



Literature study - models

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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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Abstract

The ChEmiTecs program includes eleven subprojects. In project no. 1 (P1) one of the aims is to develop a concept model regarding emissions caused by the entire process of production and use of products. This literature study aims at a limited review of the scientific literature related to models related to the ChEmiTecs model. Methods comprised search in article databases and the use of web search engines together with consultation of persons well-read in the subject. The review suggests that there have been no concept models published that resembles the whole ChEmiTecs concept model, not even close. There is however recent publications dealing with models of one certain group of emissions from one certain group of products, indicating that the question is emerging. Though there are inspirational publications out there, this study has not identified any model that cover more than parts of the ChEmiTecs concept model scope.

Task 1 – searching for any model resembling the ChEmiTecs Concept model

Purpose

The first task was to search for a model that resembles the entire ChEmiTecs concept model. That is a generic concept model that relates to a scope of emissions caused by the entire process of production and use of products covering raw material production, processing, manufacturing, use and waste handling stages of a product.

Method

The reference databases Web of Knowledge and Scopus was used, along with the Google Web Search Engine, to find references for articles. The method also included consulting colleagues and other individuals related to the area for relevant books and articles, and then going through them. For every interesting reference citations- and reference-lists have been ransacked.

Results and Conclusions task 1

This initial reference study suggests that there have been no publications of models similar to the ChEmiTecs concept model.

The closest match found (still not a very close match) is the mixed-unit EIO model for environmental LCA and MFA. The latter model is interesting for ChEmiTecs because it enables a detailed material tracking throughout a products lifecycle. The model also describes how the economical flows affect material flows or vice versa (Hawkins et al., 2007).

Reference: (Hawkins et al., 2007)

Title: A mixed-unit input-output model for environmental life-cycle assessment and material flow analysis

Abstract: Materials flow analysis models have traditionally been used to track the production, use, and consumption of materials. Economic input-output modeling has been used for environmental systems analysis, with a primary benefit being the capability to estimate direct and indirect economic and environmental impacts across the entire supply chain of production in an economy. These two types of models are combined to create a mixed-unit input-output model that is able to better track economic transactions and material flows throughout the economy associated with changes in production. A 13 by 13 economic input-output direct requirements matrix developed by the U.S. Bureau of Economic Analysis is augmented with material flow data derived from those published by the U.S. Geological Survey in the formulation of illustrative mixed-unit input-output models for lead and cadmium. The resulting model provides the capabilities of both material flow and input-output models, with detailed material tracking through entire supply chains in response to any monetary or material demand. Examples of these models are provided along with a discussion of uncertainty and extensions to these models.

Task 2 – searching for models that cover part of the ChEmiTecs concept model

Purpose

Task 2, as a continuation of task 1, deals with the suggestion that there already exist models that can be of help when developing the ChEmiTecs concept model. Therefore the aim was to find models that are close to or covers parts of the ChEmiTecs concept model scope.

As e.g. the OMNIITOX model covers the emission-fate-exposure part, this reference search has had its focus on the part of the chain that lies before; substance-material-component-product-use-emission, and the part that deals with human direct exposure, which OMNIITOX does not cover.

Method

Same method was used for task 2 as in task 1.

Results

When subdividing the references here below, the following classification categories have been adapted; 1.Chemicals, 2.Materials, 3.Products, 4.Use, 5.Human Direct Exposure, 6.Chemicals – materials, 7.Chemicals – products, 8.Materials – products, 9.Products – use, 10.Use – Human Direct Exposure. This classification is related to the different separate parts of the ChEmiTecs concept model and linked parts of the ChEmiTecs concept model chain. It is meant as guidance rather than as absolute, since one reference could belong to more than one of the classification sectors. For every subdivision, the subdivided references are listed first in a lump and then one by one with the title and an excerpt from the abstract. For some of the subdivisions one reference is more interesting than the others and is indicated with the words “most interesting reference”. This reference is presented with the whole of its abstract.

The full reference to the references in the subdivisions can be found in the “References related to the ChemiTecs model”-list. References of less interest but still worth mentioning, are listed under the heading of the “References of background interest”- list.

Figure 1 shows the results in a comprehensive way. Firstly, both the upper (*Parts of models*) and the lower (*Linked models*) parts of the figure are divided into a) models for *specific* chemicals/materials/products/uses/emissions/exposures and b) models for chemicals/materials/products/uses/emissions/exposures *in general*. Secondly the upper part is divided into parts along the chain of ChEmiTecs (illustrated by the middle part of the figure). The lower part covers most of or the whole chain.

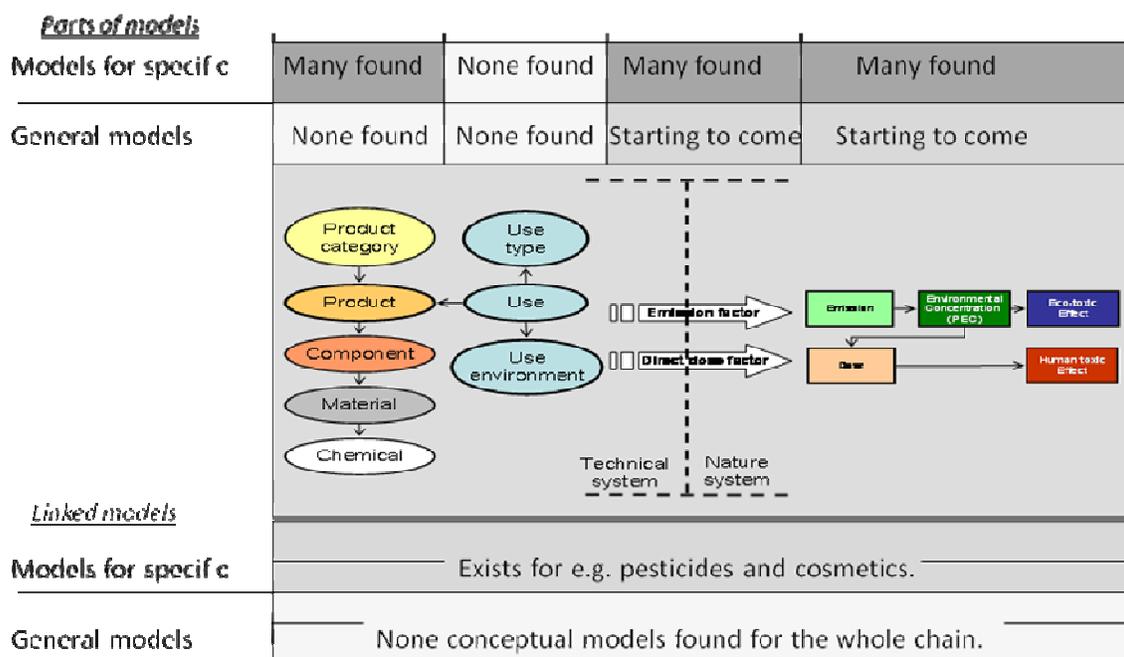


Figure 1. Results of the literature study. The figure includes models for *specific* chemicals/materials/products/uses/emissions/exposures and models for chemicals/materials/products/uses/emissions/exposures *in general*. The upper part of the figure describes parts of the ChEmiTecs chain and the lower part describes most of or the whole chain.

1. Chemicals

– references that deal with models and chemicals, substances, substance-flows, sometimes emissions. Many of these articles deal with fate processes in the natural system.

(Dalvi et al., 2006, Dodson, 2009, Guo, 2002, Hauschild et al., 2008, Hollander et al., 2009, Kawamoto et al., 2001, Kawamoto and Park, 2006, Mackay et al., 1996, Macleod et al., 2005, Månsson, 2009, Rosenbaum et al., 2007, Salthammer, 2009, Silibello et al., 2008, Tham et al., 2004, Tuia et al., 2007, Wright et al., 2008, Xu, 2009)

Most interesting references

Reference: (Wright et al., 2008)

Title: Integrating economic input-output life cycle assessment with risk assessment for a screening-level analysis

Short about: Goal, Scope, and Background The paper describes the integration of the economic input-output life cycle assessment (EIO-LCA) model and the environmental fate and transport model (CHEMGL) with a risk assessment tool. Utilizing the EIO-LCA, instead of a traditional LCA, enables a rapid, screening-level analysis of an emerging chemical of concern, decabromodiphenyl ether (DecaBDE).

Reference: (Tham et al., 2004)

Title: Emission modeling and validation of VOCs' source strengths in air-conditioned office premises

Short about: An emission model for indoor volatile organic compounds (VOCs) based on mass balance considerations has been presented and validated under steady state

conditions. Comparison were made for the measured and predicted concentrations of 37 selected VOCs and TVOC through a case intervention study on the filters of the ventilation system in a new commercial air-conditioned office building.

Reference: (Xu, 2009)
Title: Emission of Phthalate from Vinyl Flooring and Sorption to Interior Surfaces, Dust and Airborne Particles

Other references

Reference: (Tuia et al., 2007)
Title: Evaluation of a simplified top-down model for the spatial assessment of hot traffic emissions in mid-sized cities

Short about: In this paper, a simplified emission estimation model (SEEM) is evaluated. The model is based on a top-down approach and gives annual global hot emission. Particular attention is paid to the quality of the input traffic data. The quality of results is assessed by application of the SEEM model in the Chilean Gran Concepcion urban area and by comparison with a bottom-up approach that has been led for the year 2000..

Reference: (Hollander et al., 2009)
Title: Substance or space? The relative importance of substance properties and environmental characteristics in modeling the fate of chemicals in Europe.
Short about: The relative influence of substance properties and of environmental characteristics on the variation in the environmental fate of chemicals was studied systematically and comprehensively

Reference: (Kawamoto and Park, 2006)
Title: Calculation of environmental concentration and comparison of output for existing chemicals using regional multimedia modeling
Short about: The environmental fate of 40 existing chemicals is discussed using the EUSES multimedia distribution and risk assessment model with site-specific parameter setting in an urban area of Japan including a highly industrial region. There has been a strong need to assess the environmental fate of a huge number of existing chemicals. Data on the emission amounts of chemicals are essential for such prediction, and PRTR surveys may yield this data.

Reference: (Mackay et al., 1996)
Title: Evaluating the environmental fate of a variety of types of chemicals using the EQC model
Short about: The multimedia equilibrium criterion model, which can be used to evaluate the environmental fate of a variety of chemicals, is described. The model treats chemicals that fall into three categories. In the first the chemicals may partition into all environmental media, in the second they are involatile, and in the third they are insoluble in water. The structure of the model, the process equations, and the required input data for each chemical type are described.

Reference: (Macleod et al., 2005)
Title: Assessing the influence of climate variability on atmospheric concentrations of polychlorinated biphenyls using a global-scale mass balance model (BETR-global)
Short about: We introduce a new global-scale multimedia contaminant fate model (the Berkeley-Trent Global Model; BETR-Global) that integrates global climate data from the

National Centers for Environmental Prediction (NCEP). BETR-Global represents the global environment as a connected set of 288 multimedia regions on a 150 grid. We evaluate the model by simulating the global fate and transport of seven PCB congeners over a 70 year period and find satisfactory agreement between model output and observations of atmospheric PCB concentrations at 11 long-term monitoring stations in the Northern Hemisphere. We demonstrate the use of the model as a tool for understanding global pollutant dynamics by examining the hypothesis that variability in global-scale climate conditions, as reflected by the North Atlantic Oscillation (NAO), influences atmospheric PCB concentrations in the Northern Hemisphere.

Reference: (Månsson, 2009)
Title: Substance flow analysis of metals and organic compounds in an urban environment – the Stockholm example.

Short about: Dissertation containing an overview of substance flow results from many studies in Stockholm, including the use of these for mitigating emissions.

Reference: (Dalvi et al., 2006)
Title: A GIS based methodology for gridding of large-scale emission inventories: Application to carbon-monoxide emissions over Indian region

Short about: An attempt has been made in this paper to develop a geographical information system (GIS) based methodology for distributing the emissions from a broader level inventory to finely gridded emission values, considering local micro-level details and activity data.

Reference: (Dodson, 2009)
Title: Evaluating Methods for Predicting Indoor Residential Volatile Organic Compound Concentrations

Reference: (Guo, 2002)
Title: Review of indoor emission source models. Part 1, Overview
Abstract: Indoor emission source models are mainly used as a component in indoor air quality (IAQ) modeling, which, in turn, is part of exposure and risk modeling. They are also widely used to interpret the experimental data obtained from environmental chambers and buildings. This paper compiles 52 indoor emission source models found in the literature. Together, they represent the achievements that IAQ modelers have made in recent years. While most models have a certain degree of usefulness, genuine predictive models are still few, and there is undoubtedly much room for improvement. This review consists of two parts. Part 1-this paper-provides an overview of the 52 models, briefly discussing their validity, usefulness, limitations, and flaws (if any). Part 2 focuses on parameter estimation, a topic that is critically important to modelers but has not been systematically discussed.

Reference: (Hauschild et al., 2008)
Title: International consensus model for comparative assessment of chemical emissions in LCA

Reference: (Kawamoto et al., 2001)
Title: Evaluation and comparison of multimedia mass balance models of chemical fate: application of EUSES and ChemCAN to 68 chemicals in Japan

Short about: The European Union System for Evaluation of Substances (EUSES) and the ChemCAN chemical fate model are applied to describe the fate of 68 chemicals on two spatial scales in Japan. Emission information on the chemicals has been obtained from Japan's Pollutant Release and Transfer Registry and available monitoring data gathered from government reports. Environmental concentrations calculated by the two models for the four primary environmental media of air, water, soil and sediment agree within a factor of 3 for over 70% of the data, and within a factor of 10 for over 87% of the data.

Reference: (Rosenbaum et al., 2007)

Title: A flexible matrix algebra framework for the multimedia multipathway modeling of emission to impacts

Short about: When assessing human health or ecosystem impacts of chemicals several calculation steps need to be addressed. Matrix algebra solving techniques are a useful approach to structure and solve the system of mass balance equations assessing chemical fate in environmental multimedia models. We suggest expanding this matrix approach towards a framework which includes the exposure, effect, and damage assessment for human health and ecosystems, also applicable to spatial modeling. Special emphasis is laid upon interpretation of the physical meaning of different elements within the matrices.

Reference: (Salthammer, 2009)

Title: Gas/Particle Partitioning of Phthalic Acid Esters in the Indoor Environment

Reference: (Silibello et al., 2008)

Title: Modelling of PM10 concentrations over Milano urban area using two aerosol modules

Short about: To have a better understanding of the spatial distribution of PM10, a modelling system has been applied to a winter PM10 episode considering a computational domain centered on Milano metropolitan area. The modelling system software suite is based on an Eulerian photochemical model (FARM - Flexible Air quality Regional Model) and includes an emission pre-processor to apportion data from the regional emission inventory, a diagnostic meteorological model coupled with a micrometeorological module and data visualization and post-processing tools.

2. Materials

– references that deal with models and materials, components, material-flows

(Adriaanse et al., 1997, Bouman et al., 2000, Bringezu et al., 2004, Elshkaki et al., 2005, Hashimoto et al., 2004, Sörme et al., 2001b, Sörme et al., 2001a, van der Voet et al., 2002)

Most interesting reference

Reference: (Bouman et al., 2000)

Title: Material flows and economic models: an analytical comparison of SFA, LCA and partial equilibrium models

Short about: The aim of this paper is to make a first step in bridging the gap between the various types of analysis of material flows in the economy, by discussing the main differences and similarities of three often employed model types: substance flow analysis, life cycle assessment and partial economic equilibrium analysis. Instead

of submitting each model to a lengthy theoretical discussion, they are applied to a single, hypothetical example of a pollution problem.

Other references in the topic

Reference: (Bringezu et al., 2004)

Title: International comparison of resource use and its relation to economic growth - The development of total material requirement, direct material inputs and hidden flows and the structure of TMR

Short about: In this article, we study the available empirical evidence on the actual (de-)linkage of material resource use and economic growth. We compare resource use with respect to total material requirement (TMR) and direct material input (DMI) for 11 and 26 countries, respectively, and the European Union (EU-15).

Reference: (Adriaanse et al., 1997)

Title: Resource flows: the material basis of industrial economies.

Reference: (van der Voet et al., 2002)

Title: Predicting future emissions based on characteristics of stocks.

Reference: (Elshkaki et al., 2005)

Title: Dynamic stock modelling: A method for the identification and estimation of future waste streams and emissions based on past production and product stock characteristics.

Reference: (Hashimoto et al., 2004)

Title: Six indicators of material cycles for describing society's metabolism: application to wood resources in Japan.

Reference: (Sörme et al, 2001a)

Title: Century Perspective of Heavy Metal Use in Urban Areas. A Case Study in Stockholm.

Reference: (Sörme et al, 2001b)

Title: Goods in the Anthroposphere as a Metal Emission Source A Case Study of Stockholm, Sweden.

3. Products

– references that deal with models and products, commodities, product-flows (Huang and Matthews, 2008, Huppes and Ishikawa, 2007, Tukker et al., 2006, Tukker and Jansen, 2006, Huppes et al., 2006, Hertwich and Peters, 2006, Suh and Huppes, 2005, Hur et al., 2005, Wood and Lenzen, 2009)

Most interesting reference

Reference: (Huang and Matthews, 2008)

Title: Seeking opportunities to reduce life cycle impacts of consumer goods - An economy-wide assessment

Abstract: To quantify the total life cycle environmental impacts of consumption, an economy-wide assessment of goods and services is conducted using the Economic Input-Output Life Cycle Assessment (EIO-LCA) model. This research includes an assessment of total "cradle to consumer" impacts of consumption, utilization of US

Environmental Protection Agency's Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) in the EIO-LCA model, and the use of new modeling techniques for sectorial contribution analysis and subtotal supply chain impact of tier-1 supplier analysis. The results show that power generation contributes to nearly one fifth of the total embodied energy and greenhouse gas equivalent emissions in manufactured goods; and for the services and other institutions sectors, its contributions are more than one third. Sectorial contribution analyses show that mining is a major contributor of cancer effects for manufactured goods. Displacing mining production through recycling can help reduce life cycle cancer effects of goods. Consumer purchases of waste management services are found to contribute to nearly a quarter of all cancer and non-cancer impacts in the entire economy, signaling the need for producer responsibility policy aimed to reduce toxic materials that eventually enter the waste stream. Subtotal supply chain analysis of packaging materials found that on an energy basis, there exist opportunities to expand the existing applications of deposit-refund programs on beverage containers to other goods. Agencies, companies, and industry groups can use sectorial and supplier contribution analyses to identify opportunities for reducing the life cycle impacts of their products.

Other references in the topic

Reference: (Huppel and Ishikawa, 2007)

Title: Sustainability evaluation: diverging routes recombined? Tasks for a new Working Group on Modelling and Evaluation for Sustainability

Short about: In making practical decisions on technologies and products and related strategies and policies, all sustainability effects are involved, from global warming and income distribution to economic growth and habitat destruction. In the environment domain of sustainability there are at least four basically different approaches to evaluation and the underlying modelling, and at least one approach focussing on efficiency only, all with diverging outcomes. A working group involving different scientific societies is being set up to actively relate the different approaches and to see how at a practical level they might be reconciled. (C) 2007 Elsevier Ltd. All rights reserved.

Reference: (Tukker et al., 2006)

Title: Environmental impacts of products - Policy relevant information and data challenges

Reference: (Tukker and Jansen, 2006)

Title: Environmental impacts of products - A detailed review of studies

Short about: This review article brings together the conclusions of 11 studies that analyze the life-cycle impacts of total societal consumption and the relative importance of different final consumption categories. This review addresses in general studies that were included in the project Environmental Impacts of Products (EIPRO) of the European Union (EU), which form the basis of this special issue. Unlike most studies done in the past 25 years on similar topics, the studies reviewed here covered a broad set of environmental impacts beyond just energy use or carbon dioxide (CO₂) emissions.

Reference: (Huppel et al., 2006)

Title: Environmental impacts of consumption in the European Union - High-resolution input-output tables with detailed environmental extensions

- Short about: This study fills the gap between detailed LCA and low-resolution EEIOA, specifying the environmental effects of household consumption in the European Union, discerning nearly 500 sectors, while specifying a large number of environmental extensions.
- Reference: (Hertwich and Peters, 2006)
 Title: Feasibility and scope of life cycle approaches to sustainable consumption
 Short about: Household environmental impact (HEI) assessment; a description of how LCA, in combination with input-output analysis and household consumption data can be used to determine the environmental impact of consumption patterns. Short review results from studies focusing on CO₂ emissions as environmental indicator.
- Reference: (Suh and Huppel, 2005)
 Title: Methods for life cycle inventory of a product
 Short about: Methods for Life Cycle Inventory (LCI) compilation are reviewed and compared. In total, six methods are distinguished. They are LCI computation using process flow diagram; matrix expression of product system; input-output (IO) based LCI; and three different forms of hybrid analysis: the tiered hybrid analysis, the IO-based hybrid analysis, and the integrated hybrid analysis.
- Reference: (Hur et al., 2005)
 Title: Simplified LCA and matrix methods in identifying the environmental aspects of a product system
 Short about: In this study, the usefulness of life cycle assessment (LCA) and a matrix method as tools for identifying the key environmental issues of a product system were examined. For this, a simplified LCA (SLCA) method that can be applied to Electrical and Electronic Equipment (EEE) was developed to efficiently identify their significant environmental aspects for eco-design, since a full scale LCA study is usually very detailed, expensive and time-consuming. The environmentally responsible product assessment (ERPA) method, which is one of the matrix methods, was also analyzed.
- Reference: (Wood and Lenzen, 2009)
 Title: Structural path decomposition
 Short about: The authors combine Structural Decomposition Analysis (SDA) and Structural Path Analysis (SPA) in order to examine the temporal changes within a full production chain perspective. In this paper, the authors develop the mathematical model of Structural Path Decomposition (SPD) and provide two case studies of the most important changes in structural paths in Australia from 1995 to 2005.

4. Use

- references that deal with models and use, everyday life
- No references found, or they are better suited under another title.

5. Human Direct Exposure

- references that deal with models and human direct exposure; dermal exposure, inhalation etc. (Bennett et al., 2002, Fiserovaberggerova, 1990, Guinee et al., 2004, Hauschild et al., 2008, Hellweg et al., 2009, Hertwich et al., 2001, Hertwich and McKone, 2001, Hertwich et al., 1999, Huijbregts et al., 2005, Koehler et al., 2005, Lewandowski, 2008, Mackay and Webster, 2003,

MacLeod et al., 2002, Moschandreas and Saksena, 1999, Nishioka et al., 2005, Pennington et al., 2005, Rosenbaum et al., 2008, Sarigiannis and Gotti, 2007, Schneider et al., 1999, Wright et al., 2008, Babich, 2009, Fryer et al., 2006, Mueller and Nowack, 2008, Nieuwenhuijsen et al., 2006, Schripp, 2009, Semple, 2005, Wood and Lenzen, 2009, CEAM, 2009-08-03, MIMS, 2009-08-03, NCEA, 2009-08-03, NERL, 2009-08-03, Risk, 2009-08-03, RMRM, 2009-08-03)

Reference: (Bennett et al., 2002)

Title: Intake fraction for multimedia pollutants: A tool for life cycle analysis and comparative risk assessment

Short about: The intake fraction (iF) is employed as an effective tool for expressing the source-to-intake relationship for pollutant emissions in life cycle analysis (LCA) or comparative risk assessment. Intake fraction is the fraction of chemical mass emitted into the environment that eventually passes into a member of the population through inhalation, ingestion, or dermal exposure.

Reference: (Fiserovaberggerova, 1990)

Title: Application of toxicokinetic models to establish biological exposure indicators

Short about: This article is a critical review of the application of toxicokinetic models to the biological monitoring of occupational exposure to industrial chemicals.

Reference: (Guinee et al., 2004)

Title: Bringing science and pragmatism together - A tiered approach for modelling toxicological impacts in LCA

Short about: The EU 5(th) framework project OMNIITOX will develop models calculating characterisation factors for assessing the potential toxic impacts of chemicals within the framework of LCA. These models will become accessible through a web-based information system. The key objective of the OMNIITOX project is to increase the coverage of substances by such models. In order to reach this objective, simpler models which need less but available data, will have to be developed while maintaining scientific quality.

Reference: (Hauschild et al., 2008)

Title: Building a model based on scientific consensus for life cycle impact assessment of chemicals: The search for harmony and parsimony

Reference: (Hellweg et al., 2009)

Title: Integrating Human Indoor Air Pollutant Exposure within Life Cycle Impact Assessment

Short about: This paper summarizes the work of an international expert group on the integration of human indoor and outdoor exposure in LCA, within the UNEP/SETAC Life Cycle Initiative. A new methodological framework is proposed for a general procedure to include human-health effects from indoor exposure in LCA. Exposure models from occupational hygiene and household indoor air quality studies and practices are critically reviewed and recommendations are provided on the appropriateness of various model alternatives in the context of LCA.

Reference: (Hertwich et al., 2001)

Title: Human toxicity potentials for life-cycle assessment and toxics release inventory risk screening

- Short about: This article presents cancer and noncancer HTP values for air and surface-water emissions of 330 compounds.
- Reference: (Hertwich and McKone, 2001)
Title: Pollutant-specific scale of multimedia models and its implications for the potential dose
Short about: This paper extends the concept of a pollutant-specific model scale through the introduction of a characteristic atmospheric scale height. It is the height of the atmosphere that would be needed to contain all the pollutant if the entire atmosphere had ground-level concentration, taking into account deposition and degradation. The spatial range is defined as the expected advection-driven travel distance of a pollutant molecule released to a specific compartment.
- Reference: (Hertwich et al., 1999)
Title: Parameter uncertainty and variability in evaluative fate and exposure models
Short about: The human toxicity potential, a weighting scheme used to evaluate toxic emissions for life cycle assessment and toxics release inventories, is based on potential dose calculations and toxicity factors. This paper evaluates the variance in potential dose calculations that can be attributed to the uncertainty in chemical-specific input parameters as well as the variability in exposure factors and landscape parameters.
- Reference: (Huijbregts et al., 2005)
Title: A comparison between the multimedia fate and exposure models CalTOX and uniform system for evaluation of substances adapted for life-cycle assessment based on the population intake fraction of toxic pollutants
Short about: In life-cycle assessment (LCA) and comparative risk assessment, potential human exposure to toxic pollutants can be expressed as the population intake fraction (iF), which represents the fraction of the quantity emitted that enters the human population. To assess the influence of model differences in the calculation of the population iF ingestion and inhalation iFs of 365 substances emitted to air, freshwater, and soil were calculated with two commonly applied multimedia fate and exposure models, CalTOX and the uniform system for evaluation of substances adapted for life-cycle assessment (USES-LCA).
- Reference: (Koehler et al., 2005)
Title: Rethinking environmental performance from a public health perspective - A comparative industry analysis
Short about: To date the most common measures of environmental performance used to compare industries, and by extension firms or facilities, have been quantity of pollution emitted or hazardous waste generated. Discharge information, however, does not necessarily capture potential health effects. This article proposes an alternative environmental performance measure that includes the public health risks of toxic air emissions extended to industry supply chains using economic input-output life-cycle assessment.
- Reference: (Lewandowski, 2008)
Title: Modeling chemical exposure in risk assessment
Short about: Risk assessment is increasingly concerned with assessing risks from environmental exposure pathways beyond those typically considered, i.e., direct ingestion, inhalation or dermal exposure to chemicals in air, water, and soil. A number of models have been developed to facilitate analysis of these more complex exposure

Situations. Such models also enhance Our ability to assess both aggregate and Cumulative exposures. Three different modeling approaches are described which address some of these issues; the U.S. EPA's IEUBK model for lead, the multipathway health risk assessment (MPHRA) methodology developed for assessing risks of incinerators and waste combustors. and the U.S. EPA's Stochastic Human Exposure and Dose Simulation (SHEDS) model.

Reference: (Mackay and Webster, 2003)

Title: A perspective on environmental models and QSARs

Short about: A general review is presented of the roles of QSARs and mass balance models as tools for assessing the environmental fate and effects of chemicals of commerce. It is argued that all such chemicals must be assessed using a consistent and transparent methodology that uses chemical property data derived from QSARs, or experimental determinations when possible and applies evaluative or region-specific environmental models.

Reference: (MacLeod et al., 2002)

Title: Evaluating and expressing the propagation of uncertainty in chemical fate and bioaccumulation models

Short about: First-order analytical sensitivity and uncertainty analysis for environmental chemical fate models is described and applied to a regional contaminant fate model and a food web bioaccumulation model. By assuming linear relationships between inputs and outputs, independence, and log-normal distributions of input variables, a relationship between uncertainty in input parameters and uncertainty in output parameters can be derived, yielding results that are consistent with a Monte Carlo analysis with similar input assumptions.

Reference: (Moschandreas and Saksena, 1999)

Title: 14th Meeting of the Scientific-Group-on-the-Methodologies-of-Safety-Evaluation-of-Chemicals (SGOMSEC)

Short about: Exposure assessment, a component of risk assessment, links sources of pollution with health effects. Exposure models are scientific tools used to gain insights into the processes affecting exposure assessment. The purpose of this paper is to review the process and methodology of estimating inhalation exposure to particulate matter (PM) using various types of models. Three types of models are discussed in the paper.

Reference: (Nishioka et al., 2005)

Title: A risk-based approach to health impact assessment for input-output analysis - Part 1: Methodology

Short about: In this study, an LCIA tool is developed which takes into account the geographical variability in both emissions and exposure, and which can be applied to all economic sectors in I-O analysis. The method relies on screening-level risk calculations and methods to estimate population exposure per unit of emissions from specific geographic locations.

Reference: (Pennington et al., 2005)

Title: Multimedia fate and human intake modeling: Spatial versus nonspatial insights for chemical emissions in Western Europe

Short about: Multimedia fate and multipathway human,exposure models are widely adopted in assessments of toxicological risks of chemical emissions at the regional scale. This

paper addresses the question of how much spatial detail is necessary in such models when estimating the intake by the entire population in large, heterogeneous regions such as Europe. The paper presents a spatially resolved multimedia fate and multipathway exposure model for Western Europe, available as IMPACT 2002. This Model accounts for relationships between the location of food production and drinking water extraction as well as where population cohorts live relative to where chemical emissions occur.

- Reference: (Rosenbaum et al., 2008)
Title: USEtox-the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment
Short about: In 2005, a comprehensive comparison of life cycle impact assessment toxicity characterisation models was initiated by the United Nations Environment Program (UNEP)-Society for Environmental Toxicology and Chemistry (SETAC) Life Cycle Initiative, directly involving the model developers of CalTOX, IMPACT 2002, USES-LCA, BETR, EDIP, WATSON and EcoSense. In this paper, we describe this model comparison process and its results-in particular the scientific consensus model developed by the model developers. The main objectives of this effort were (1) to identify specific sources of differences between the models' results and structure, (2) to detect the indispensable model components and (3) to build a scientific consensus model from them, representing recommended practice.
- Reference: (Sarigiannis and Gotti, 2007)
Title: Biology-based dose-response models for health risk assessment of chemical mixtures
Short about: In this work a pharmacokinetic/pharmacodynamic (PBPK/PD) model for benzene, toluene, ethylbenzene and all xylenes that accounts for the interactions among these chemicals at the sites of metabolism is presented.
- Reference: (Schneider et al., 1999)
Title: Conceptual model for assessment of dermal exposure
Short about: A consistent terminology based on a multicompartiment model for assessment of dermal exposure is proposed that describes the transport of contaminant mass from the source of the hazardous substance to the surface of the skin. Six compartments and two barriers together with eight mass transport processes are described.
- Reference: (Wright et al., 2008)
Title: Integrating economic input-output life cycle assessment with risk assessment for a screening-level analysis
Short about: The paper describes the integration of the economic input-output life cycle assessment (EIO-LCA) model and the environmental fate and transport model (CHEMGL) with a risk assessment tool. Utilizing the EIO-LCA, instead of a traditional LCA, enables a rapid, screening-level analysis of an emerging chemical of concern, decabromodiphenyl ether (DecaBDE).
- Reference: (Babich, 2009)
Title: Consumer Exposure to Flame Retardant (FR) Chemicals in Upholstered Furniture
Short about: SETAC Conference 2009, Abstract

- Reference: (Fryer et al., 2006)
 Title: Human exposure modelling for chemical risk assessment: a review of current approaches and research and policy implications
 Short about: A wide variety of exposure models are currently employed for health risk assessments. Individual models have been developed to meet the chemical exposure assessment needs of Government, industry and academia. These existing exposure models can be broadly categorised according to the following types of exposure source: environmental, dietary, consumer product, occupational, and aggregate and cumulative. Aggregate exposure models consider multiple exposure pathways, while cumulative models consider multiple chemicals. In this paper each of these basic types of exposure model are briefly described, along with any inherent strengths or weaknesses, with the UK as a case study.
- Reference: (Mueller and Nowack, 2008)
 Title: Exposure modeling of engineered nanoparticles in the environment
 Short about: The aim of this study was to use a life-cycle perspective to model the quantities of engineered nanoparticles released into the environment. Three types of nanoparticles were studied: nano silver (nano-Ag), nano TiO₂ (nano-TiO₂), and carbon nanotubes (CNT). The quantification was based on a substance flow analysis from products to air, soil, and water in Switzerland.
- Reference: (Nieuwenhuijsen et al., 2006)
 Title: New developments in exposure assessment: The impact on the practice of health risk assessment and epidemiological studies
 Short about: The field of epidemiology is about to undergo a sea change with respect to the exposure component because each year better environmental and exposure models, statistical techniques and new biological monitoring techniques are being introduced. This paper reviews these techniques and discusses where additional research is likely to pay a significant dividend.
- Reference: (Schripp, 2009)
 Title: Distribution of Semi Volatile Organic Compounds in the Indoor Environment
 Short about: SETAC Conference 2009, Abstract
- Reference: (Semple, 2005)
 Title: Assessing occupational and environmental exposure
 Short about: Exposure modelling, particularly for the environmental fate of chemicals has undergone many recent developments and Monte Carlo techniques can be used to characterize model uncertainty and variability. This approach to exposure assessment can now be used in the setting of the wider environment and will enable a far better understanding of the relationship between exposure and disease.
- Reference: (Wood and Lenzen, 2009)
 Title: Structural path decomposition
 Short about: The authors combine Structural Decomposition Analysis (SDA) and Structural Path Analysis (SPA) in order to examine the temporal changes within a full production chain perspective. In this paper, the authors develop the mathematical model of Structural Path Decomposition (SPD) and provide two case studies of the most important changes in structural paths in Australia from 1995 to 2005.

Reference: (CEAM, 2009-08-03)
 Title: Center for Exposure Assessment and Modeling (from the EPA website)
 Short about: Center for Exposure Assessment and Modeling (CEAM) provides models that assess air and water pathways for the spread of organic metals and pollutants.

Reference: (MIMS, 2009-08-03)
 Title: Multimedia Integrated Modeling System (from the EPA website)
 Short about: Multimedia Integrated Modeling System (MIMS) addresses and simulates a variety of air, water, and soil changes.
 Linking Air Quality & Human Health/Linking Local-Scale and Regional-Scale Models for Exposure Assessments

Reference: (NCEA, 2009-08-03)
 Title: NCEA Risk Tools- Human Health (from the EPA website)
 Short about: NCEA Risk Tools- Human Health lists tools used by the National Center for Exposure Assessment to analyze human health damages from toxin exposure.
 Catreg Software for Categorical Regression Analysis - The software was developed to support toxicity assessment for acute inhalation exposures

Reference: (NERL, 2009-08-03)
 Title: ORD Exposure Research Models created by NERL (The National Exposure Research Laboratory) (from the EPA website)
 Short about: ORD Exposure Research Models contains models that address chemical exposure to humans and ecosystems.
 Exposure Related Dose Estimating Model (ERDEM) for assessing human exposure and dose. ERDEM solves a system of ordinary differential equations that describe the organ system consisting of lung, gastro-intestinal, dermal, liver, kidney, and other compartments, as needed. Metabolism, binding, and enzyme inhibition are modeled.

Reference: (Risk, 2009-08-03)
 Title: Risk Assessment Tools (from the EPA website)
 Short about: Risk Assessment Tools lists EPA tools and models used for risk assessment.
 Dietary Exposure Potential Model is a model using extant food databases to estimate dietary exposure to chemical residues
 Human Exposure Modeling - Hazardous Air Pollutant Exposure Model (HAPEM)
 The HAPEM model has been designed to estimate inhalation exposure for selected population groups to various air toxics. Through a series of calculation routines, the model makes use of ambient air concentration data, indoor/outdoor microenvironment concentration relationship data, population data, and human activity pattern data to estimate an expected range of inhalation exposure concentrations for groups of individuals.
 Ecotox Thresholds EPA has developed software that calculates Ecotox Thresholds (ETs) for selected chemicals and can print out a table of ETs and their sources.
 Databases: Consolidated Human Activity Database (CHAD) contains data obtained from pre-existing human activity studies that were collected at city, state, and national levels. CHAD is intended to be an input file for exposure/intake dose modeling and/or statistical analysis.
 HEDS is the Human Exposure Database System. HEDS is an integrated database system that contains chemical measurements, questionnaire responses, documents,

and other information related to EPA research studies of the exposure of people to Environmental contaminants.

Reference: (RMRM, 2009-08-03)

Title: Risk Management Research Models (from the EPA website)

Short about: Risk Management Research Models lists numerous models and databases used by the Risk Management Research Division.

Indoor Air Quality Modeling Using the latest EPA research, the Indoor Environment Management Branch has developed an indoor air quality model for analyzing the effect of emissions sources, sinks, ventilation, and air cleaners on indoor air quality.

RISK Model The RISK computer model is designed to calculate individual exposure to indoor air pollutants from emissions sources. The model can calculate exposure due to individual (as opposed to population) activity patterns and source use. It can also determine risk from the calculated exposure to indoor air pollution.

IAQX: Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure Model

This model is an indoor air quality simulation software package that supplements existing simulation programs. It performs conventional indoor air quality simulations, computes the time concentration profile and inhalation exposure, and estimates the adequate ventilation rate for improving indoor air quality.

6. Chemicals – materials

– references that deal with models and chemicals/substances/substance-flows linking to materials/components/material-flows

(Bouman et al., 2000, Guinee et al., 2006, Hawkins et al., 2007, Morf et al., 2008,)

Most interesting reference

Reference: (Hawkins et al., 2007)

Title: A mixed-unit input-output model for environmental life-cycle assessment and material flow analysis

Abstract: Materials flow analysis models have traditionally been used to track the production, use, and consumption of materials. Economic input-output modeling has been used for environmental systems analysis, with a primary benefit being the capability to estimate direct and indirect economic and environmental impacts across the entire supply chain of production in an economy. These two types of models are combined to create a mixed-unit input-output model that is able to better track economic transactions and material flows throughout the economy associated with changes in production. A 13 by 13 economic input-output direct requirements matrix developed by the U.S. Bureau of Economic Analysis is augmented with material flow data derived from those published by the U.S. Geological Survey in the formulation of illustrative mixed-unit input-output models for lead and cadmium. The resulting model provides the capabilities of both material flow and input-output models, with detailed material tracking through entire supply chains in response to any monetary or material demand. Examples of these models are provided along with a discussion of uncertainty and extensions to these models.

Input: Material flow data and EIO requirements matrix. Case study question: What will the (seven) Pb/Cd Flow Sectors look like if there was an additional final demand of \$10 million in the (twelve) Dollar Flow Sectors?

Output: Detailed material tracking through entire supply chains in response to any monetary or material demand. Case study results: Results presented in form of a

matrix, in which is given the increase in tonnes of Pb/Cd that is needed in each Flow Sector for an additional final demand of \$10 million in each Dollar Sector at a time.

Use: This model describes how the economical flows affect material flows or vice versa. Maybe it can be useful as a continuation of the program; looking at changes in emissions from use of commodities due to changes in the economical, raw material and social flows.

Other references

Reference: (Guinee et al., 2006)

Title: Human and ecological life cycle tools for the integrated assessment of systems (HELIAS)

Short about: Relationships between life cycle decision support tools (particularly SFA, MFA and LCA) from an empirical side: which combinations of tools have actually been used, and what is the added value of combining tools in practical case studies? It is concluded that there is not one generally valid protocol for which tools to use for which question. The essential idea of using a combination of tools is exactly the fact that research questions are not simple by nature and cannot be generalized into protocols.

Reference: (Bouman et al., 2000)

Title: Material flows and economic models: an analytical comparison of SFA, LCA and partial equilibrium models

Short about: The aim of this paper is to make a first step in bridging the gap between the various types of analysis of material flows in the economy, by discussing the main differences and similarities of three often employed model types: substance flow analysis, life cycle assessment and partial economic equilibrium analysis. It appears that the results of the three models are complementary rather than contradictory. A sequential application of a number of limited models may therefore be an approach that provides more useful information than the tedious construction and application of an encompassing model that integrates these models.

Reference: (Morf et al. 2008)

Title: Dynamic substance flow analysis as a valuable risk evaluation tool - A case study of or brominated flame retardants as an example of potential endocrine disrupters.

Short about:

7. Chemicals – products

– references that deal with models and chemicals/substances/substance-flows linking to products/commodities/product-flows

(Harper, 2008, Månsson et al., 2008, Tasaki et al., 2004)

Most interesting references

Reference: (Harper, 2008)

Title: A Product-Level Approach to Historical Material Flow Analysis.

Abstract: Studies of material cycles, which have a solid history in biogeochemistry, include characterization of technological materials cycles that quantify the way in which materials move through the economy and environment of a region. One of the most important aspects of historical technological materials cycles is determining how much material goes into various uses over time and modeling its lifetime in each use. A material flow analysis methodology is presented by which a historical

(i.e., 1975 to 2000) study of tungsten use in the United States was constructed. The approach utilized in this study is twofold: the traditional approach by which material going into end-use sectors is approximated (the “end-use sector model”), and a second approach by which end-use products are specifically addressed (the “finished product model”). By virtue of the latter method, a detailed historical account of a material’s end uses was developed. This study shows that (1) both models present a detailed treatment of trade of finished products over time for a variety of highly disaggregated products, (2) the end-use sector model provides a method to combine quantitative and qualitative data about products in various sectors to estimate domestic production for a metal about which little is known in terms of its end uses, and (3) the finished product model produces detailed estimates of domestic production. for a large number of highly disaggregated products.

Reference: (Tasaki, 2004)
Title: Substance flow analysis of brominated flame retardants and related compounds in waste TV sets in Japan.
Abstract: We conducted time-series substance flow analysis of two types of brominated flame retardants (BFRs) – polybrominated diphenyl ethers (PBDEs) and tetrabromobisphenol A (TBBPA) – and two types of related compounds – Sb (used with BFRs for flame inhibition) and polybrominated dibenzo dioxins and furans (PBDDs/DFs: unintended byproducts) – in five size categories of waste TV sets in Japan. Two scenarios were created with BFR substitutions and compared to a “business as usual” scenario in order to obtain basic information for strategic product management. The results showed that the use of DecaBDE in rear and front covers of TV sets began in fiscal 1987–1990 and 1993–1996, respectively, and that TBBPA was used to some extent as a substitute for DecaBDE in the 90s. The amount of waste Br in the plastic covers is predicted to increase until at least fiscal 2020 due to the increasing size of TV sets. Although substitution of BFRs with non-BFRs in Japan by 2006 will reduce waste Br, the amount in waste TV sets will not peak until fiscal 2009. The results will help inform decisions in Japan regarding the recovery and disposal of waste TV sets. The methods used would benefit waste managers faced with similar issues in other countries.

Reference: (Månsson et al., 2008)
Title: Sources of alkylphenols and alkylphenol ethoxylates in wastewater - a substance flow analysis in Stockholm, Sweden..
Short about: The study identifies textiles as an important source of the substances in waste water.

8. Materials – products

– references that deal with models materials/components/material-flows linking to products/commodities/product-flows

Most interesting reference

Reference: (Oguchi et al. 2008)
Title: Product flow analysis of various consumer durables in Japan.
Abstract: We conducted a product flow analysis (PFA) for 94 consumer durables in Japan to obtain a complete picture of the domestic flow. Data on domestic shipment, average weight and average lifespan of each product was surveyed and estimated based on statistics and product catalogues of manufacturers.

Then, the amount of domestic shipment and waste from households and enterprises was estimated as inflow and outflow of the system. This is the first report on the complete picture of domestic product flow of consumer durables in Japan.

From the results, the target items of Japan's recycling laws are considered reasonable from the viewpoint of landfill waste reduction because the total waste weight of the nine target items accounts for 68% of the total of 94 items. The number of waste products was relatively large for items such as cellular phones, VCRs and notebook PCs, which contain numerous hazardous and/or valuable substances, although their waste weight was small. The waste product collection ratio for the nine target items remains at 2–56% on a weight basis (4–59% on a number basis) due to the fact that some waste products are taken to industrial waste treatment facilities and exported. In addition, in the post-consumer stage, the flow has not yet been identified for 46–68% of the waste products of the 94 items in weight (82–86% in number). These products might be treated as municipal or industrial waste, exported, or illegally dumped and their flow should be clarified through further research.

9. Products – use

– references that deal with models and products/commodities/product-flows linking to use/everyday life

(Joshi, 2000, Barrero et al., 2006, Gunschera et al., 2009, Guo and Murray, 2000, Guo, 2002, Katsoyiannis et al., 2008, Katsoyiannis et al., 2005, Kwon et al., 2007, Larsen et al., 2009, McKellop and D'Lima, 2007, Niemela et al., 2007, Ohlmeyer et al., 2008, Zhu et al., 2005, Girman, 1987, Hu et al., 2007)

Most interesting reference

Reference: (Guo, 2002)

Title: Review of indoor emission source models. Part 1, Overview

Abstract: Indoor emission source models are mainly used as a component in indoor air quality (IAQ) modeling, which, in turn, is part of exposure and risk modeling. They are also widely used to interpret the experimental data obtained from environmental chambers and buildings. This paper compiles 52 indoor emission source models found in the literature. Together, they represent the achievements that IAQ modelers have made in recent years. While most models have a certain degree of usefulness, genuine predictive models are still few, and there is undoubtedly much room for improvement. This review consists of two parts. Part 1-this paper-provides an overview of the 52 models, briefly discussing their validity, usefulness, limitations, and flaws (if any). Part 2 focuses on parameter estimation, a topic that is critically important to modelers but has not been systematically discussed.

Other references

Reference: (Joshi, 2000)

Title: Product Environmental Life-Cycle Assessment Using Input-Output Techniques

Reference: (Barrero et al., 2006)

Title: Emission tests from office equipment in the indoortron environmental chamber

Reference: (Gunschera et al., 2009)
Title: Surface-catalysed reactions on pollutant-removing building products for indoor use
Short about: In order to evaluate the potential for emission of secondary reaction products from building materials designed to remove pollutants from indoor air, four samples of ceiling tiles-three commercially available and one custom-made - were investigated in chamber experiments.

Reference: (Guo and Murray, 2000)
Title: Modelling of emissions of total volatile organic compounds in an Australian house
Short about: A simplified indoor air quality (IAQ) model has been applied to predict IAQ in an Australian house, using environmental chamber measurements of source strengths, house ventilation and room size. Total volatile organic compounds (TVOCs) was used as the model pollutant in this study.

Reference: (Katsoyiannis et al., 2008)
Title: VOC and carbonyl emissions from carpets: A comparative study using four types of environmental chambers
Short about: Emissions of Volatile Organic Compounds (VOCs) and carbonyls from carpets of different type (wool, synthetic) over a time period of three days at 23 degrees C, at 45% relative humidity, 0.5 air change rate and a loading factor of 0.4 m² m⁻³ were measured. The experiments were carried out at four different environmental chambers (volumes of 0.02/0.28/0.45/30 m³).

Reference: (Katsoyiannis et al., 2005)
Title: Determination of volatile organic compounds emitted from household products. The case of velvet carpets (moquettes)
Short about: Three environmental chambers with controlled temperature, humidity and ventilation have been used to evaluate the emissions of total volatile organic compounds (TVOCs), emitted by various types of carpets. TVOC emissions were tested as a function of time. Sampling was conducted after 0, 24, 48 and 72 hours in all experiments. The results show that emissions of TVOCs by carpets vary significantly between the various types of carpets, reaching extremely high concentrations.

Reference: (Kwon et al., 2007)
Title: Characterization of emissions composition for selected household products available in Korea
Short about: The present study investigated the emission composition for 59 household products currently sold in Korea, using a headspace analysis.

Reference: (Larsen et al., 2009)
Title: Life cycle assessment of offset printed matter with EDIP97: how important are emissions of chemicals?
Short about: In this paper the impacts from chemicals emitted during the life cycle of sheet fed offset printed matter is included. This is done by making use of some of the newest knowledge about emissions from the production at the printing industry combined with knowledge about the composition of the printing materials used

Reference: (McKellop and D'Lima, 2007)
Title: How have wear testing and joint simulator studies helped to discriminate among materials and designs?

Reference: (Niemela et al., 2007)
Title: A virtual indoor environment model - a useful tool for design
Short about: The aim of this paper is to present an integrated approach, in terms of a virtual room model, for visualizing the model predictions of various indoor environment parameters in order to enhance interaction between the members of the design team and the occupants. The approach is based on room model and virtual room model concepts. By enhancing collaboration and integration in the design phase, the approach should reduce the design cycle and make the design and construction phases more accurate.

Reference: (Ohlmeyer et al., 2008)
Title: Influence of panel thickness on the release of volatile organic compounds from OSB made of *Pinus sylvestris* L
Short about: Emissions from building products are considered to be a major source of elevated volatile organic compound (VOC) concentrations in indoor air. To investigate the effect of panel thickness on the release of VOC three oriented strandboards (OSB) of different thicknesses were characterized. The emissions deriving from the panels made of Scots pine were investigated over a period of 125 days using environmental test chambers.

Reference: (Zhu et al., 2005)
Title: Prediction of initial emission rates of 2-butoxyethanol from consumer products using equilibrium headspace concentrations: An application of the vapor pressure and boundary layer (VB) model
Short about: The initial emission rate of volatile organic compounds (VOCs) from consumer products is important for assessing potential human exposure to VOCs in products. The vapor pressure and boundary layer (VB) model developed in the past was used to predict the emission rates of VOCs in the fast decaying phase from petroleum-based wet materials. This study has extended the model to largely water-based products.

Reference: (Girman, 1987)
Title: Considerations in evaluating emissions from consumer products
Short about: While several indoor air quality studies suggest consumer products (e.g. aerosol sprays, paint removers, etc.) can be significant sources of volatile organic compounds, until recently characterizing emissions from consumer products has received relatively little attention. Many considerations that must be addressed in designing studies of consumer product emissions are similar to those addressed in studies of the emissions from building materials and combustion appliances. These similarities are discussed and, in addition, the considerations unique to studies of consumer product emissions are discussed with reference to an ongoing study of consumer products that contain methylene chloride. When conducting an experimental study on emissions from consumer products following eight considerations are proposed: (1) defining the potential health hazard; (2) acquiring application technique and usage pattern information; (3) establishing study goals; (4) assessing instrumental and facility capabilities; (5) writing protocol; (6) pretesting; (7) conducting the study; (8) post-study considerations.

Reference: (Hu et al., 2007)
Title: An analytical mass transfer model for predicting VOC emissions from multi-layered building materials with convective surfaces on both sides
Short about: An analytical mass transfer model for predicting emissions of Volatile Organic Compounds (VOCs) from multi-layered building materials and the instantaneous VOC material-phase distribution is developed.

10. Use – Human Direct Exposure

– references that deal with models and use/everyday life linking to human direct exposure (Birkved and Hauschild, 2006, McNamara et al., 2007, Schneider et al., 1999, Vermeire et al., 1993, Vermeulen et al., 2000)

Most interesting reference

Reference: (Vermeire et al., 1993)
Title: Estimation of consumer exposure to chemicals – application of simple-models.
Abstract: Occupational and consumer exposure only recently has become an issue meriting a more systematic approach. This paper offers a method for the estimation of consumer exposure on the basis of limited data sets. Following a selection of exposure route(s) of concern, acute, subchronic and chronic exposure scenarios are identified based on the expected exposure frequency and duration. Algorithms for the estimation of the external exposure are presented and illustrated by example calculations. The external and internal exposure assessment is further integrated into a hazard assessment scheme for consumer products including the determination of no-effect levels for man and the calculation of hazard quotients.
Input: Data for the exposure scenario: duration, frequency, acute, subchronic, chronic. Physical and other parameters: concentrations, amounts, bioavailability. Human parameters: weight, ventilation, area of skin. Example of question that can be investigated: How extensive is the dermal exposure for a specific human situated in a specific environment or dealing with a specific product?
Output: No-effect levels for humans and hazard quotients. Example answer: The dermal exposure is X mg/cm³.
Inclusions: Algorithms for oral, dermal and inhalation exposure.
Use: Vermeire sets up a method, built on algorithms, for assessing occupational and consumer exposure, based on physical properties of the material/product and of the human receiver. Seems to me it will give some general ideas for the concept model.

Other references

Reference: (Birkved and Hauschild, 2006)
Title: PestLCI - A model for estimating field emissions of pesticides in agricultural LCA.
Short about: PestLCI is a modular model for estimation of pesticide emissions from field application to the different environmental compartments. It estimates the fractions of the applied quantity which is emitted to the air, surface water, and groundwater compartment based on information which will normally be available to the model user.

Reference: (McNamara et al., 2007)
Title: Probabilistic modeling of European consumer exposure to cosmetic products.
Short about: Statistical analysis of the usage profile of the European population to seven cosmetic products (body lotion, shampoo, deodorant spray, deodorant non-spray,

facial moisturiser, lipstick and toothpaste) resulting in a new model of European exposure to cosmetic products.

Reference: (Schneider et al., 1999)

Title: Conceptual model for assessment of dermal exposure.

Short about: Consistent terminology based on a multicompartment model for assessment of dermal exposure. The terminology describes the transport of contaminant mass from the source of the hazardous substance to the surface of the skin. Six compartments and two barriers together with eight mass transport processes are described. The importance of measuring the concentration of contaminant and not mass per area in the skin contaminant layer is stressed, as it is the concentration difference between the skin contamination layer and the perfused tissue that drives uptake.

Reference: (Vermeulen et al., 2000)

Title: Identification of dermal exposure pathways in the rubber manufacturing industry.

Short about: Using the Schneider concept model for dermal exposure Vermeulen et al. designs an exposure assessment strategy for dermal pathways in the rubber manufacturing industry.

Short discussion and Conclusion task 2

There are recent publications regarding models of emissions from products. These publications are still on a “one certain group of chemicals emanating from one certain group of products “-level including environmental chamber experiments. No concept models have been found on this subject but the publications show that there are more people out there posing the same question; Are the emissions from commodities a problem?

The most studied area, looking at the amount of publications found, seems to be the human exposure area. There are various types of exposure models; fate-exposure models, dose-response models and models including risk assessment, life cycle assessment, human toxicology, ecotoxicology etc. There have been attempts at the beginning of this century, to integrate human direct exposure models with use of certain products (cosmetics and pesticides), however finding recent publications dealing with this matter have proven to be impossible. The reason to this observation is unclear.

Models concerning materials and products separately are often economical models e.g. economic input-output models combined with material flow analysis and/or with life cycle assessment. Also these models work with specific materials or products and do not introduce a top down concept model.

The overall conclusion is that inspirational publications exist; but alas, this study has not yielded a “direct hit” – no model has been found that covers more than parts of the ChEmiTecs concept model scope, but models exist that can be of immediate assistance in the further development of the ChEmiTecs concept model and for the further development of the ChEmiTecs programme.

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