal as waste from a specified product. Normally, no emissions are considered during the use of a product unless direct emissions are an inherent function of the product such as the case with pesticides. Much focus of LCA has also been on the larger flows related to carbon dioxide, sulphur dioxide and a few more. Related to LCA, but applying more extended system boundaries, is the so called input-output LCA model that uses an economy wide approach linking econometric data to environmental concerns. There are also a few attempts to use this approach for dealing with chemicals (Wright et al. 2008)

The concept modelling methodology originally is based on information management methodology mostly applied in information technology development and has proven a useful tool to deal with complex environmental issues.

1.2.1 SPINE – Generic environmental information

Due to the interdisciplinary nature of environmental assessment a number of concept models have been developed for areas related to the scope of Chemitecs.

Based on a general need for structuring information for Life Cycle Assessment a generic model called the SPINE model was developed to describe the main aspects of environmental information (Carlson et al. 1995). The core concepts of the SPINE model is shown in figure 1.

The SPINE model divides the universe in three distinct systems where the physical reality encompasses the Technical and Nature Systems. The subjective evaluation of the physical world is given within the Social system. The Nature system includes all natural materials and processes in the world without artificial manipulation. The Technical system encompasses artificial technical and organisational constructs for extracting and refining natural resources into more useful goods. Also, this manipulation causes changes in the Nature system. If effects in the Nature system caused by the Technical system are evaluated as adverse in the Social system we refer to them as environmental problems.

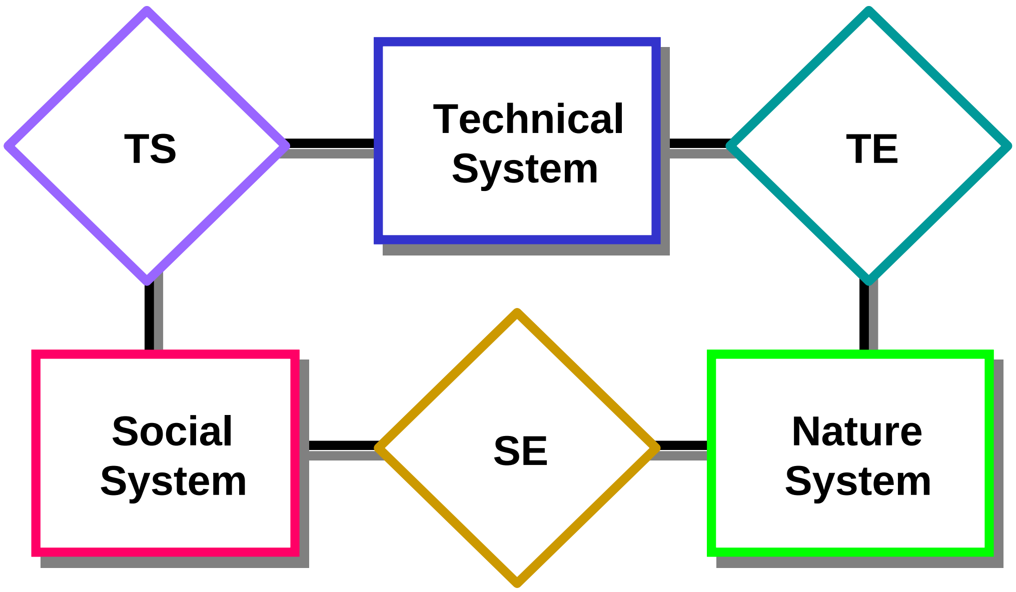

Figure 1 The generic SPINE model of envrionmental information (Carlson, 2006).

In environmental assessment the generic issue is ultimately to perform an evaluation of goods from the Technical system and/or effects from the Technical System in the Nature system. Information is needed from all three systems to understand what actions and constructs in the Technical system are causing effects in the Nature system, what added value is provided from the technical constructs, and at the same time what the effects on nature are worth.

In Chemitecs the focus is primarily to understand the physical relation of using products and how this effects the environment, e.g. how using cars in the Technical system causes increased levels of toxic substances in aquatic ecosystems in the Nature system. Describing the evaluation in the Social system is at an initial study not a focus issue but will be considered qualitatively.

1.2.2 OMNIITOX – concepts for the nature system

Each of the three systems in the SPINE model can be broken down into sub-concepts with higher resolution. An effort to do this was done in the OMNIITOX project which purpose was to harmonize different environmental modelling approaches including Risk Assessment and Life Cycle Impact Assessment (Molander et al. 2004). The core of the OMNIITOX concept model is presented in figure 2 (Tivander et al. 2004).

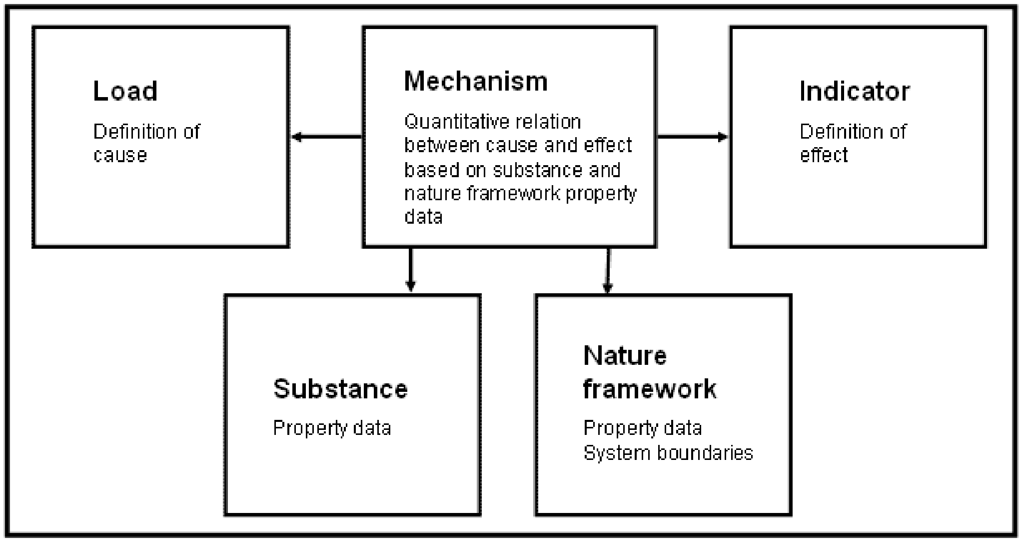

Figure 2 The core of the OMNIITOX concept model (Tivander et al., 2004).

The main idea of the model is to link phenomena in nature in a cause and effect chain. The part of nature being studied is defined as the Nature Framework with well defined system boundaries. Specific phenomena in nature of interest are defined as Indicators, e.g. concentrations of chemicals in the fresh water, biodiversity, etc. A change – a stress – is introduced in the Nature system represented by the Load concept, e.g. an emission of formaldehyde into air. The Mechanism is the link describing how a Load affects an Indicator. In order to provide a quantified description of the mechanism, property data is needed on ambient parameters in the Nature Framework, e.g. precipitation and temperature, and also data related to substances such as chemical and toxicological properties of the substance in the emission.

The Load-Mechanism-Indicator link can be extended into longer cause effect chains by interconnection of mechanisms, as shown in Figure 3. This implies a widening of the overall system boundaries of the model, i.e. the connected sub-mechanisms are all members of a superior aggregated mechanism.

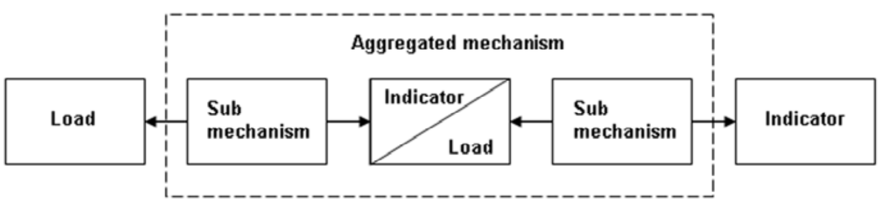

Figure 3 A cause-effect chain can be modelled if the indicator of a mechanism is identical to the load of a subsequent mechanism. The aggregated mechanism encompassing sub-mechanisms can be regarded as a 'unit' mechanism (Tivander et al., 2004).

If the inner sub-mechanism structure of the aggregated mechanism is disregarded, the aggregated mechanism can be regarded as a 'unit' mechanism. The superior mechanism can in turn be incorporated as a sub-mechanism of yet another mechanism. In this way an arbitrary number of sub-levels of mechanisms with different levels of detail can be transparently interconnected in the same model by using the same core concepts. This kind of conceptual hierarchies are often revealed when unbundling the complexity of the physical world. Detailed breakdown and descriptions of all concepts in the OMNIITOX are given in the report *Concept model for the OMNIITOX Information System Including OMNIITOX Data Format Definition* (Tivander et al. 2004).

In Chemitecs the focus is not on the development of a concept model covering the events after an emission and therefore a selected cause effect chain for assessing the environmental system will be applied, see figure 4. Chemicals are released into nature due to the use of products in society. How the emissions disperse in nature and give rise to changes in concentrations in different environmental compartments such as fresh water, air, and soil is described in the Fate mechanism. The modelled concentrations are referred to as Predicted Environmental Concentrations or PEC based on the terminology used in environmental risk assessment. The changed environmental concentrations in turn give rise to further effects. Eco-toxicological effects are estimated based on comparing the concentration with measured laboratory toxicological data on how organisms respond to such changes in concentration. Toxic effects on humans are first assessed in terms of exposure i.e. how much of the substance is taken up into the body, also referred to as dose. Based on this dose the toxic effects are estimated mainly based on laboratory toxicity test data on mammals.

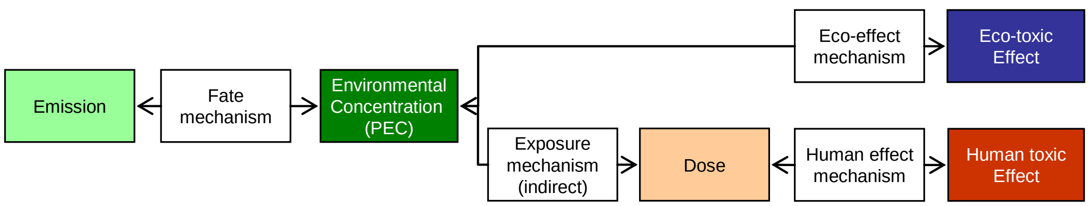

Figure 4 A selected set of loads indicators and mechanism constituting a conceptual environmental system cause effect chain applied in Chemitecs. Compare with the generic OMNIITOX core concepts.

1.2.3 RAVEL – concepts for products, components and materials

The RAVEL project was a project focussing on incorporating environmental performance in product design within the railway industry. A concept model was developed for structuring information for the calculation of environmental performance indicators based on properties of products, components, and materials (Carlson, Forsberg, 2000). Figure 5 shows a conceptual outline of the general method developed in the project. This breakdown of a product designs into components and materials provides a core structure of how to describe the relation between materials and products in the Chemitecs concept model. Each material and component is attached with values of properties relevant for the calculation of environmental performance indicators for the product design.

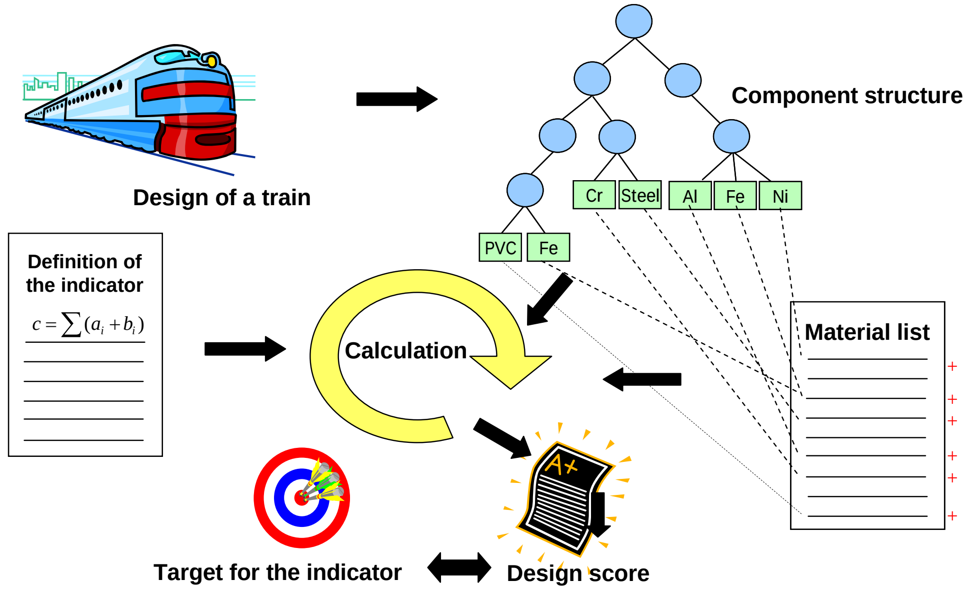

Figure 5 Conceptual approach from the RAVEL project for calculation of Environmental Performance Indicators of product designs (Carlson, Forsberg, 2000).

1.2.4 REACH - guidelines for assessing chemical exposure

The European Chemicals Agency ECHA (2008) has published Guidance documents for the implementation of the REACH legislation (EC, 2006). The guidance on "Estimation of exposure of articles" has a related scope to Chemitecs. A concept model developed by ECHA based on mass pools and flows provides an interesting approach with the focus perspective on a given chemical, as outlined in figure 6. Assuming a steady state of chemical flows and pools, ECHA provides a practical quantitative approach to estimate emission factors for chemicals from products which may prove helpful when developing a the quantitative model in Chemitecs.

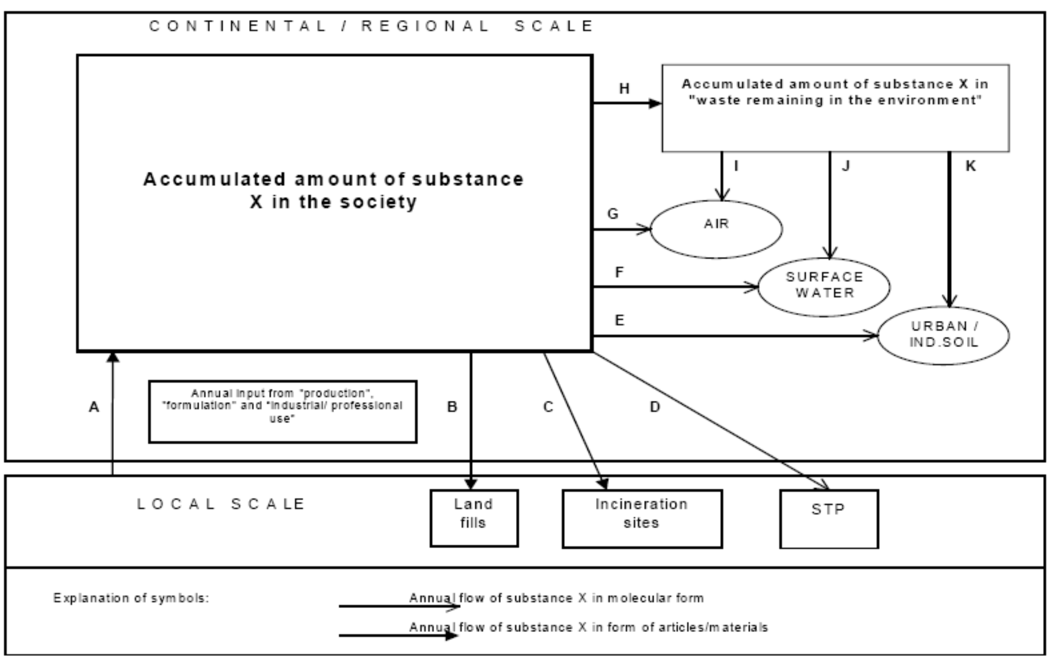

Figure 6 Concept model for exposure assessment from the guidance document from the European Chemicals Agency for the implementation of REACH (ECHA, 2008).

2 The Chemitecs concept model

2.1 Overview of the Chemitecs concept model

An overview of the Chemitecs concept model is presented in figure 7. As previously described the environmental system is assessed through the cause effect-chain starting from emissions and also through direct exposure to products. The main issue in the Chemitecs project to assess the magnitude of the environmental problems related to emissions of chemicals from using products. This puts the focus on describing and quantifying these emissions and direct doses which serves as a link between the technical and nature part of the product use system.

The core concepts of the technical system part of the model are product and use. Products may be sorted into categories such as chemical products, consumer goods, foodstuff, building products, etc. The product concept hence includes any physical products not limited to a specific category. Each product consists of one or several components, which in turn are made of one or several materials, which consists of one or several chemicals. Different types of properties and descriptions are related to each of the levels of physical representation from product category to chemical level.

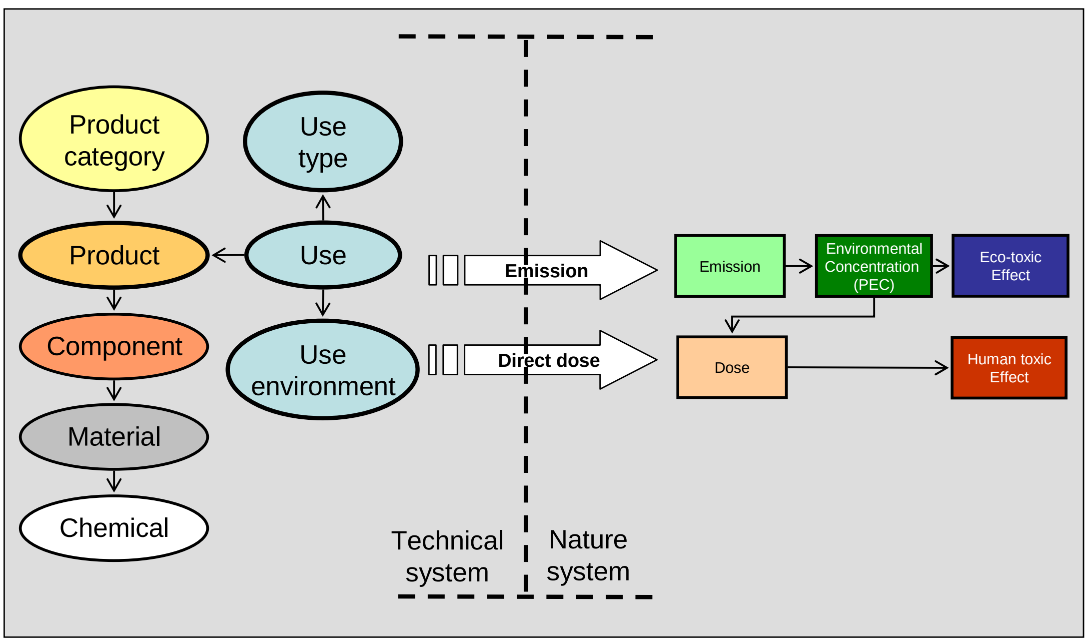

Figure 7 Overview of the Chemitecs concept model

The “use” concept is describing an episode of a given product. This includes active use e.g. “driving a car” and passive use e.g. “parked car in garage” or “demolishing of car”. How much chemical substances are emitted from a product depends on the type of use, the length of time it is used and the ambient environmental conditions in the direct vicinity where use takes place. The “use” concept is not limited to end-use of final consumer products but applies to any product. E.g. industrial manufacturing is considered a use of the products required for the manufacturing process.

2.2 Detailed descriptions of Chemitecs concepts

2.2.1 Product

The term product is defined in the project as any physical matter that is produced or designed for a use purpose; mostly products are traded on a market, but not necessarily. This definition is close to the terminology of economics where a tangible (physical) product is "a good" (Swedish "vara"). A product is the result of a physical production process of some sort, e.g. assembling components, processing material, preparation or reactions of substances.

As the focus in Chemitecs is on emissions from products i.e. physical flows of matter, the product concept used here only includes physical products. A product consists of one or several components that in turn are made of different materials. The commercial trading of *services* is only relevant in this context as they often imply usage of physical products. E.g. a commercial taxi service requires the use of products including cars and fuel etc. Hence commercial services are considered as a part of the use concept.

At this generic conceptual level there is no distinction between different types of products. This includes everything from consumer commodities, pharmaceuticals, food, cosmetics, chemical products, to infrastructure and production plants. Confer to the Product Category concept for a further elaboration of ways and rationales for categorizing products.

For comparison, the related term "Article" is defined by the European Commission (2006) within the REACH legislation on chemicals. Regulation (EC) No 1907/2006 defines an article as "an object which during production is given a special shape, surface or design which determines its function to a greater degree than does its chemical composition". This definition is intended as a distinction from chemical products which is the primary concern of REACH. The term "Chemical product" is defined in the Swedish Environmental Code (Swedish Government 1998) as "a chemical substance or preparation of chemical substances that is not an article". In the perspective of total material flows in society, as in Chemitecs, all concrete matter that is used by humans is included. In the Chemitecs concept model both articles and chemical products according to the above legal definitions are considered as products.

A product is generally something produced or imported and made available on a commercial market. This is important as the transfer of physical products between producers and users is mostly only indirectly registered in terms of monetary transactions. However, not all products are sold. A product could be given for free or produced for personal use or it may be an intermediate product or component in a more complex production process. In these cases very little information is available regarding the product quantities. This is also the case regarding the second-hand market. Monetary data on commercial product trade are however regularly collected and compiled covering the bulk part of product flows in society. This opens for a modelling of the link between monetary data and physical flows.

All products are unique. No product is exactly as another. This means that even when considering a specific product model of a specific brand, e.g. a specific shoe model it is a "product category" as it is a group of products and not a unique specific physical product.

One result of product use is waste generation. In essence waste is very similar to products. Like products waste involves a material flow and it is managed and used which gives rise to emissions. Hence in the Chemitecs concept model the concept of waste can be seen as a subset of the product concept. A main difference between waste and other products is that products are primarily designed to be useful and fulfil a function. When this usefulness is ended the product is discarded and considered to be waste. Only to a minor degree the inevitable management of the waste resulting from the product is considered in the design of new products.

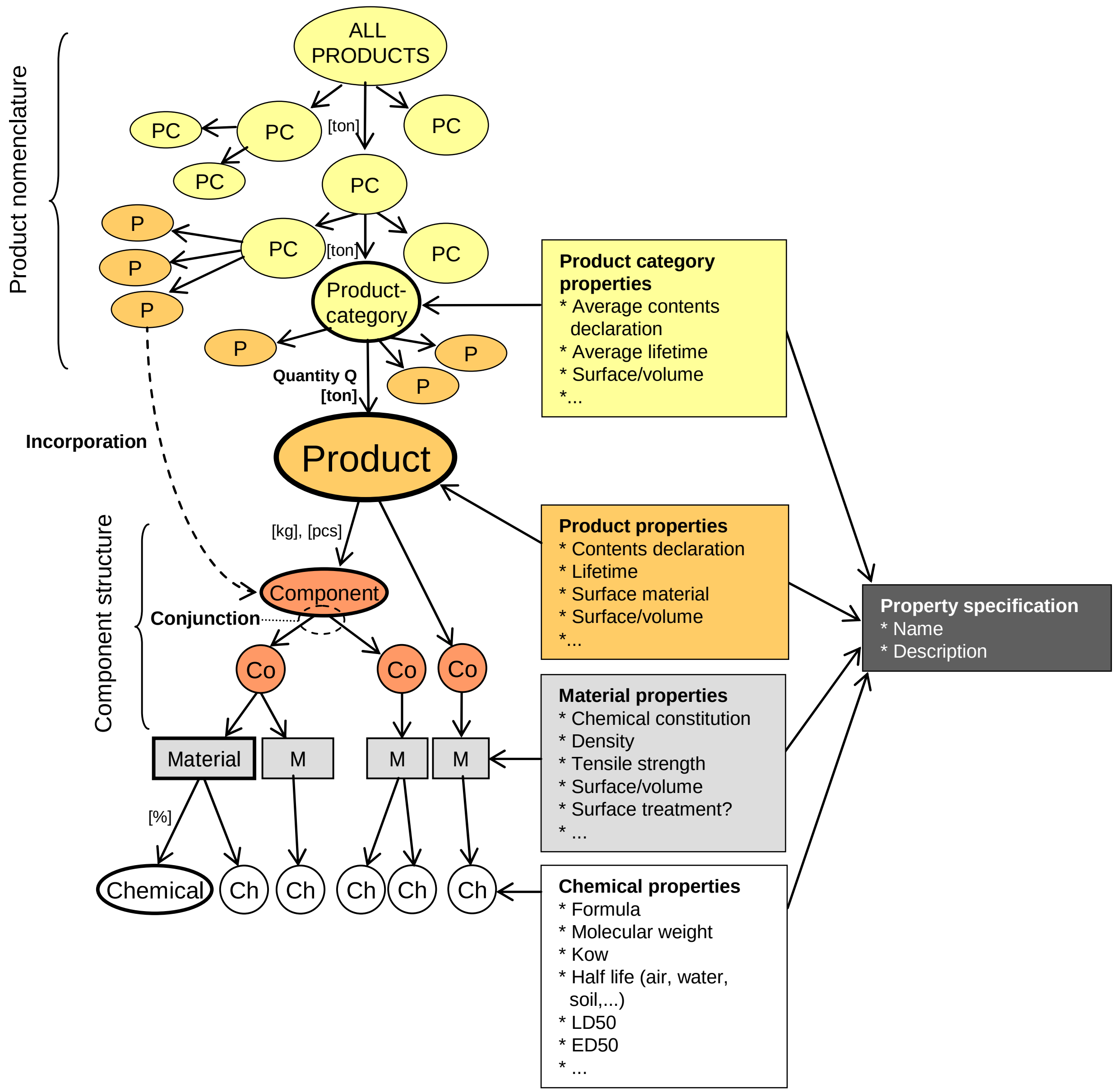

Figure 8 The concepts related to products in Chemitecs concept model: from chemicals via material, components, product to product categories.

2.2.2 Product property

The commercial aspects of products are linked to subjective evaluation based on functionality, aesthetics, comfort, safety and also more intangible properties such as brand, PR, status, etc. Such properties genuinely distinguish products from the other concepts of physical matter including materials and chemicals. These properties are used in the perspective of assessing the market and may be relevant to the overall understanding of the problem context. However, the Chemitecs concept model focus on the physical properties of the product that contribute to the products potential to emit chemicals. These properties include lifetime, age, component structure, material content, surface material, etc.

For a specific product each property is given by a property value, e.g. the product property "lifetime" of a certain model of a mobile phone has the value "3.5 years". Numerical property values may be given with statistical parameters to illustrate the domain and likelihood of possible values. Metadata about the origin and acquisition method of a property value can be documented as an inherent part of the product property.

2.2.3 Property specification

Each property of products, product categories, materials, and chemicals needs a definition to ensure they are consistently acquired, documented, and interpreted. A property specification is such a definition with a specific property name and a descriptive explanation of its physical representation. Depending on perspective the description may be more or less strict. For example the material property specification "tensile strength" may be defined with a requirement that a specific measurement method must be applied to obtain a property value with a defined resulting statistical parameterisation. In contrast, the product property specification "content declaration" may be described without any restrictions in observation method or required level of detail.

The level of requirements defined on data depends of course on the application. For a product developer strict material property specifications may be required to work efficiently. In the vast majority of cases, within the scope of Chemitecs, property data need to be gathered where possible, so it is abundantly clear that it is not practical to put very strict requirements on data but rather to leave as many options as possible to obtain the property values. However, focus is put on a description of the physical representation of the property to avoid misinterpretation of any property values.

2.2.4 Product category

Products can be categorized into groups of products in order to avoid dealing with each unique product at a time. There are many reasons for categorizing products that can be applied but some typical aspects are: legal "chemical products", "foodstuff", "pharmaceuticals"; intended use of the products e.g. "footwear", "personal vehicles", "detergents"; material content e.g. "bulk polymer plastics", "wood products"; size and shape "polymer tubes with diameter < 10 cm", "wooden rods". Aspects can be combined such as "organic solvents" where both material content and intended use are inherent.

Product categories can be organised in a hierarchy starting with all products divided into finer categories. At the lowest possible level the unique specific product level is reached. The possible ways and rationales for categorizing products are limited only by our imagination.

An ideal product categorisation in the Chemitecs perspective would be based on similarities of product of key physical properties contributing to the emission potential, such as material content. The available trading data on product category quantities however is mainly created from other principles such as function or legislation. Probably more physically related or LCA-stage related descriptions are to be preferred.

As waste is considered a subset of product concept waste categories based on waste generating sector and waste fraction type are additional types of product categories.

2.2.5 Product category property

Product category trading data is continuously collected in terms of how much imported, exported or sold from new production. This product category property data is generally given in monetary value and sometimes in physical quantities (e.g. mass or volume) it is possible to track how products flow in the technosphere. Also, it is possible to extrapolate many product properties into averages for product categories enabling quantification of emissions from many products simultaneously. For example an average content declaration or average life time of the product category "tyres" can be generated.

2.2.6 Component

A component is a part of a product with a distinguishable shape, material content, and function in the product. Every product consists of one or several components, e.g. a train engine consists of thousands of components while a plastic cup consists of one single component. In more complex products it can be useful to describe a component structure where components are divided into sub-components. At the lowest level in the component structure each component is made of materials. Through this branched (hierarchical) structure each part of the component structure can be unambiguously quantified and eventually the contents of the entire product can in principle be determined.

Some products are produced and sold with the direct intention to become components in other more complex products, such as a steering wheel may be produced and sold to become a component of a car. See also the Incorporation concept for managing this distinction in order to avoid double counting of emissions from such products and from the product in which the product is a component. See also the RAVEL information model (Carlson, Forsberg, 2000).

2.2.7 Conjunction

A conjunction is a description of how components are connected to each other. The relative location of the components can be described as "adjacent" or "encapsulated". The conjunction concept also includes the mode of connection, e.g. glued, welded, screwed, etc.

2.2.8 Incorporation and lifetime

When considering the entire domain of products in a society it is important to distinguish between whether emissions are regarded to emanate from the use of components or from use of products of which the components are parts. In order to avoid double counting when quantifying these emissions the incorporation concept is introduced. Incorporation means that a product is used as a component in another more complex product.

Regarding (chemical) products that are used as ingredients mixed or reacted into a more complex product the same incorporation concept applies.

The lifetime and hence all uses of the incorporated (component-)product is considered to end the moment the new more complex product is sold and is starting to be used. Consider for example a steering wheel for a car that is manufactured and sold to a car manufacturer. Uses of the steering wheel include transportation to the car manufacturer and assembly into the car. During this use any emission emanating from the steering wheel is attributed to the steering wheel as a specific product. The lifetime of the steering wheel product can either end at the time of mounting or when the car is sold from the manufacturer; the steering wheel is now a component of the car. Any emissions from the steering wheel component after this point are considered to emanate from using the car product. However, at a later stage, during scraping and waste handling, components can "re-emerge" as a waste product, a type of "second life" of a product to consider in the conceptual model (see below).

2.2.9 Material

A material is physical matter with a defined, mostly homogenous, structure and chemical composition. Materials in the forms we know them in daily life are in different shapes and composition such as metals and alloys, polymers, preparations and substances. There might be exceptions to consider, but at this stage of the conceptual model the development can proceed without considering high-tech materials such as self-polishing windows.

Gases and liquids and powders are also considered to be materials in the Chemitecs concept model. E.g. when a bottle containing water is sold as a product, the liquid water is considered as a material.

At the material level certain physical properties are of interest such as tensile strength, brittleness, density, water absorption capacity, flammability, etc. In comparison with the product concept, the material concept has no inherent commercial aspects. A material can however be commercialized by making a product out of it. All products ultimately consist of materials.

Materials consist of one or several chemicals, either included for their functional properties or as impurities, i.e. chemicals with no function or even with impairing properties on the overall intended function of the material. In solid materials the composition of chemicals constituting the material are often described as a matrix, e.g. a polymer matrix may consist of main polymer strands with a pattern of distributed added functional chemicals such as fillers, flame retardant, ultraviolet-stabilizers etc.

Functional chemicals in polymers are either reactive or additive. Reactive chemicals react with and bind chemically to the host polymer whereas additive functional chemicals are monomer molecules that are not chemically bound to the polymer. For a more thorough description on this subject see Appendix 2 Polymers and functional chemicals.

It is common that the exact chemical composition of materials used in products is not fully known. This is problematic when assessing how much of the different chemicals are emitted from products. A reason for this loss of information is that focus lies on the desired functional properties of the included chemicals rather than exact molecular structure. Different chemicals may have the same function or nearly the same function in a material and are sometimes regarded as interchangeable. This leads to material content described based on functionality, e.g. polystyrene with 2 % flame retardants, 0.5 % UV stabilizers, etc. The communication of actual material content is also often limited by commercial protection of property rights making data acquisition more difficult. Nevertheless is there a commonly acknowledged need for detailed and available declaration of real chemical contents.

2.2.10 Material property

At the material level a number of properties are relevant for the assessment of emission potential. Some examples are chemical constitution, structure, surface/volume ratio, etc. Emission factors for some chemicals exist for some materials. Functional material properties such as tensile strength, heat conductivity, fire resistance, etc are also relevant to assess emission potential of chemicals.

As the exact chemical composition of materials is often not fully known it is difficult to estimate the emissions from a specific material in a specific product. Bulk data on functional chemical use in society may provide a possible way to estimate the overall emissions of such chemicals.

2.2.11 Chemical Substances

Chemical substances are defined based on their molecular structure, i.e. the elemental composition and structure of molecules. In the REACH legislation (EC 2006) a substance is defined as "a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition".

The chemical substance concept does not imply any commercial or intentional aspects on function as may be implied by legislative texts regarding producers and importers of chemical products. The concept only concerns the physical structure and properties of elements and molecules. A chemical substance is the resulting chemical product of a chemical reaction.

In both human and eco-toxicological discourse the chemical substance perspective has traditionally been the starting point. When assessing the environmental effects of an emitted substance it is common that the fate, exposure and effect of one single chemical substance at a time are analysed in isolation from other chemicals. Environmental studies of chemicals are mainly done on how the chemical behaves in the nature system based on data obtained from laboratory tests. To gain control of the development towards a society free of toxic chemicals in the environment, the origins and flow of chemicals in the technosphere must also be assessed; from their creation, as building blocks of materials into products and emissions.

There are large gaps of knowledge and data regarding chemical properties, complete material compositions, emission processes related to product structure and use, routes of chemicals in nature, chemical derivates and metabolites, and interaction between chemicals. The sheer number and combinations of different chemicals, products, uses, emissions and finally environmental distribution, transport, transformation processes and effects makes it very difficult to account for them all in a broad system perspective.

2.2.12 Chemical property

Properties relevant to the chemicals are e.g. molecular weight, vapour pressure, melting point, half life in air, and LD50. The properties are relevant both for the amount of chemical substance emitted from products and for the assessment of effects in the environment.

In order to track how chemicals are flowing in the product stream a possible approach is to also account for the functional properties of chemicals, i.e. what function the chemical serve as a part of a material. This can be particularly useful for tracking additives often added in low concentrations in materials.

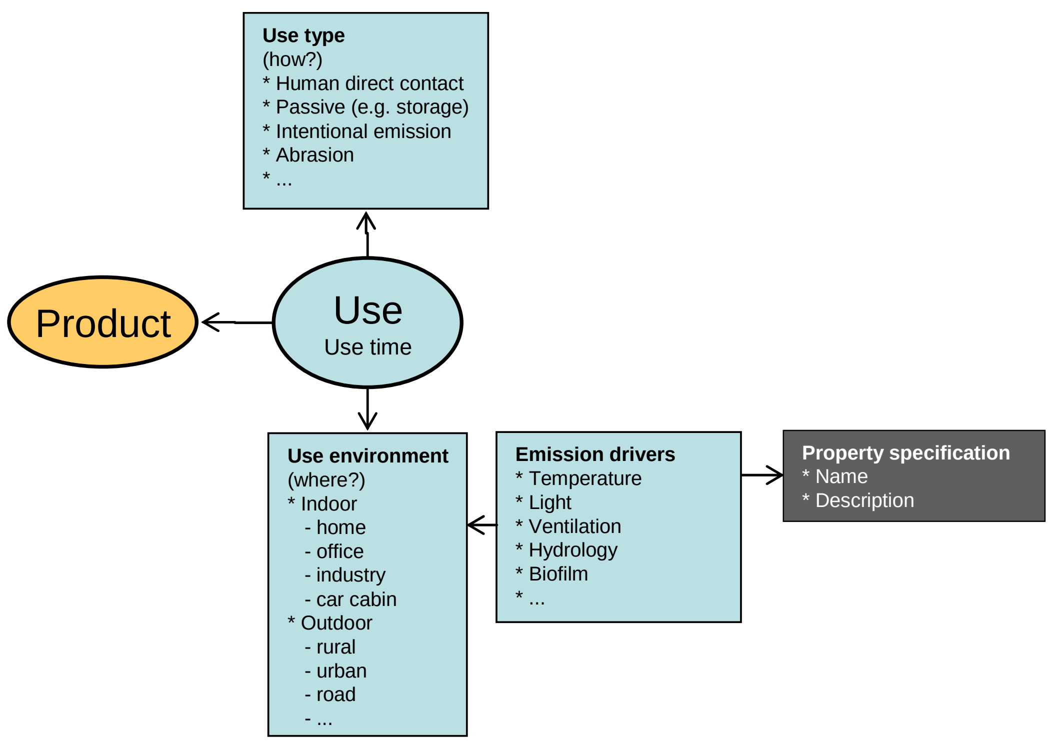

Figure 9 The use concept in the Chemitecs concept model

2.2.13 Use

The use concept encompasses all uses of products. All episodes of how products are handled, actively or passively, are included.

To this definition Chemitecs concept model adds the same use of chemical products. Hence the Chemitecs use concept includes all uses of products defined in the model.

A clear distinction must be made from the concept of product *function* which is an idealized description of the intended use and not necessarily what actually happens to a product. Taking a pencil as an example its primary function is writing or drawing, but for most pencils that is only a part of how they are actually used. For the most part of its lifetime it is passively stored somewhere (on a desk or a drawer or a pocket), it can be used as a toy, be chewed on, poking holes in the ground with, etc, etc.

A use of a product is a combination of product (*what* is used) use type (*how* the product is used), use environment (*where* the product is used), and use time (*how long* the product is used).

The REACH legislation defines use of an article as; "any processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, production of an article or any other utilisation" (EC 2006). This definition provides examples of uses related to chemical products and articles.

Product use-time and product lifetime

A lifetime of a given product can be divided into episodes of uses where each use occurs over a time span called use-time. Adding all use-times of a product equals the product's lifetime.

The lifetime can be defined to start at the point when the finished product is delivered from the producer to the customer. Such a product transaction generally involves a monetary exchange when the product is sold. As such economic data on transactions exists for all commercial product exchanges it can be used to provide bulk information of the flow of products.

However, an exact definition of the start of a product lifetime might be problematic as not all product transactions are traceable through commercial data. For instance products can be handed over internally in a company, they can be given for free, they can be sold second-hand or on the black market etc. However for industrially produced products the start of a product lifetime based on commercial trade data covers the bulk majority of products flowing in society.

A possible definition of when the lifetime of a product ends is when it is considered to be waste. According to the current EC regulations[1] the definition of waste is defined as follows:

"'waste shall mean any substance or object in the categories set out in Annex I which the holder discards or intends or is required to discard;". As the 16 categories in Annex I referred to in the definition contains a final category stating: "Q16 Any materials, substances or products which are not contained in the abovementioned categories", it means that the legal definition of waste in practice collapses to: any substance or object which the holder discards or intends or is required to discard. This legal waste definition is however not fully compatible with the Chemitecs definition of products and product use. Concerning the mere intention or the legal duty to discard is it unclear how to

[1] DIRECTIVE 2006/12/EC OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 5 April 2006 on waste, Article 1(a)

quantify the amount of such "intended" waste as well as any emissions occurring until the time the product is actually discarded. A more practical delimitation of the end of a product lifetime is when the product is actually discarded.

Data on collected waste exists with different waste fractions from different sectors. Some of the waste streams are however not handled with controlled waste treatment activities such as littering, dumping or burning in open fires. As there are little data on the amounts of these unmanaged waste streams it is difficult to estimate what emissions they cause.

As soon as the product becomes waste its lifetime is considered to have ended and it enters another stage, the end-of-life stage. Hence any waste treatment of a product is not considered as a use of that product, but can be considered as the creation of a new product – a waste product or a waste handling product. Many waste treatment activities results in *new* waste treatment products, such as compost from composting, syngas from thermal gasification, etc. This is also the case with re-use and material recycling processes. These products are considered as new products just as any other virgin product.

The specific case of re-use poses a difficulty to adequately account for the life-time of a product. In the case of direct re-use with the same function it is quite straightforward, e.g. the case with re-using glass bottles. It becomes more difficult when a product is re-used but with entirely different function such as a rubber tyre that may become too worn out for a car but instead can function as a swing in a playground or impact protection barrier on a dock or a race course. Some of these re-uses are traceable through commercial transaction data of e.g. how many used tyres are sold.

It could also be argued that waste treatment is considered as the final use of a product. Any emissions occurring during the waste treatment can either be allocated to the "old product" or to a new "waste product".

However the considerations regarding the conceptualization of products end-of-life and the waste-handling stage must be regarded as preliminary. There are reasons to link the further development to the so called cradle-to-cradle approach, which maintain the ideas that all materials need to be re-cycled. Therefore the chains of products, starting with raw materials (a product according to our concepts), production of material (also a product) and the further production of components (products) can be seen as the root system of a tree, that after entering the waste handling stage is "componentized" or "de-produced" into waste products and further made into materials (also products) and so on.

The *unpacking of a product* is a specific question worth mentioning due to the fact the packaging materials is of huge significance both for product quality, marketing, as a significant (waste related) material stream and for emissions occurring during this stage. It is possible to view the packed product as a specific product and to consider "componentization" to start with the unpacking of the product (packaging being a component and the useable product also as a component (in comparison to the packed product). By this kind of somewhat extended definitions the "component/product"-terminology can be maintained from the very start of the value chain with raw material extraction into the very end of the chain where either resources are gained from the waste handling or valueless and harmless emissions are released to the ecosphere.

2.2.14 Use environment

When using a product the amount of chemical emissions released from the product differs depending on the immediate environment where the use takes place. Also, the receiving environment of the emission may differ. Different use environment may be defined such as "Indoor home", "Indoor car cabin", "Indoor industrial" and "Outdoor urban", "Outdoor rural", etc. The use environment types are characterized by key parameters that influence the emissions, see the Emission driver concept. Preset combinations of default values on the emission drivers can be defined for the types.

2.2.15 Emission driver

An emission driver is a property that has a particular influence on the emission from the product. Some examples of such drivers are connected to the use environment such as temperature, light, ventilation, humidity, etc. Others depend on the use type such as internal heating when using the product or whether abrasion occurs or not.

2.2.16 Use type

The use type concept concerns *how* a product is used. Examples of use types are "Storage", "Transportation", "Active handling" etc.

A use type can be described through assigning values to predefined parameters such as "direct skin contact", "Passive/Active", "Intentional emission", "Abrasion" etc.

2.2.17 Emission factor and Direct dose factor

An emission factor is a quantitative multiplier estimating the emission of a substance from a defined set of descriptors of the technical system. In mathematical terms an emission E_c of chemical c is given as

$$E_c=F_c*X$$

where, F_c is the emission factor and X represents a product use situation defined with a set of descriptors. The emission factor can be given on different levels of detail e.g. the amount emitted from a specific material, product, and use. It is also possible to define such factors on aggregated levels such as the emission per product category, or per material accumulated in all products, or per use environment. The concept model provides many different entry levels for such assessments but the general issue remains to quantify emissions.

Direct dose factors are similar to emission factors but apply where products are used in direct contact with humans and thereby shortcutting the environmental fate model in the nature system.

2.2.18 Emission Driver profile, Emission Velocity profile and Total Product Emission

In reality emissions are dynamically changing and depend on the continuous changes of use environment and the associated emissions drivers, use type and changes in the product geometry and contents. An emission factor is therefore a simplification relating to an assumed specific or aggregated use situation.

A more generic approach to determine emissions is to apply emission driver profiles which describe how relevant emission driving parameters change over time during the product's lifetime, such as temperature variations, and use type.

Time profiles can also be described of the physical geometry and chemical substance contents of the product, which also may change over time. This includes surface materials, encapsulation, and whether the shape of the product changes at any point, e.g. by opening a cover of a box or unfolding a tent, etc.

Emissions velocity profiles describe how fast substances are emitted from the product over its lifetime. These velocity profiles can be calculated based on the driver profiles. Integration of the emission velocity profile over the product lifetime yields the total emission from the product.

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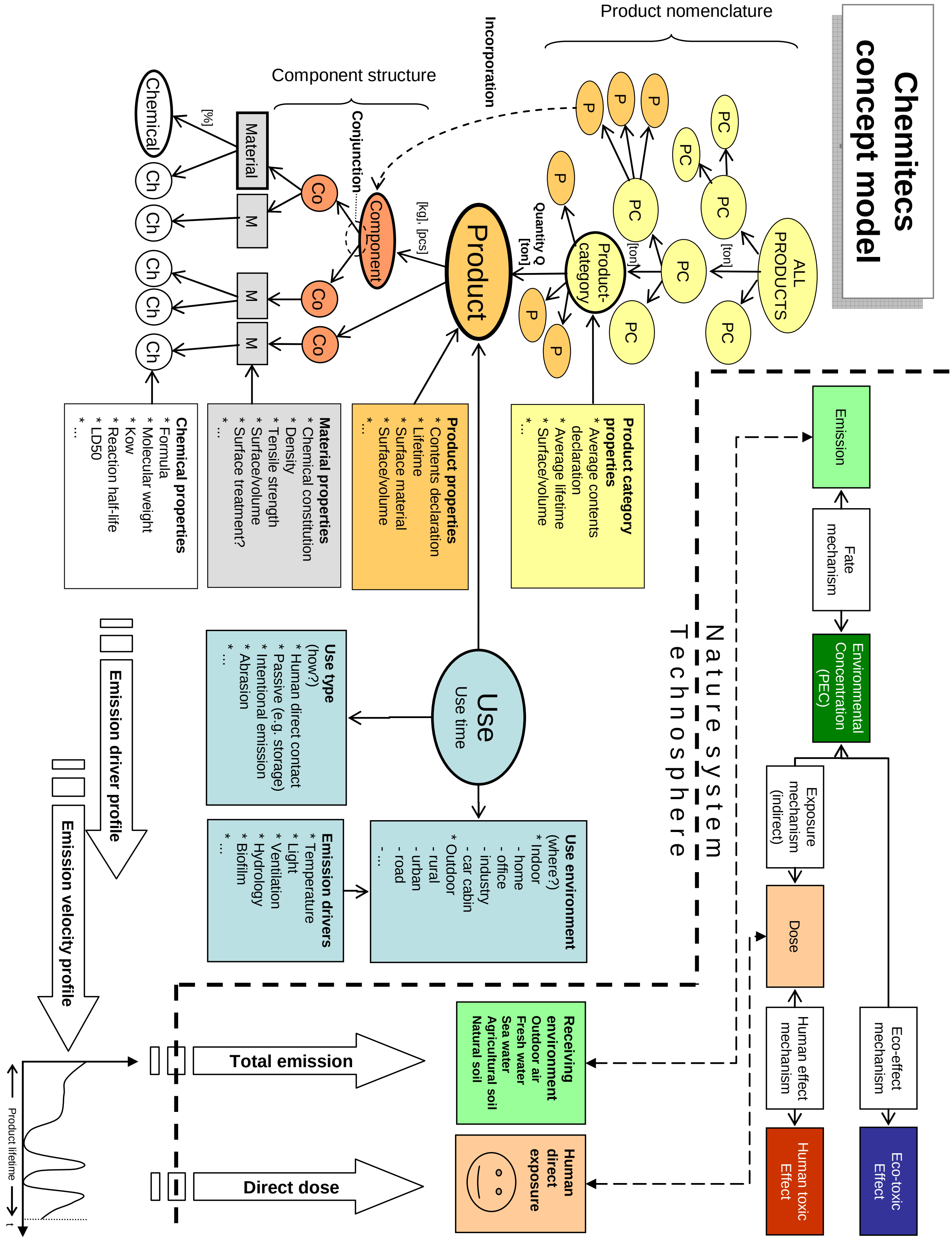
Appendix 1 The Chemitecs concept model illustration



Appendix 2 Polymers and functional chemicals.

By Stefan Posner, Swerea

The term polymer is an extensive term of materials that are made of large molecules built up by small and simple chemical units in several repetitive ways. Polymers are formed by nature or by man. The latter kinds of polymers are either synthetic of regenerated from natural occurring polymers such as cellulose. The basic properties of these polymers either there have their origin from nature or man there is sometimes a need to adopt their native behaviour into preferred technical and quality properties i.e. stiff polymers into a softer polymer, an easy burning polymer into a fire retardant polymer etc. In order to achieve these technical modifications there is a need to incorporate functionalities, either as chemicals or groups of chemicals that interact in such a way that they achieve these preferred functionalities under certain critical circumstances that could inflict the polymer during its uses. Beside the preferred functionalities the chemicals incorporated in the polymer may cause non preferred properties to the polymer that may inflict its suitability to be used on the market in a feasible way. (As many properties of these chemicals need to be defined and understood on their functional characteristics as much as possible before and during use.)

In order to understand and predict the physical behaviour of chemicals we need to define different categories depending on the purpose for their presence in a certain material. On the basis of this philosophy, three main categories of chemicals may be distinguished namely

- Chemicals with certain functionality/ies in the final product, mentioned as functional chemicals
- Chemicals with no functionality/ies in the final product, mentioned as impurities.
- Chemicals that occur through unintended production by man or nature, mentioned as impurities.

Functional chemicals
Functional chemicals represent a very large group of chemicals of inorganic and organic compounds. They are either additive or reactive. They should be clearly separated by definition from chemicals that are addressed as impurities that have very low or no logical explanatory history of their presence in the polymer, since they don't contribute to the preferred technical properties of the polymer. This does not mean that they are less relevant concerning their possible impact on health and/or environment, but they are beyond any explanatory and predictable control at later stages of the polymer life cycle.

Reactives
Reactive functional chemicals are added during the polymerisation process and become an integral part of the polymer and form a co-polymer. The result is a modified polymer with required functional properties and different molecule structure compared to the original polymer molecule.

Additives
Additive functional chemicals are incorporated into the polymer prior to, during, or more frequently after polymerisation. Additive functional chemicals are monomer molecules

that are not chemically bounded to the polymer. They may therefore, in contrast to reactive functional chemicals, be released from the polymer and thereby also discharged to the environment.

Some additives can appreciably impair the properties of polymers. The basic problem is the trade-off between the decrease of performance of the polymer caused by the functional chemical and the preferred requirements. In addition to fulfilling the appropriate technical and quality requirements set by the market and society, a feasible functional chemical shall, at most, fulfil all of the qualities mentioned below.

Preferred functional properties

- Fillers
- Plasticisers and softeners
- Lubricants and flow promoters
- Anti-ageing additives
- Flame-retardants
- Colourants
- Blowing agents
- Cross-linking agents
- Ultra-violet degradable additives
- etc

Mechanical properties

- Not significantly alter the mechanical properties of the polymer
- Be easy to incorporate into the host polymer
- Be compatible with the host polymer
- Should be stable under processing and service of life conditions

Physical properties

- Be colourless or at least non-discolouring properties
- Have good light stability
- Be resistant towards ageing and hydrolysis
- Not cause corrosion
- Should not bleed or bloom
- Should be stable under processing and service of life conditions

Health and environmental properties

- Not have harmful health effects

- Not have harmful environmental properties

Commercial viability

- Be commercially available and cost efficient

Fillers

Fillers are a certain category of additives that are usually applied to solid additives incorporated into the polymer to modify its physical, and usually mechanical, properties. Air and other gases should be considered as fillers in cellular polymers if their functionality is explicit for required porosity or flexibility properties of which they are for example for polyurethane foams.

There is a wide range of filler classifications which could be divided as follows

- Particulate fillers that include reinforcing and inert fillers
- Rubbery fillers that include non reactive and reactive fillers
- Resins that include nonreactive and reactive fillers
- Fibrous fillers that include random whiskers and laminar organic or inorganic fillers.

For each kind of additive there are some fundamental factors that have extensive importance on their potential to emit to the environment in its original form or as any form of degradation product namely their compatibility to the polymer. The coming chapter will give a theoretical explanatory picture of interactions between additives and polymers depending on their chemical characteristics and molecular structures. A basic rule in chemistry is "Equal solve equal" which is the fundament for this reasoning. Basically the theoretical descriptions are based on thermodynamic prediction models of substance vis-à-vis polymer solubility factors. If this is not fulfilled there is no interaction between the polymer and chemical, which could result in emissions from the material.

Polymer solubility

A chemical will be a solvent for another material if the molecules of the two materials are compatible which means that they can co-exist on the molecular scale and there is no tendency to separate. This statement does not indicate the speed at which solution may take place since this depends on additional considerations such as the molecular size of the potential solvent and the temperature. Molecules of two different species will be able to co-exist if the force of attraction between different molecules is not less than the forces of attraction between two like molecules of either species. If the average force of attraction is between to dissimilar molecules, A and B, is FAB, between similar molecules of type B is FBB and between similar molecules of type A is FAA, then for compatibility FAB > =FBB and FAB >=FAA.

Every material is unique and need to be considered separately. Such material systems are

- Amorphous non-polar polymers and amorphous non-polar solvents
- Crystalline non-polar polymers and amorphous solvents
- Amorphous non-polar polymers and crystalline solvents

- Amorphous polar polymers and solvents
- Crystalline polar polymers and solvents
- Vulcanised rubber and thermosetting plastics
-

It is assumed in these circumstances by analogy with gravitational and electrostatic attraction that FAB will be equal to the geometric mean of FAA and FBB. If by arbitrary definition we take FAA>FAB then

FAA>FAB>FBB.

Since we have already seen that solution will only occur when

FAB>= FAA and FAB>=FBB

then compatibility between amorphous non-polar polymers and solvents can only occur when

FAA=FAB=FBB

Appendix 3 Om kemiska produkter

Kemiska produkter är en typ av varor som faller inom ramarna för följande definition enligt Miljöbalken 1998:808 kap14 2 §:

> ”Med kemisk produkt avses ett kemiskt ämne och beredningar av kemiska ämnen”.

Vidare definieras i Kemikalieinspektionens föreskrifter om klassificering och märkning av kemiska produkter KIFS 2005:7

> 1 §) *Ämnen*: kemiska grundämnen och deras föreningar i naturlig eller framställd form, inklusive eventuella tillsatser nödvändiga för att bevara produktens stabilitet och eventuella föroreningar som härrör från tillverkningsprocessen, men exklusive eventuella lösningsmedel som kan avskiljas utan att detta påverkar ämnets stabilitet eller ändrar dess sammansättning;
>
> *Beredningar*: blandningar eller lösningar som består av två eller flera ämnen;
>
> *Kemiska produkter*: ämnen och beredningar

Denna definition ger ingen knivskarp tolkningshjälp om vilka varor som klassificeras som kemiska produkter då alla fysiska varor undantagslöst består av olika *ämnen*. Vad som avses med kemisk produkt är i praktiken kopplat till det administrativa ansvar som innehas av KemI och hur det uttolkas. I KIFS 2005:7 står det vidare:

> 5 §) Dessa föreskrifter gäller inte följande beredningar i bruksfärdigt skick, avsedda för slutanvändaren:
> a) Humanläkemedel och veterinärmedicinska produkter som de definieras i direktiv 2001/83/EG5 och 2001/ 82/EG6.
> b) Kosmetiska produkter som de definieras i direktiv 76/768/EEG7.
> c) Ämnesblandningar som i form av avfall omfattas av direktiv 75/442/EEG8och 78/319/EEG9.
> d) Livsmedel.
> e) Djurfoder.
> f) Radioaktiva ämnen som avses i direktiv 80/836/Euratom10 eller beredningar som innehåller sådana ämnen.
> g) Sådana medicintekniska produkter som införs i (invasiva) eller som används direkt på kroppen, i den utsträckning som det i gemenskapsföreskrifter fastställs bestämmelser om klassificering och märkning av farliga ämnen och beredningar, vilka säkerställer samma nivå på information och skydd som direktiv 1999/45/EG.

För detta projekt är även varor som faller inom undantagen a)-g) relevanta för helhetsbilden om ”hur stort är problemet med emissioner från varor”. Dock är hanteringen av kemiska produkter belagt med ett lagstiftat regelverk som även innebär en konsistent analys och dokumentation av egenskaper hos varan. Denna information är nödvändig men inte tillräcklig för att kvantifiera emissioner och effekter.