Complex problems - simple models? An integrated and flexible modelling approach to address human health and environmental impacts of anthropogenic emissions

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EXTENDED ABSTRACT

Policy attaches an increasing importance to human health and a sound environment. Scientific support, hence, needs to provide more reliable answers to questions of environmental concern which are inherently complex and require an integrated perception. Process models can be used to assist this. However, existing models usually do not represent all aspects of such complex questions. Therefore, two main approaches for extending existing models are discussed: setting up one rather rigid but 'fully integrated' model, and linking models by either coupling modules forming a complex modelling framework or integrating parameterised modules into other models in a very simplified manner.

We found that for our models, i.e. the environmental fate and exposure models *EcoSense* and *WATSON* as well as the optimisation tool *OMEGA*, linking is to be preferred to fully integrated modelling in order to be more flexible and to avoid very computing time-consuming calculation steps.

Linking options primarily depend on the questions to be answered and thus we applied the modular design for questions at wider, e.g. European, scales and parameterisation when it comes to the tight time constraints of an optimisation problem. According to requirements of the policy questions we selected two exemplarily problems with regard to modularisation: (i) calculating total damage costs of heavy metal emissions via both inhalation and ingestion and (ii) calculating external costs of anthropogenic emissions at different scales and for various receptors. Both questions could be answered adequately by linking our models appropriately.

In general, our work shows that the concept of linking models has proven to be a viable approach to run models in an integrated way because single models are well-engineered, robust, tested and can be coupled concisely. Nevertheless, it is important to entirely understand the complexity of all questions, not only those related to impacts on human health and the environment due to anthropogenic emissions, to determine the best available strategy to link existing models.

1 INTRODUCTION

In policy an urgent need for scientific consultation arose to tackle environmental and human health problems due to contamination of the environment by 'man-made' emissions. According to Mackay (2001), Jorgensen (2001) and many others models are an expedient instrument, representing various aspects, from environmental conditions to impact assessment. However, as most questions are of complex nature models need to be linked in order to provide a more comprehensive picture of the question and conduct an integrated assessment.

In the present study we couple different environmental fate and exposure assessment as well as optimisation models to determine strategies to minimize human health and ecosystem impacts in Europe. Although the definition of integrated assessment is still under debate (e.g. Gough et al., 1998, Tolba, 2003) most agreement is on that it involves several disciplines, follows the causal chain from human actions to their consequences, should provide added value compared to single disciplinary sources assessments and should offer decision-makers useful information (e.g. CIESIN, 1995). In this context integrated assessment is used as the multidisciplinary process of synthesizing knowledge across scientific disciplines with the purpose of providing all relevant information to policy makers to help to make a decision. For integrated modelling we adapt Argent's view (2004) who defines integrated modelling as a process where "different components of the natural and other systems are modelled in a linked way, ideally with representation of feedbacks, loops, responses, thresholds and other features of system behaviour".

We will show that the main advantage of an integrated modelling approach by coupling models compared to applying one single complex model lies in the possibility to take an application focussed approach. This means that the involved models are more flexible and thus various types of questions can be answered by choosing different model compositions. Integrated modelling hereafter implies covering all relevant aspects of the questions of interest by following the impact pathway approach as shown in Figure 1, starting with the emission of a pollutant into the environment; regarding its dispersion in the different environmental media; identifying the exposure of the receptors and calculating the related impacts and damages which then are expressed as monetary values (external costs). Costs of policy options such as mitigation measures are taken into account as well as behavioural changes of the population. The integration of the modelling is justified by considering all relevant sources, stressors, exposure pathways, environmental media as well as temporal and spatial scales, using methods from different scientific disciplines, such as engineering, natural sciences and economics.

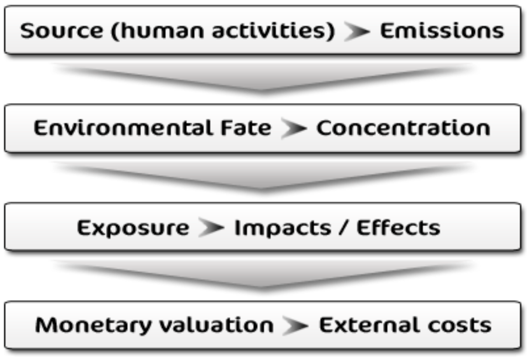

Figure 1. The impact pathway approach allows for monetary valuation of impacts of pollutants on receptors (cf. DPSIR approach (EEA)).

2 MODELLING OF ENVIRONMENTAL FATE AND EXPOSURE ASSESSMENT

2.1 *EcoSense* – atmospheric model

Krewitt et al. (1999) developed the atmospheric dispersion and exposure assessment tool *EcoSense* (cf. Software tools developed and used within ExternE - Externalities of Energy) which implements the impact pathway approach developed within *ExternE* (Bickel and Friedrich, 2005). It was designed for the analysis of single energy sources (electricity and heat production, transport processes) in Europe but it can also be used for analysis of multiple emission sources in certain regions.

EcoSense was developed to support the assessment of priority impacts resulting from the exposure to airborne pollutants, namely impacts on human health, crops, building materials and ecosystems. The current version of *EcoSense*, *EcoSenseWeb*, covers the emission of classical air pollutants SO_2, NO_x, primary particulates, and NMVOC (non-methane volatile organic compounds), as well as some of the most important heavy metals. It includes also impact assessment due to emission of greenhouse gases. Impacts are calculated on different spatial scales, i.e. local (50 km around the emission source), regional (this means Europe-wide) and (northern) hemispheric scale.

As health and environmental impact assessment is a field of large uncertainties and incomplete, but rapidly growing understanding of the physical, chemical and biological mechanisms of action, the model is continuously developed and extended.

2.2 *WATSON* – water and soil model

A multi-media extension of *EcoSense* named *WATSON* was developed by Bachmann (2006). *WATSON* performs exposure assessment and as well as *EcoSense* is based on the impact pathway approach. This framework facilitates the coverage of exposures towards hazardous substances through ingestion of various food items as well as through drinking water in a spatially-resolved pan-European setting based on an environmental fate model for the media soil and water. The contaminants‘ environmental fate is described with the help of a spatially-resolved climatological box model similar to Mackay level III/IV models (Mackay, 1991).

The subsequent environmental fate model is spatially differentiated according to catchment information. It assumes long-term average conditions in order to describe the environment. *WATSON*s exposure assessment for ingestion is very complex due to both the variety of food items to which human beings might be exposed and the spatial distribution of the food production. The estimation of ingestion-related exposures builds on the site-specific risk assessment approach recommended by the US-EPA for hazardous waste combustion facilities (US-EPA, 1998). Trade is seen as an extension of the (natural) environmental fate.

WATSON is at present able to calculate the exposure, impacts and external costs of heavy metals due to ingestion but will be further extended to rather volatile compounds, such as persistent organic pollutants and pesticides.

2.3 *OMEGA* – optimisation model

In contrast to the environmental fate and exposure assessment models *EcoSense* and *WATSON* the *OMEGA* tool is an optimisation model for environmental assessment which mainly focuses on optimal emission control strategies. Its main purpose thus is to optimise sets of emission abatement measures, further on also called strategies, to meet some user-defined air quality targets with least costs. Typical measures are the usage of certain filters for power plants or catalysts for passenger cars. The targets can be national emission ceilings, limit values of concentrations on the EMEP 50 km grid or external costs. For the latter, *OMEGA* maximizes the difference of savings of external costs and additional money needed to reduce emissions.

So far, there are two versions of *OMEGA*, one for classical air pollutants and the second one for heavy metals. The first one is able to assess the atmospherical effects of NH_3, NMVOC, NO_x, particulate matter and SO_x. It also calculates the national emissions of greenhouse gases and CO. Until now, *OMEGA* calculates the external costs autonomously, only covering the linear exposure-response functions used in *EcoSense*, concerning effects of ozone on crops and of ozone and particulate matter on human health.

OMEGA-HM works with another database of emission factors and abatement measures. It models the impact pathway for heavy metals concerning inhalation. It also calculates the depositions of heavy metals per grid cell according to different land use types, which serve as input data for *WATSON*. Currently, the model is expanded to cover also PCBs (polychlorinated biphenyls) and dioxins.

3 POSSIBILITIES OF LINKING MODELS

Since several approaches exist for coupling models to enable integrated assessments this paragraph focuses on selected options of linking models together in order to answer different questions of interest. Firstly, the fully integrated modelling approach will be discussed in contrast to the concept of linking models or independently working modules (cf. Paragraph 3.1). Secondly, we will delineate how to set up a flexible approach based on modules (cf. Paragraph 3.2) which can be composed in a modelling framework while finally, parameterisation is presented as an option to provide complex modelling frameworks to be used within another model with tight runtime constraints (cf. Paragraph 3.3).

3.1 The ‘fully integrated’ modelling approach

What are the most significant differences between the concepts of ‘model coupling’ and ‘fully integrated modelling’ and when is coupling of models more suitable than modelling fully integrated? Before answering these questions a brief definition of the term ‘fully integrated’ is required.

When it comes to model the environmental fate of substances which show complex interaction processes[1], such as gas transfer between different media, it is essential to figure out if these processes can be covered by a modelling framework. As an example the use of a dynamic, two or three-dimensional air, water or groundwater quality model may be required in order to predict effects of such multimedia substances at specific times and places. This apparently points to the advantage of making an environmental fate model fully integrated with respect to all media involved, all relevant chemicals and all interactions between both, media and chemicals. Fully integrated in this context means that all interaction processes between two media can be formulated as a whole within one and the same model. If in this case the fully integrated approach is to be preferred to a coupled modelling framework will be discussed in the following by means of the gas transfer process across the air-water interface.

Gas transfer, whose importance has been highlighted amongst others by the role of the oceans for being the largest sink of fossil fuel-produced CO_2 (Donelan and Wanninkhof, 2002), is controlled by parameters such as different turbulence levels (Herlina, 2005). In order to calculate the gas transfer we need the derivation of the concentration which

[1] hereafter referred to as ‘multimedia substances’

is proportional to the difference between the gas concentration at equilibrium stage $\dot{c}$ and the current gas concentration c as shown in the following equation:

$$\frac{\delta c}{\delta t} = \hat{k} \cdot (\dot{c} - c) \qquad (1)$$

where $\hat{k}$ denotes the volumetric gas transfer coefficient. Calculating the gas transfer at every specific space and time by using this equation may result in immense computational effort. Thus, the fully integrated approach is suitable to only a limited extent when it comes to higher temporal and spatial resolutions.

However, the overall gas transfer process of the substance can also be taken into account in a coupled modelling framework (e.g. an model to assess damage costs of air pollutants, such as *EcoSense*, coupled to a water and soil model, such as *WATSON*) when rather predefining than calculating the air quality model's gas transfer and those of the respective water surface within the water and soil model. This goes in line with the findings of Margni and co-workers (Margni, 2003; Margni et al., 2004) who found that coupling a single-medium air quality model to a water and soil multimedia type of model is a justifiable approach for assessing average environmental concentrations of at least certain volatile substances. Furthermore, for the bulk of substances which are not true multimedia substances (Klepper and den Hollander, 1999) the intermedia exchange is assessed to be small (Margni, 2003; Margni et al., 2004). This indicates that for these substances linking models in a way of individually working modules will be a suitable approach to systematically describe and analyse the interplay of release, phase partitioning, degradation and both intra- and intermedia transport. Thus, the concept of modular design is described in the following.

3.2 Modules and their application in modelling frameworks

Both, parts of models and whole encapsulated models can be regarded as modules. These modules are normally well-engineered, robust, tested and therefore reliable. Argent (2004) uses the principle of object orientation as the basis for the construction of modules. For transferring a legacy model into a module which can be used together with other modules he suggests that the legacy models can be embedded into methods which pre-process data, create files, run the model in different modes and process the results for further use. To provide management and linking of the modules and enable a flexible, simple and correct usage frameworks are needed. The core condition here is to precisely describe the modules in a way that only compatible modules can be connected. This applies not only for data format but even more for the underlying assumptions and methodologies.

The information exchange between modules depends on how they are linked. If the framework enables an automated linkage, as may be the case for intra-model modules, data transfer may be processed directly or otherwise by exchanging files. Also a database oriented approach is possible (e.g. Kokkonen et al., 2003). In case that whole models are used as modules it sometimes has advantages to perform the data transfer manually as the intermediate results can be checked and validated more easily.

In the HarmonIT project (HarmonIT), whose objective was to provide a mechanism to link models in the water domain, the modular approach was realised in a highly sophisticated manner. The developed OpenMI standard defines an interface for time-dependent models (modules) to exchange data during runtime (Moore, 2005) that allows for flexible linking.

The linkage of modules is a very powerful and flexible approach. Yet, in situations characterised by tight CPU time constraints it cannot be applied properly. In this case parametrising the respective module can be used to represent its functionality in a simplified way. This is explained in the following paragraph.

3.3 Parameterisation

Whenever there is an interactive model, like the optimisation model *OMEGA*, CPU time becomes very important. So it is often not advisable to link a whole complex model to it. To overcome this problem, we just look at this 'server model' as a black box that requires some figures as input values and produces another set of figures as output. The idea behind parameterisation is now to find a mathematical function f, that gives a more or less good estimate of the output figures - or at least the subset of the output that the client model is interested in $\vec{y} = (y^1, ..., y^m)$ - depending on the input values $\vec{x} = (x^1, ..., x^n)$. The relevant ones can be identified by doing a sensitivity analysis.

In general, one could assume some formula for f with some number l of unknown parameters. To assign values to them, running the model l times gives a linear equation system, with exactly one solution for the parameters, as long as one manages to avoid linearly dependent equations. Of course, one might want to do some additional model runs, just to be able to check the quality of the parameterisation's estimation.

The most simple possibility to do this is to run the model for some reference scenario $\vec{x}_0$ and for all scenarios, where one input value is reduced for example by some amount λ: $\vec{x}_{\lambda,i} = \vec{x}_0 - \lambda \vec{e}_i$, where $\vec{e}_i$ denotes the i-th unit vector. Now any other output value can be interpolated out of these results with the formula

$$f(\vec{x}) = f(\vec{x}_0) + \sum_{i=0}^{n} \frac{x_0^i - x^i}{\lambda} * (f(\vec{x}_0) - f(\vec{x}_{\lambda,i})) \qquad (2)$$

Often, the changes of some k-th coordinate of the image y^k is more or less independently influenced by the changes of the values x^i. Therefore, one can assume that there are one-dimensional functions δ^i with

$$f(\vec{x}) = f(\vec{x}_0) + \sum_{i=0}^{n} \delta^i(x_0^i - x^i), \text{ with } \delta^i(0) = 0 \quad (3)$$

For this case, the only question is what kind of one-dimensional curves δ^i one wants to put through the sampling points as interpolating functions. Most times, polynomials or splines (piecewise polynomial functions) are used. Although this property of the model is not vital to use the general ideas presented here to find a good interpolating function f, it allows to use less sampling points and actually, all our models do have this property.

A typical example of parameterisation are the Source-Receptor Matrices (or Country-to-Grid Matrices) derived from runs of a Chemical Transport Model (CTM). Those matrices are used by several models. Besides *EcoSense* and *OMEGA* also RAINS respectively GAINS (GAINS) use these data sets. *OMEGA-HM* additionally is provided with quite similar data on heavy metal dispersion in the atmosphere, allowing to calculate heavy metal impacts together with *WATSON*. The data for this were prepared by the Norwegian Meteorological Institute (met.no) (respectively by MSC-East (msc-e) for heavy metals) by running a full CTM time and again on a computer cluster.

4 LINKING EXISTING MODELS

In the previous paragraph we introduced different options to flexibly link models or modules, respectively. The way how to link models primarily depends on the questions to be answered. Thus, in this paragraph we start with a discussion of how to utilize the linking options for particular questions related to impacts on human health and the environment due to anthropogenic emissions. Finally, we exemplarily test the modular design as one of our main linking options on the basis of two questions which are of current concern within European policy.

As mentioned in paragraph 3.1 with a fully integrated model it is possible to calculate almost every single process of a system, due to the complexity of nature preferably at the local scale. An example could be the question: How do different chemicals influence each other in a specific catchment area? Many of the questions of environmental concern, however, are based on at least national or even continental scale and furthermore, when it comes to sustainability, deal with large time scales. An example is the question: What are the total human health costs of anthropogenic emissions of heavy metals in Europe? (cf. Paragraph 4.1) In those cases it is impossible to cover all relevant processes within the same model spatially and temporarily resolved. To overcome this problem we used a modular design where individually working models operate as a system of modules linked via specific interfaces further described in the following examples. Those modules can easily be reused, re-sorted, and connected in a way applicable to the question of interest.

The use of the concept of modularisation for its part is limited to only few runs due to the fact that according to the calculated processes and the resolutions it still can be relatively time-consuming. When focussing on optimisation strategies we therefore introduced the concept of parameterisation, where the model functionality is condensed to some functions and data. One example could be: What mitigation measure strategy should be used in order to maximize the difference between avoided external costs and costs of implementation? Thus, we recommend to always try to fully understand the specific requirements of a question before thinking about how to link the different available modules or models.

4.1 Calculation of heavy metal emission impacts

One example of modularisation was realised, when calculating external costs caused by heavy metal emissions. For this, first *OMEGA-HM* is run to evaluate the damages caused by inhalation and to calculate mean annual deposition values for every grid cell and every compartment, both times using the Source-Receptor Matrices (cf. Paragraph 3.3) for heavy metals.

Then the deposition values are inserted into the database of *WATSON*. This step is done manually, simultaneously checking the data for inconsistencies and incompleteness, although an interface for automatic data transfer will be created soon. *WATSON* now calculates the damages due to ingestion with different discounting schemes. Figure 2 shows the result-

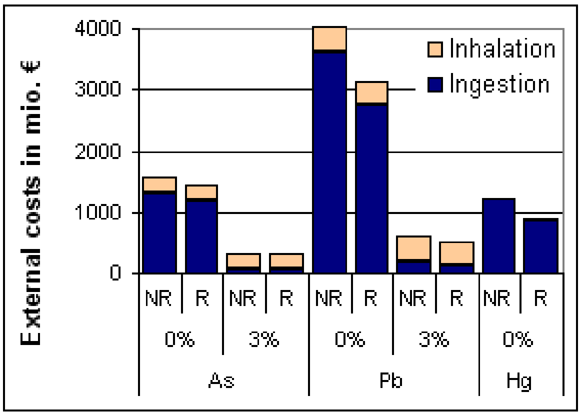

Figure 2. Comparison of external costs due to inhalation and ingestion (NR: no reduction scenario; R: reduction scenario) with 0% , 3% discounting.

ing external costs for arsenic, lead and mercury for the business as usual (NR: 'no reduction') and the maximum feasible technical reduction scenario (R: 'reduction'), comparing damages due to inhalation and ingestion for 0 % and 3 % annual discounting. Since it usually takes a long time for emitted heavy metals to reach the human body via ingestion, the discounting factor plays a very important role for future damages. However, as most heavy metals' residence in the atmosphere and bioaccumulation probably are quite significant, their impacts via the ingestion pathway for 3% discounting will most likely be less important. For the complex environmental fate behaviour of mercury no discounting factor can be applied. It was rather necessary to use a simplified model, assuming that today's emissions are proportional to current ingestion values without influencing future exposure.

4.2 External costs of anthropogenic emissions

In this paragraph we tackle the fundamental problem to assess effects on human health at different scales – local, regional and hemispherical – due to air emissions from a point source. Alongside we describe the assessment of impacts on crops, material and ecosystems at the regional scale. This assessment is partly covered by *EcoSense* (cf. Paragraph 2.1) but for a complete answer heavy structural changes and extensions are needed.

Given that *EcoSense* is grown over decades some technical and structural limitations were reached. Thus, to improve and enhance the model, the selected solution was to break down *EcoSense* in stand-alone modules (cf. Chaper 3.2). Due to this reconfiguration we obtained a more flexible and adaptable tool. The interfaces between the modules are similar to the ones described in Argent (2004). The modular design guarantees well encapsulated code and also allows to switch to the best suited programming language when adding new modules which ensures interoperability. Third party programs are as well encapsulated into modules and provided with interfaces to be included in the pool of modules.

As singled out in Paragraph 3.2 the modules have to be described in a common description language to state the functionality, prerequisites and the interfaces, i.e. input and output data, of a module. The description language has to be general enough to represent any sort of module in the given context. We chose XML-files to describe modules, because of many benefits as partly listed in Kokkonen (2003). One advantage is the structured way to describe the semantics of information where the structure is stated by XML-schemes. We used this concept to define a scheme representing the required items of a module definition. All modules have their own XML-file derived from the scheme. This allows an automatic interpretation of modules and enhances the human readability. The interfaces of the modules are as well described by XML-schemes where concrete data are entities of the scheme. Only data in the correct form are accepted by the module.

Finally, to choose and connect modules in a flexible way in a model framework to automatically start and control the run of modules and to organize the exchange of data was realized. The data transfer is processed directly by exchanging files or, if more appropriate, a database oriented aproach is applied.

We used the modular design and the modelling framework to make a calculation for a hypothetic coal fired power plant in Germany near Stuttgart with an electricity production of 3900 GWh per year and an emission of approx. 1000 tons of $\mathrm{SO_2}$, 1800 tons of $\mathrm{NO_x}$, and 200 tons of $\mathrm{PM_{2.5}}$ per year. The modules are selected in such a way that effects on human health at the local, regional and hemispheric scale are assessed. We had to connect Chemical Transport Models (CTM) for different spatial scales to modules to assess impacts, damages and external costs. For regional and (northern) hemispheric scale we used the modules that encapsulate Source-Receptor Matrices prepared by the Norwegian Meteorological Institute (cf. Paragraph 3.3). The Industrial Source Complex model (Brode and Wang, 1992) is used for transport modelling of primary air pollutants in an area of $50\mathrm{km}$ around the facility where chemical reactions in the atmosphere have little influence on the concentrations of primary pollutants. This model needs detailed meteorological data for the considered point source provided by another module in our framework. To calculate impacts on ecosystems an additional module has to be used in the calculation.

The external costs for the power plant are calculated automatically by starting the described model connection in the framework applying the contigent valuation method (cf. Bickel, Friedrich, 2005) . The results expressed in €-Cent per kWh are for the local scale 0.0002, for the regional scale 0.77, and for the local/regional scale 0.77. Due to the high stack of $240m$ the local effects are very low. The module to consider the hemispheric scale modifies the overall results by 0.013 €-Cent to assessed external costs of 0.79 €-Cent per kWh. Regarding the receptors crops and materials our model calculates an impact of 0.049 €-Cent per kWh. Impacts on ecosystems due to acidification and eutrophication in Europe are estimated as 0.09 €-Cent per kWh. They are calculated by estimating the biodiversity loss of ecosystems.

5 CONCLUSION

On the one hand, individually working models or modules respectively can be recommended to be used for questions based on large spacial and temporal scales, such as questions concerning sustainability at the European scale. On the other hand, the concept of parameterisation is suitable when optimisation needs to be taken into account as in the question of finding the best mitigation measure strategy to reduce emissions of classical air pollutants.

Generally, in addition to the benefit of applying standalone models used in order to support policy makers coupling models enhances the possibility to appropriately answer complex questions which cannot be answered adequately by only using models individually. The most sensitive and important point within this process - while the linking itself is done rather easily - is to identify the requirements of a question to be able to select the appropriate modules and coupling methods to answer it.

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