Modelling chemical emissions from products

– a first iteration of a Swedish case study of polymers and related chemicals

Objective

The objective of this research was to develop and apply a simple method for an initial approximation of emissions of a set of organic chemicals from products containing a selected number of materials, mostly plastics, used in Sweden.

Background

Estimating the size of the problem with release, fate, exposure and effects from the human use of chemical substances of materials and consumer products is daunting. More than 100 000 chemical substances are in commercial use and a reasonable description of their existence in, and release from, plastic polymers, glues, paints, fibres, lubricants and so on comprise a big challenge.
Still there is a need to cover the vast range of substances in order to get an initial indication of relative amounts emitted and to know what chemicals to focus regarding risk reduction measures.

References

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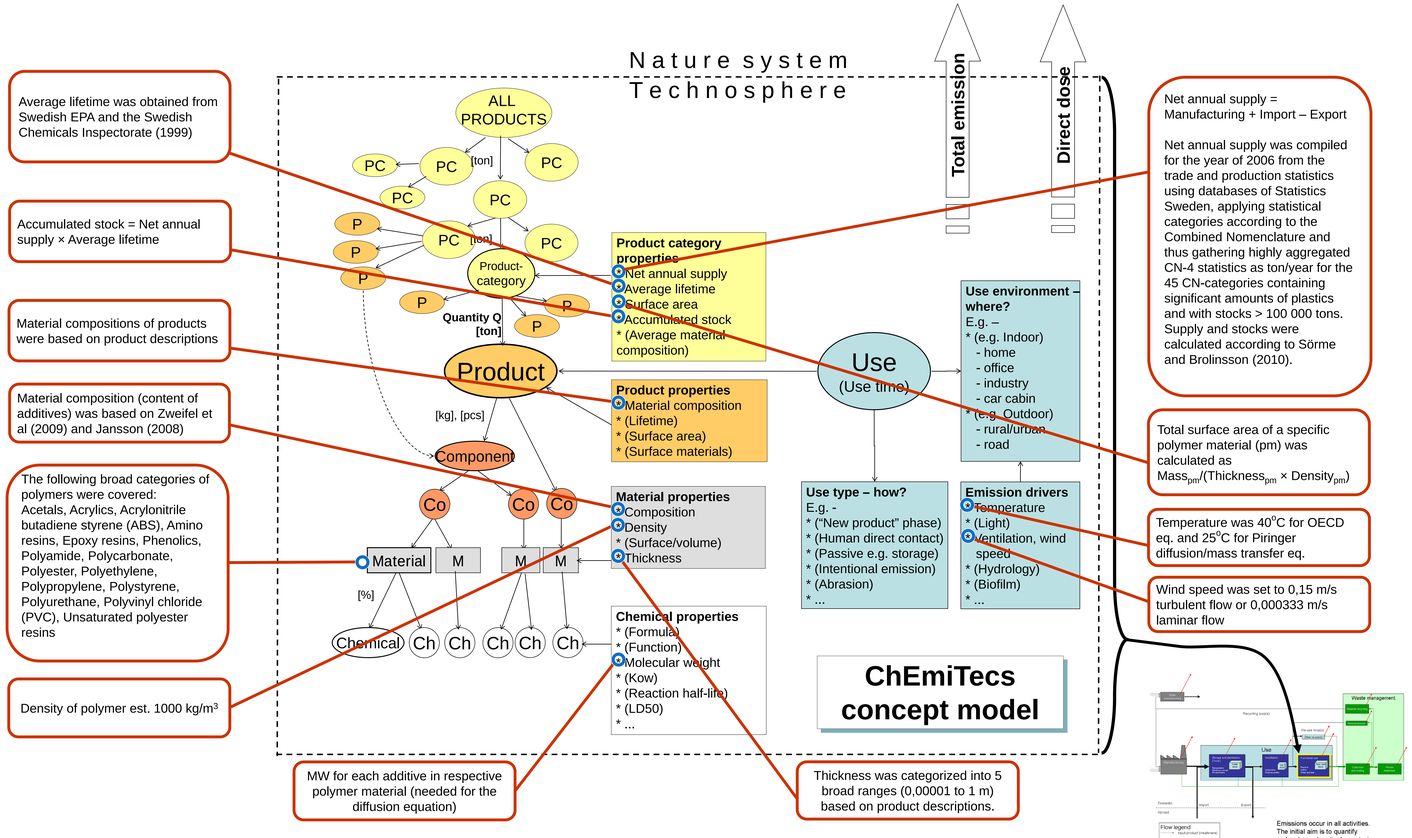
ChEmiTecs Research program - http://www.chemitecs.se/

Model & Algorithm

Emissions of additives from all goods containing plastic non-fibre polymers were based on estimates of total area for each plastic type and an empirical diffusion equation (OECD 2009) or a new equation based on a Piringer-type diffusion coefficient and convection mass transfer predictions. Below are further specifications of the algorithm given in conjunction to its place in the conceptual model's calculation hierarchy. Bracketed factors were not included in this first iteration of the calculations.



First results

Regardless of diffusion equation used the 8 substances with the highest emissions from the list of chosen additives are sorbitan monolaurate, triphenylphosphate 2,4-dibromophenol, 2,4,6-tribromophenol, oleic acid amide, di(ethylhexyl)phthalate, benzylbuthylphthalate, dibutylphthalate and di(n-hexyl,n-octyl,n-decyl)phthalate. All of these substances are to be expected due to their ubiquitous use and chemical properties. In general the OECD equation overestimates emissions 300-500 times (extreme is 10000 times).

On-going work

The uncertainty is currently huge due to several factors. The diffusion model is e.g. under improvement based on empirical work. Furthermore are the total areas of polymers uncertain due to uncertain amounts of different polymers and their thicknesses in various goods. The amount of unbound additive in materials is another considerable uncertainty. However these and other uncertainties will be brought down during the development of the model and its database, which include further work based on case-studies and the on-going refined identification of additives in the materials and their amounts.

Sverker Molander, Johan Tivander, Filippa Fuhrman – Environmental Systems Analysis, Chalmers University of Technology, Gothenburg, Sweden
Patrik L. Andersson, Peter Haglund, Tomas Holmgren – Department of Chemistry, University of Umeå, Umeå, Sweden
Elisabeth Hallberg, Tomas Rydberg, Jenny Westerdahl, Andreas Öman – IVL Swedish Environmental Research Institute, Gothenburg, Sweden