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"Methodical Optimization of Model Approaches on Pollutant Balancing in River Basin Districts to Promote the Implementation Strategy for the Water Framework Directive"

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Summary

In compliance to the reporting commitment within the framework of international river basin and marine conventions as well as the EU water framework directive the ongoing updating and development of model systems for quantifying emissions into surface water in Germany is needed. The aim of this research project therefore was to methodically further develop the existing quantification approaches within a feasibility study and to test their adequacy for modeling in the scale of large river basins as well as to implement input data sets of spatially and temporally higher resolution. Furthermore, a consistent and transparent instrument is to be developed which will facilitate the reporting commitments and complies with the follow-up and development capabilities concerning the consideration of scenarios.

The initial point for this project is a project of the Federal Environment Agency of Germany which was completed in 2010 (Fuchs et al., 2010). In two sub-projects a homogenous data basis and modeling approaches were developed for all German river basins for all relevant substance groups (nutrients and pollutants) and integrated into the model system MONERIS (Behrendt et al., 1999).

By technically re-implementing the MONERIS approach into the open source model system MoRE a flexible and transparent tool for quantifying and visualizing emissions into surface waters was developed. MoRE comprises all input data and modeling approaches according to Fuchs et al. (2010) that are relevant for balancing pollutant emissions. The transparent documentation concept facilitates the understanding of the input data, approaches and results. The architecture of MoRE allows users without any knowledge of programing to be able to add other input data and quantification approaches as well as embed other substance groups. This way different variants of input data and modeling approaches can be integrated as variants of the basic variant and the produced results can be compared. Furthermore, the implementation of different variants allows the analysis of sensitivities in the model as well as the consideration of scenarios when modeling emissions.

In the completed project of Fuchs et al. (2010) the most important emission pathways were identified. On the basis of these results the following modeling approaches were be developed based on their relevance for pollutant emissions:

- the modeling approach for water balance and runoff components
- the data basis and modeling approaches for quantifying the emissions via sewer systems
- the data basis and model approaches on erosion and sediment delivery into surface waters
- the in-stream retention of particulately transported pollutants
- the metrological recording of river loads in case of floods.

For the purpose of further developing the hydrological approach it was tested whether a conceptional water balance model is suitable for mapping the water balance and runoff characteristics in the analytical units as a basis for modeling the emissions. For this the model system PRMS (Precipitation Runoff Modeling System) was used exemplarily for the catchment area of the Ruhr (4,485 km²). For encompassing the heterogeneous structure of the catchment area (land use and soils) hydrologically homogenous zones were allocated according to the runoff characteristics. Furthermore, the temporal resolution was increased to be able to encompass the dynamics of the runoff processes. The Ruhr example showed that

unsealed areas (e.g. woodland, grassland or arable land) can be distinguished from sealed areas (settlements and commercial areas) in regard to their runoff reaction. Conceptional water balance models are therefore good for generating land use specific runoff components as input data for modelling emissions.

When quantifying the emissions via sewer systems the stormwater runoff from sealed areas plays a significant role. The key parameters are the size of these areas and their substance-specific surface load. Within this project both input data sets were improved considerably. The data basis for sealed areas was generated by intersecting a database on the degree of soil sealing with a database on urban areas. In addition, the surface load for copper and zinc as a function of anthropogenic activities was designated for two types of settlements. At first, representative concentrations in stormwater runoff were derived for lowly and highly urbanized areas. Then the sealed area within the settlements was classified along these lines. In conclusion, the surface load was derived for both settlement types. The result showed no change for the overall emissions via sewer systems for copper, but zinc emissions declined by 13 %. But the new input data lead to a more realistic illustration of the spatial dispersal of the total emissions by improving the illustration of agglomerations and areas of low population density in a map showing total emissions.

For the improvement of the data base to quantify emissions via the pathway erosion, detailed data on soil loss from agricultural areas (based on the ABAG factors derived by Wurbs and Steininger (2011) and a survey on the percentage of conservation tillage methods) were implemented into the MoRE system. Based on these data a consistent spatially lumped approach to quantify the sediment input into surface waters was derived and validated using long term suspended solid loads at monitoring stations. Furthermore, the top soil concentrations of heavy metals were regionalized according to the different bedrocks of Germany. Compared to the results of Fuchs et al. (2010) no significant changes of emissions via erosion for the analytical units, strong regional variations are obvious. Local emission hot spots in the river basins can thus be more adequately captured by detailed input data.

A portion of the suspended solids that is delivered to surface water bodies from the catchment areas can be re-deposited in the river system. The example of the Danube basin has shown that the consideration of local sedimentation rates in lakes and impoundments leads to a good adaptation of monitored suspended solid loads.

To validate the model results the modeled river loads are compared with the loads that were observed through the standardized measurement programs. An optimized measurement concept was developed to improve the database as these measuring programs do not sufficiently comprise the sediment and pollutant transport during flood events. The measurement concept is designed to take specific samples of a medium sized river during flood events. The evaluation of the data shows that standardized measurement programs do not map the transported river loads sufficiently as the sediment loads during a flood event are 80 times higher than at average flow. Consequently, the pollutant concentrations are significantly higher, by 4 to 30 times. The concentration of phosphor during the measurement came up to the concentration at mean water, contrary to the heavy metals.

Within the framework of this project the potential of the methodological development of chosen modeling approaches was investigated in the context of a feasibility study. The feasibility study lay the foundation for an optimal adaptation of the complete model in a

subsequent phase of model development and to transfer the approaches to the whole of Germany.

1 Introduction

In compliance to the reporting commitments within the framework of the river basin and marine conventions as well as the EU Water Framework Directive the ongoing updating and development of model systems for quantifying emissions in surface water is demanded. Within the framework of this project the potential of a methodological enhancement of chosen modeling approaches is investigated in the sense of a feasibility study in order to guarantee in the next project phase a professional development of the model an adaptation of the complete model. Furthermore, a consistent and transparent instrument should be developed with which the reporting commitments can be fulfilled and the implementation of the EU water framework directive can be supported.

With the conclusion of the predecessing projects "Model-based Quantification and Internetbased Visualization of Emissions into Rivers in Germany" and "Development of a Management Tool on Emissions into Surface Waters within the Framework of the International Reporting Commitment" a harmonized variant of the MONERIS model system has been available (Venohr et al., 2008; Fuchs et al., 2010). The modeling results for nutrients (nitrogen and phosphor) and pollutants (heavy metals and PAH) were generated based on harmonized basic data and modeling approaches and stored in a database. For the first time it then became possible to visualize the emissions into surface waters for all analytical areas in Germany.

Based on this, selected modeling approaches for pollutant emissions were to be further developed methodically. In summary the work was focused on:

- Optimization and further development of the database, the user interface and the calculation module towards the ability of enabling scenarios and fulfilling the report commitment for the Federal Environment Agency
- Improvement of individual modeling approaches (water balance, sewer systems, erosion and retention for particulately transported matters)
- Development of an optimized measurement concept to record river loads in case of floods
- Warranty of applicability of the model in international river basins (interfaces, regional specifics)
- Organizing a workshop to coordinate with state authorities and river basin communities

The results achieved for the individual points of the project will be carried out as follows. At first chapter 2 shows the technical initial situation of the project. Then the implementation of the MONERIS approach in the modeling tool MoRE is explained. In chapter 3 the improvements to individual approaches on emissions modeling are shown: Hydrology (chapter 3.1), sewer systems (section 3.2), erosion and retention (section 3.3). Chapter 3.4 describes an optimized model concept to comprise substances transported during flood events and its results.

Finally, chapter 4 summarizes the most important conclusions from the feasibility study. Further steps are explained in short regarding the future transfer of the model on to the whole of Germany and foreign river basin areas. In addition, suggestions are made for further adaptations of particular quantification approaches.

2 Development and Optimization of the dp-technical tools

In this chapter the initial situation will be outlined first, then the aims set will be presented. Following that will be a description of the technical implementation of the MONERIS (**Modeling N**utrient Emissions into **RI**ver **S**ystems) concept to the modeling tool MoRE.

2.1 Initial situation and intention

The completion of the project "Model-based Quantification and Internet-based Visualization of Emissions into Rivers in Germany. Nutrients, heavy metals and further priority substances"(Fuchs et al., 2010) produced a homogenous instrument that makes it possible to identify the most important emission pathways and pollution hotspots for different substance groups in larger river basins. Based on this it is possible to identify measures to reduce emissions into surface waters and to estimate their effectiveness. Within the framework of that project the general and substance specific input data, chosen intermediate results and final results for nutrients (nitrogen and phosphor), heavy metals (cadmium, chromium, copper, mercury, nickel, lead and zinc) and PAH (polycyclic aromatic hydrocarbons) for all analytical units, years and substance groups were consolidated in one database. In addition, individually linked MS Excel files were available which used the general and substance specific input data to model emissions for nutrients, heavy metals and PAH. By merging the data into a database it was possible to also visualize emissions into surface waters for all analytical units in Germany via an appropriate graphical user interface.

For the first time this produced modeling results for nutrients and pollutants for Germany which were based on harmonized input data and approaches. However, the PostgreSQL database as well as the Excel files were not documented to a sufficient extent so the results can only be reproduced to a certain degree. Besides, Excel-MONERIS reached its performance limits with the amount of data that had accumulated over the 23 balancing years, the large amount of analytical units as well as the diversity of substances.

This initial situation called for a technical reimplementation considering the following aspects:

- establishing the calculating capacity and implementing the existing methodical approaches (MONERIS concept) into a new tool (software),
- complete and meticulous documentation (with the guarantee of reproducible and traceable results),
- open, flexible structure,
- calculating with different input data sets or modeling approaches parallel to the basic variant to assess the quality of input data and analyse the sensitivities,
- extension to other substance groups such as nutrients and further priority substances without the effort of having to reprogram and
- user-friendliness.

The modeling tool for balancing pollutant emissions that is emerging in this project should be able to map the MONERIS results so far from 1983 till 2005 on the basis of all general and substance specific input data as well as the modeling approaches by Fuchs et al. (2010).

This new implementation is a development of the PostgreSQL database which emerged from the mentioned project of the Germany Federal Environment Agency while including the approaches from the Excel files and a newly developed calculation engine to create a modeling tool for pollutant emissions into surface waters. The open and flexible structure allows this tool to be extended for other substance groups e.g. nutrients and further priority substances as well as for other sets of input data and approaches.

2.2 The modeling tool MoRE

In this section the system architecture of MoRE is explained and the individual components of MoRE are described in short. Further details on MoRE can be found in the manual (Fuchs et al., 2012). The technical implementation of the modeling approaches will be shown in section 2.2.3. Further topics are in the documentation in MoRE (section 2.2.4), the handling of the results (section 2.2.5) and the applicability to international river basins (section 2.2.6). This is followed by a summary in section 2.2.7.

2.2.1 The system architecture of MoRE

To implement the mentioned aims it was necessary to develop a completely new model architecture which regulates the interaction amongst the newly developed components of MoRE. The fundamental components of MoRE being as follows: (Figure 1):

- an open source PostgreSQL database,
- an independent, generic calculation engine
- as well as two graphical user interfaces: the developer interface "MoRE Developer" and the visualizing interface "MoRE Visualizer".



Figure 1: System architecture of MoRE

The user interfaces were developed to interact with the PostgreSQL database. The content of the PostgreSQL database can be read, edited and extended with the help of the user interface *MoRE Developer*. *MoRE Visualizer* is then used to visualize the modeling results. The modeling is done by a generic calculation engine which is accessed via the user interface MoRE Developer and has a dynamic connection to the PostgreSQL database. The modeling results can either be listed as tables by the MoRE Developer or as maps as well as graphs by the MoRE Visualizer. The users can use MoRE either via a network connection as multi-user access or as a standalone application for a PC.

The individual components of MoRE will now be explained.

2.2.2 Individual components of MoRE

2.2.2.1 Database

The PostgreSQL database of MoRE contains all necessary data, approaches, the obtained results and the appropriate meta data for modeling.

Apart from general input data (e.g. mean elevation, land use, soil type, rainfall, connection rate, etc.) and substance-related input data (e.g. topsoil content, rainfall concentrations, effluent concentrations of wastewater treatment plants) the data needed for modeling is model constants. The database comprises values of input data for each analytical unit and, where applicable, for each year. This is supplemented by metadata. For example this means that every entry to the database is given a distinct origin. In addition, information on references to pathway and substance is included. The database also contains the spatial reference of modeling in the form of analytical units.

Furthermore, all modeling approaches (empirical equations) are stored in the database. The modeling approaches also have assigned metadata such as e.g. origin and substance reference.

Finally, the database comprises the model results. These are saved on two levels, as preliminary and final results. After being computed all results have a provisional character. After an assessment the user can decide to either discard the results or classify them as final. The visualization only uses finalised result. After being modeled the results also can be exported to MS Excel.

2.2.2.2 Calculation engine

One of the main aims in developing MoRE was to supply a flexible modeling tool. Therefore, the calculation engine is generic and was designed and programed as autonomous unit of the MoRE system. During a calculation run (modeling) it reads the input data from the database and computes according to the underlying modeling approaches. As the calculation engine does not contain any formulas but merely the logical structure of the database, it does not have to be adapted to new computing algorithms as long as the structure stays the same. This means the user does not need any programing skills and can embed and test new computational approaches without any big efforts.

The calculation engine was optimized for speed and therefore executes as many operations as possible in the RAM. With that the interactions with the PostgreSQL database were reduced to a minimum. This achieves obvious benefits for the performance as only chosen variables are saved during one computation step. This choice can be adapted by the user as pleased. In addition, there is a choice between a fast calculation run, which only saves the

chosen variables, and a slower protocol that not just saves the chosen variables but also all input data and all generated intermediate results.

The calculation engine was developed as API (Application Programing Interface) in the programing language C#. It can therefore easily be used by other applications such as a web server. This means the calculation engine can be executed everywhere, where a .NET framework can run, e.g. in Windows, Linux or Mac OS X.

2.2.2.3 Developer interface MoRE Developer

With the help of the user interface MoRE Developer input data can be imported into the database and metadata can be allocated to them. MoRE Developer allows for new calculation approaches to be integrated or existing ones to be adapted. Flowcharts can be deposited to document the approaches so these can be retraced properly. Finally, the MoRE Developer drives the calculation engine to compute the emissions into surface waters as well as river loads.

The developer interface MoRE Developer allows different settings to be made for the visualization interface. E.g. all changes in the final results made in the MoRE Developer will have a direct influence on the results shown in the visualization interface.

2.2.2.4 Visualization interface MoRE Visualizer

The MoRE Visualizer offers the possibility to show and analyse the basic data and the results. It is a browser-based application that can be used via an internet connection and works with a direct connection to the MoRE database.

The main use of the visualizer is to depict area-specific emissions into surface waters for the analytical units in the form of maps. For this the following criteria must be selected: catchment area (e.g. administrative units, river basin districts), substance and period. In addition, the visualizer can aggregate the depicted results according to the chosen criteria. One special feature is the selective comparison of different periods as well as visualizing different result sets.

Finally, the modeling results can also be illustrated as a report and be exported to MS Excel. There are further functions such as printing and user-defined classification of the results.

2.2.3 Technical implementation of the modeling approaches

The modeling approaches in MoRE are stored in the database as text and are interpreted by the calculation engine together with the input data during modeling. As the modeling does not refer to a compiled file the user has the possibility to change the approaches at any time if desired without any knowledge of programing.

Balance parameters for the modeling are the following components: inhabitants, areas, runoff, emissions and river loads. These are generally calculated by empirical equations. The modeling has three levels. The smallest unit is defined as a formula (equation). The aggregation of several formulas in a certain order is called algorithm. Several algorithms in a defined order make a calculation stack (Figure 2). The calculation stacks generally map a component.

Flowcharts were stored for the calculation stacks to achieve a high transparency and a good outline of the implemented approaches (also see section 2.2.4).



Figure 2: Structure of the modeling approaches in MoRE

MoRE is modular so that approaches for different emission pathways can be adapted independently from another. This enables the user to calculate an emission pathway with different input data or different modeling approaches as variant to the basic variant. The obtained results can then be compared to assess the quality of new input data and approaches. The variants also help to analyse sensitivities.

The calculation engine models the components inhabitants, areas, runoff and emissions for each analytical unit independently from other analytical units. As a supplement to this, a topologically dependent calculation along the runoff tree was implemented for the modeling of river loads, in which the upstream and downstream areas of an analytical unit were taken into account. In addition, factors for splitting the area's runoff and river loads in different downstream areas were considered.

2.2.4 Documentation in MoRE

A documentation concept was developed in MoRE to be able to reproduce the results and to facilitate the traceability of input data, modeling approaches and results.

This concept requires that the input data, intermediate results and results from the database not just get a variable name and a description but also further information. For example, this could be an origin in the form of a literature citation, a reference or pathway reference or a unit.

The modeling approaches are documented in a similar way. Each empirical equation in MoRE has a distinct variable name, a description and an origin assigned to it. And the operations are implemented in text form so that the user can retrace them without any programing knowledge. The underlying model approaches for each emission pathway are

also available in the form of flowcharts. They visualize the order of the calculations, the formula content as well as the input variables needed and their units. Different symbols make it easy to differentiate between input variables, model constants, intermediate results and results. Examples can be found here in Appendix 6.

To document the results, MoRE can create a protocol during a calculation which saves all used input data, intermediate and final results as well as all equations used.

2.2.5 Management of the results

To fulfill reporting commitments of the Federal Environment Agency, the reported results must be documented. Additionally, a possibility was provided in MoRE to carry out model calculations with different input data or approaches to swiftly assess the quality of input data or the effect of changes in the approaches.

To be able to manage the amount of generated results each calculation process and protocol respectively is given a unique identification number. The results produced from the calculations/protocols all have – as already described in section 2.2.2.1 – a provisional character and are marked as preliminary results. Where required the user can discard them after checking them. Selected results can be classified as final result sets. Only these result sets can be displayed with the help of the visualization interface.

2.2.6 Guarantee of applicability in international river basins

As already described in section 2.2.2.2 the database can be extended at any time as long as the architecture of the database system is maintained. For the applicability of the model system in other river basins MoRE thus offers a flexible and easy integration of new input data and analytical units. For instance, new topologies can be integrated with the help of an import tool and the modeling can be extended to other river basins. In addition, the model structure facilitates the use of input data with different quality without that any further programing effort is needed. The data has to be in Excel format to be able to be imported.

The model can be used to calculate results from the level of analytical units up to the level of river basins as well as for administrative borders.

2.2.7 Summary and outlook

Within the framework of this project the flexible and transparent open source model system MoRE was developed on the basis of the MONERIS concept (Behrendt et al., 1999) to quantify and visualize emissions into surface waters. In MoRE all input data and modeling approaches on pollutants of the previous project (Fuchs et al., 2010) are implemented as basic variant. Based on this basic variant a completely correct reproduction of the results for pollutants from the previous project can be guaranteed.

Based on the results from the previous project a new model architecture was developed. MoRE consists of a PostgreSQL database in which the input data, modeling approaches, results and the corresponding metadata are stored. To achieve the calculation capacity a generic calculation engine was programed as a unit that is independent from the MoRE database. It therefore does not need to be adapted to changes in the modeling approaches as long as the architecture of MoRE is maintained. This enables the user to create variants of input data and modeling approaches as supplement to the basic variant as well as to integrate other substance groups without any programing skills. Further components of MoRE are the user interface MoRE Developer to change the input data and modeling approaches as well as the user interface MoRE Visualizer which can display and analyze the final results.

MoRE offers an optimal base for designing and implementing modeling approaches, alternative input data (e.g. in a higher resolution), formulas and scenarios. The system is modular so that modeling approaches for different emission pathways can be adjusted independently from each other. This way different variants of input data and modeling approaches can be created parallel to the basic variant for an emission pathway and the generated results can be compared. On the one hand the quality of the input data can be evaluated. On the other hand the implementation of different variants enables the analysis of sensitivities in the model. Both points are of major importance for the priority pollutants as there are no consistent databases and hardly any affirmed modeling approaches for most of the substances. Furthermore, the possibility of creating variants in MoRE provided the necessary technical requirements to be able to include scenarios when modeling emissions.

3 Improving individual approaches for material flow modeling

The following section will illustrate the improvements of individual approaches for modeling the water balance, the emissions via sewer systems, emissions via erosion as well as for the modeling of retention. Additionally, a procedure will be shown that enhances the recording of river loads in cases of floods.

3.1 Enhancements of the hydrological approach

3.1.1 Initial situation and the necessity of adjustment

Mapping emissions into surface waters as accurate as possible depends strongly on the knowledge of the spatially and temporally spread runoff characteristics and the corresponding runoff balances. The model concept MONERIS, which was implemented within the framework of this project in the MoRE tool, balances on the basis of a semi-empiric, conceptional approach the nutrient and pollutant loads into surface waters on the catchment scale. The determination of the water balance, as a basis for balancing loads, has been carried out with the MONERIS model concept with a temporal resolution of annual values. This means that the emissions are also accounted for in annual values. A description of the used approach can be found in Behrendt et al. (1999) and Fuchs et al. (2010).

On the background of a larger temporal differentiation of nutrient and pollutant emissions modeling the superior aim of this work is to further develop the hydrological approach. Here the aim for the temporal resolution for modeling loads is to be monthly in order to improve the model results.

To be able to provide a more reliable basis for balancing loads into surface waters, the aim of this project is to enhance the approach used so far for assessing the water balance. It is necessary, even for an aspired monthly resolution, to simulate the hydrological balance on the basis of daily values to be able to map the seasonal dynamics and characteristic hydrological regime. This high temporal resolution of the hydrological model is necessary to be able to reproduce runoff dynamics, runoff volumes and with that the water balance on the spatial basis of the Analytical Units in a way which is more process-orientated than the previous approach. On that basis the loads from urban and rural areas into rivers can be measured more detailed and differentiated. The enhancements of the hydrological model approach are also needed to be able to spatially as well as temporally calculate the hydrological behaviour of catchment areas within the framework of changing scenarios (e.g. climate, land use) in a suitable way.

In the following it will be shown which basic requirements are set for the water balance simulation with a hydrological model to be able to facilitate a detailed calculation of the water balances in river basins with the help of a comprehensively available data basis. For a first test run of the improved hydrological model approach the catchment area of the Ruhr was chosen within the framework of a feasibility study. With the help of this pilot area the new hydrological model approach is explained and the results of the water balance calculation are illustrated. Subsequently, the possible development potentials as well as the general transferability of the approach to all river basins nationwide are discussed.

3.1.2 Demands on the hydrological model

A hydrological model concept suitable for modeling loads with MoRE should reproduce both the runoff behaviour and the water balance on river basins spatially and temporally as well as possible.

Generally, for the choice of a hydrological model the spatial and temporal as well as the basic methodological model requirements of the implemented approaches to model emissions should be considered. The hydrological approach for calculating the water balance of meso- and macro-scaled catchments should principally reproduce the hydrological behaviour and runoff processes as simple as possible. By this means it is also necessary to achieve an adequate degree of detail that matches the purpose of the emissions modeling so that no conflicts can evolve between the components of the model chain.

The smallest spatial resolution allocated in MoRE was based on hydrological properties, socalled analytical units, which in average (within Germany) are about 130 km² (Fuchs et al., 2010). These analytical units are to be transferred as elementary spatial units for the hydrological modeling. Each Analytical Unit exists of smaller spatial units which all have different runoff behaviour depending on the existing spatial characteristics (soil characteristics, land use, slope). Especially rural areas (agriculturally used areas and forested areas) and urban (built-up) areas feature diverse runoff behaviours. Therefore, based on the analytical units, the runoff rates for urban and rural areas must be calculated separately.

Simulation of runoff from **rural areas** should be calculated for three separate runoff components, which differ from each other by their hydrological response time to a rainfall event:

- fast reacting runoff
- temporally slightly deferred runoff
- temporally highly deferred runoff

The runoff reacting quickly tends to occur on the surface or the near-surface areas, often rooted and bulked soil areas. Whereas the runoff components with short and long delays can be allocated to the other unsaturated and saturated soil zones.

Urban areas always have fast runoff components which are fed back to the surface waters via the canalisation to rain water release points or via wastewater treatment plants. For the modeling of emissions the runoff from the built-up (partially sealed) areas has to be calculated separately.

The total runoff for an Analytical Unit is obtained by the superposition of the mentioned fractions of runoff from different partial areas which are assumed to be homogeneous in regard to their runoff behaviour.

Besides detecting the spatial heterogeneity it is also necessary to properly map the temporal differences in the runoff behaviour and runoff dynamics of catchment areas. Therefore, the runoff behaviour of the analytical units must be simulated on a basis of daily values. For the emissions modeling monthly values are then to be derived from these daily values.

A further important precondition for the hydrological modeling is that the necessary spatial and temporal database for all catchment areas (within Germany) is uniformly available. For enhancing the hydrological approach it is not necessary to develop a completely new model. It should rather be a hydrological model that conforms to the above mentioned requirements for modeling emissions and has already proven of value in large river basins.

3.1.3 Analysis of approved water balance models

As described in the previous section the analysis concentrates on existing models which

- work on the catchment scale,
- are applicable in larger areas with heterogeneous area characteristics (meso- and macro scale),
- do not contradict the empirical approach of emissions modeling,
- can comply with the spatio-temporal requirements for modeling emissions.

The hydrological model for simulating the water balance at first has to comply with the spatiotemporal requirements to be able to calculate the water balance spatially distributed for catchment areas in a high resolution. Based on the available data basis the choice of the hydrological model depends on the ability of the calculation approach to map the individual hydrological sub-processes and finally the complete water balance.

In general there are many hydrological models which comply with the requirements and are used nationally and internationally. These hydrological models always use comparable methods of calculation to reproduce the hydrological behaviour of catchment areas. They mainly differ in the processing of the procedures to describe the hydrological processes as well as in the management and output of computations and intermediate results. In Germany each federal state has a different hydrological model. For example, Baden-Wuerttemberg and North-Rhine Westphalia use the water balance model LARSIM (Large Area Runoff Simulation Model) (Bremicker, 2000), whereas in Thuringia and Saxony the rainwater runoff model NASIM (Hydrotec, 2011) is in use. A summary of the models used in Germany, Austria and Switzerland for simulating flood events can be found in DWA (2010) for example. In neighbouring Europe amongst others the HBV-model has successfully been applied (Bergström, 1992). The mentioned models are all based on hydrological calculation concepts which map the hydrological system and the running natural processes in a more or less simplified manner by presumptions and estimations, e.g. by a linear storage approach.

A further hydrological model which complies to the necessary requirements (spatially and temporally) is the Precipitation Runoff Modeling System (PRMS) (USGS, 2009). PRMS is also a conceptional water balance model which is successfully deployed in Germany (Bende, 1997) and internationally (Hay et al., 2003).

In the catchment area of the Ruhr PRMS is the hydrological model basis with which the reservoirs of the Ruhrverband have been managed for many years (Ruhrverband, 2002a). An essential advantage of PRMS is that the whole source code (Fortran) is available for free in the internet. The open, modular program structure of the hydrological model allows to further optimize and adapt the calculation approaches and data processing in the future if necessary. A complete detachment from the chosen model basis PRMS is therefore imaginable, too. In doing so the fundamental concept of the model could be adopted and implemented in a way that a tight link with the load model is made possible.

For this reason the PRMS model was chosen. It fulfills all prerequisite requirements. PRMS works related to catchment areas on the meso- and macro scale. The model harmonizes methodically with the empirical approach of the load modeling and fulfils all necessary spatio-temporal requirements. The model further offers the requirements to realistically reproduce

the runoff characteristics in river catchments and thus calculate the water balance with sufficient accuracy. PRMS is freely available and offers a high flexibility in matters of development and adaptation to existing load modeling.

The following section will describe in more detail the general functionality of the hydrological water balance model PRMS and will also specify the data basis needed to calculate the water balance.

3.1.4 The water balance model PRMS

3.1.4.1 The Precipitation Runoff Modeling System

PRMS is a deterministic, distributed-parameter, conceptual hydrological watershed and water-balance model. The model, developed by the U.S. Geological Survey (USGS) has been in use since 1983 to examine the impact of manifold combinations and changes in precipitation, climate and land use on watershed response of different sized catchment areas (Flügel et al., 1993; Dudley, 2008).

With PRMS the water balance of a catchment area is calculated on the basis of so-called Hydrological Response Units (HRUs). The HRUs are the spatially differentiated elemental parameterisation and calculation units of the hydrological model. Within the HRU it is assumed that the system reaction is homogenous concerning the runoff characteristics in consequence of hydrometeorological events. By designating HRUs it is possible to take account of spatial heterogeneities in a catchment area, e.g. differences in soil characteristics, in gradient, in land use but also in rainfall events and then simulate the runoff characteristics spatially distributed.

The definition of different HRUs is always guided by the question being looked at. In this case the identification of the HRUs results from the superimposed information on soil and land use. Homogenous soil information and superimposed homogenous land use form an HRU. A comprehensive description of the HRU concept can be found at Flügel (1996).

Concerning the circumstances for load modeling with MoRE this means that the analytical units allocated within the framework of the hydrological modelling simulation can be further subdivided into HRUs according to their spatial characteristics. The HRUs can thus be rural or urban partial areas. Based on the meteorological input data (precipitation, temperature etc.) the hydrological model simulates the water balance within an Analytical Unit (catchment area) separately for each HRU (homogenous partial area) in daily time steps. In principle the PRMS simulates the vertical water flow in an HRU with the help of storage elements and exchange processes between these storages (Brudy-Zippelius, 2003). At the same time the temporally variable vegetation, a possible layer of snow, depressions on the ground surface and the complete soil zone are simulated as a series of different storage modules (Figure 3).



Figure 3: Scheme of the hydrological water balance model PRMS (modified after Leavesley et al., 1995)

The runoff from an analytical unit results from superimposing the partial runoffs from the different HRUs. A detailed description of the process algorithms can be found at Leavesley et al. (1983) und USGS (2009) for example.

3.1.4.2 Data basis

Different spatial information on catchment characteristics is needed to use the water balance model. In addition, time-dependent hydrometeorological values in daily steps are needed to simulate the water balance and to calibrate the model. The data basis used is shown in Table 1.

Data Type	Scale/Resolution/ Unit	References	Data Description
Stream network		Umweltbundesamt	GIS-data set of watercourses
Elevation data	30 x 30 m²	ERSDAC (2009)	Worldwide information on elevation in Digital Elevation Models
Soil data	1:1,000,000	BGR (2004)	General soil map of Germany (BÜK1000); Explicit use of soil types
Geology	1:1,000,000	BGR (2002)	Digital Geological map of Germany (GK1000)
Land use	100 x 100 m²	EEA (2010)b	CORINE Land Cover 2006 raster data
Hydrometeorological D	ata (12 climate station	s)	
Precipitation	mm		Daily value
Temperature	°C		Minimum, maximum, mean
Relative humidity	%		14 o'clock LT
Discharge data	m³/s		Daily value

 Table 1: Overview of the data basis for the hydrological modeling

Precipitation is the most important input parameter for the water balance of a hydrological system and is therefore the decisive driving value to simulate the runoff behaviour. The required time series in daily steps are available for the whole of Germany e.g. at the German Weather Service (DWD) as REGNIE raster data set (1 km x 1 km) (Dietzer, 2000).

The meteorological status parameters temperature and relative humidity are needed to calculate the evaporation processes in a catchment area. To calculate the evapotranspiration the daily maximum temperature as well as the relative humidity at the maximum of the daily temperature curve are needed. Further temperature values (e.g. minimum temperature) are used to map the accumulation of snow and snow melting processes. The correct measurement of these procedures plays a significant role in calculating the water balance. The necessary time series of daily values for the used model input data precipitation, temperature and humidity and further meteorological parameters can be found as digital data set e.g. at the Potsdam Institute for Climate Impact Research (PIK) (Österle et al., 2006).

Time series of measured discharges are used to calibrate and then validate the quality of the model runoff. These time series can be found at the hydrological data services of the federal states as well as at the Federal Institute of Hydrology.

3.1.5 Feasibility study for water balance modeling

In the following the results of the feasibility study for the hydrological water balance model will be illustrated with the example of the Ruhr catchment.

3.1.5.1 Characterizing the catchment area

The Ruhr, with a catchment area of 4,485 km², originates from a spring about 670 m above sea level on the northern slope of the Ruhrkopf in the Hochsauerland (about 842 m a.s.l.) and joins the Rhine at Duisburg-Ruhrort (about 20 m a.s.l.) after 219 km. The landscape characteristics of the Ruhr catchment reach from densely wooded and scarcely populated lower mountain ranges in the Sauerland to widely sealed urban areas in the river valleys and in the western part close to the mouth. The areas can be attributed to the geological-geographical unit of the Rhenish Slate Mountains to the east of the Rhine (Brudy-Zippelius, 2003). The average discharge when it flows into the Rhine is about 76 m³/s (Ruhrverband, 2011a).

With a total of 8 dams and 5 reservoirs the Ruhr with its tributaries forms a very complex hydrological system. With a total floodwater of up to just under 35 km² the volume of all retained water of all damming structures amounts to about 480 million m³ (Ruhrverband, 2011a).



Figure 4: Water withdrawal from the Ruhr catchment area (Ruhrverband, 2011)

An intensive use of water resources takes place to supply almost 5 million people with drinking and processing water along the Ruhr and in its catchment area. Due to the intensive use of water in the Ruhr area a large extent of the water is lost completely (Ruhrverband, 2009). Because of water being exported to neighbouring catchment areas (Figure 4) but also because of a high evaporation rate from the water surface areas of the numerous reservoirs a certain percentage of the precipitation never runs off or runs off in other catchment areas.

3.1.5.2 Spatial reference for the hydrological modeling

In MoRE the catchment area for the Ruhr was split into 23 analytical units (see Figure 5). These have an average size of 180 km². To consider the heterogeneity of the Ruhr catchment as well as to map the most important spatial parameters that affect the hydrological dynamics, suitable HRUs were derived. Apart from the soil type the type of land use is an important parameter. To generate the HRUs the soil information is superimposed with the land use information. In this case the HRU concept assumes that the soil type and specifically superimposing land use have a homogenous hydrological behaviour. Therefore each soil type with a superimposed land use forms a new HRU.



Figure 5: Analytical units and river system in the Ruhr catchment

Three different soil types were found in the Ruhr catchment area from the digital general soil map (BÜK 1000) of Germany (BGR, 1998):

- sand,
- clay,
- silt.

Land use classes were identified based on the raster data of the CORINE Land Cover 2006 (EEA, 2010b). In compliance to the requirements of the load model concept (Fuchs et al., 2010) 6 land use classes were identified:

- cropland,
- forest area,
- grassland,
- opencast,
- water surface,
- developed area.

By intersecting the three assigned soil data with the assigned land use classes (apart from the developed areas) 13 different possible rural HRU types were identified for the rural,



unsettled areas of the Ruhr catchment (Figure 6 and Table 2). The water surfaces were assigned as a single type of HRU.

Figure 6: Ruhr catchment with HRU types for the rural areas

Independently from the underlying soil information, the urban (settled) areas were differentiated into three urban URU types:

- dense development
- loosened-up development
- dispersed development

The differentiation of each of the settled areas in the different HRU types results from the allocated occupancy according to the CLC 2006 classification (EEA, 2010b). For the urban areas (land use class "developed area") the subclasses of level 3 were considered respectively according to the expected runoff behaviour. For example the areas with dense development and expected high grade of surface sealing were assigned to the urban HRU type "dense development". Railway networks on the other hand were always assigned to the urban HRU type "dense development". Railway networks on the other hand were always assigned to the urban HRU type "loosened-up development" and areas that were marked as leisure facilities were assigned to the urban HRU type "dispersed development". A different methodical procedure had to be chosen especially for those areas which were classified in the CLC 2006 as areas with "discontinuous urban fabric". The classification of areas of this most common area type in one of the three mentioned urban HRU type "dense development", areas above 1 km² were assigned to the urban HRU type "loosened-up development" and areas smaller than 0.5 km² to the HRU type "dispersed development".

Table 2: Combination of soil types and land use for the derivation of rural HRU types (upper chart) and urban HRU types (lower chart)

Rural Areas					
	Cropland	Grassland	Naturally covered area	Opencast	Lakes
Clay	HRU1	HRU2	HRU3	HRU4	
Sand	HRU5	HRU6	HRU7	HRU8	HRU13
Silt	HRU9	HRU10	HRU11	HRU12	

Urban Areas				
Dense Development	Loosened-up Development	Dispersed Development		
HRU14	HRU15	HRU16		

Therefore the catchment area for the Ruhr was able to be assigned to three urban HRU types according to the expected hydrological behaviour (Figure 7). The grade of surface sealing for the developed area type "dispersed development" is about 15 % in average, for the developed area type "loosened-up development" about 30 % and rises for the inner city densely developed areas ("dense development") up to 60 %. The hydrological system was

therefore simulated within the Analytical Unit on the basis of potentially 16 different HRU types (Table 2). Based on this the scenic heterogeneity of the catchment and the differences in the runoff were able to be detected.



Figure 7: Ruhr catchment with analytical units and urban HRU types

3.1.5.3 Time-dependent input data

The simulation and the verification of the calculated water balance in the catchment area of the Ruhr with the model PRMS needed meteorological and hydrological input data in daily time steps (Figure 8). For validating the model time-dependent data was available for April 2002 till March 2006.

For the meteorological parameters precipitation, air temperature and relative humidity a measurement network made up out of 12 climate stations could be used. The precipitation for the sub-catchments was transferred to the analytical units with the help of the polygon procedure by Thiessen (1911). The temperature data was delivered as average daily values and also the maximum and minimum values of the daily measured temperature curve were used.



Figure 8: Meteorological model input data for an analytical unit in the area of the Bigge reservoir: Precipitation, relative humidity and temperature in daily values for the period November 2003 – October 2004

Furthermore, the daily runoff values were available for the calibration and subsequent validation period at gauge Hagen-Hohenlimburg (catchment surface area (AE) \approx 1,320 km²) in the sub basin of the Lenne, the largest tributary of the Ruhr, and at the two Ruhr gauges Villigst (AE \approx 2,010 km²) as well as Hattingen (AE \approx 4,120 km²). The Lenne gauge Hagen-Hohenlimburg is located about seven kilometres upstream of the mouth into the Ruhr (Ruhrverband, 2011b). The gauge at Villigst is situated just upstream of the Lenne mouth whereas Hattingen is about half way down the Ruhr between Lenne and the mouth into the Rhine (Figure 4).

3.1.5.4 Results and assessment

The hydrological water balance model simulates the hydrological system on the temporal basis of daily values. Differentiated into the existing land use classes the following runoff components were calculated for the 23 different analytical units of the Ruhr catchment:

fast reacting runoff [m³/s]

temporally slightly deferred runoff [m³/s] - rural area

- temporally highly deferred runoff [m³/s]
- fast reacting urban runoff [m³/s]
 urban area

The hydrological model was calibrated by using the water management years 1992 and 1993 (Figure 8Figure 9). With a coefficient of determination of $R^2 = 0.89$ the PRMS reproduces the hydrological runoff behaviour of the Ruhr catchment area in this time stretch with a high accuracy.



Figure 9: Comparison of the measured and simulated hydrographs at gauge Hattingen in the calibration period November 1991 - October 1993

Figure 10 shows exemplarily the calculated runoff for the complete Ruhr catchment area for the water management year 2003 within the validation period (2002 to 2006) as cumulative hydrograph from all analytical units for the mentioned runoff components (fast reacting runoff components combined) as well as the derived total hydrograph. For further checking the plausibility of the calculated runoff components a separation of the measured runoff hydrographs could not be conducted as there was no information on the origin of the water. For this reason the hydrological simulation tried to map the individual runoff amounts as precisely as possible and with that calculating the runoff hydrographs as overall reaction of different components as exactly as possible.



Figure 10: Cumulated hydrographs of the 23 analytical units in a daily time step for the different simulated runoff (fast reacting rural and urban runoff portions are combined)

Visual comparisons with the measurements of the available gauges show that the hydrological model maps the runoff dynamics well in the test area. With model efficiencies according to Nash and Sutcliffe (1970) between 0.58 and 0.67 the good results are confirmed by all means.

Due to the large influence on the runoff behaviour by the above mentioned water export and evaporation from the reservoirs the use of the model efficiency according to Nash and Sutcliffe is rather inappropriate for estimating the quality of a model in the Ruhr catchment. A comparison with the clearly affected observation time series generally rules out high model efficiencies as the water balance model reproduces the unaffected hydrological system without the use of water resources.

The example of the gauge at Hagen-Hohenlimburg shows that the low flow periods are mapped well as well as the flood peak values (Figure 11). To check the plausibility the measured and simulated water balances were compared with each other. For this the cumulative hydrograph volumes for the whole validation period were used. Figure 12 shows this comparison for the gauge at Hagen-Hohenlimburg. As expected this comparison of both cumulative frequency polygons shows that due to the intensive use of water resources the measured total discharge is overestimated by approx. 9 %.



Figure 11: Comparison of the measured and simulated hydrographs at gauge Hagen-Hohenlimburg



Figure 12: Comparison of discharge volumes: measurement and simulation at gauge Hagen-Hohenlimburg

This overestimation, however, is explicitly caused by the large amount of water extracted from the Ruhr for supplying the neighbouring areas with drinking water and by the high amount of evaporation from the different reservoirs. These water losses correspond in sum to the difference between the calculated and measured discharge volumes. An average annual amount of extracted water for the complete Ruhr catchment area in the simulation period can be specified as being about 240 million m³ (Ruhrverband, 2002b; 2003; 2004; 2005; 2006). Due to the known inundated areas an annual evaporation amount of about 35 million m³ can be estimated by using the empirical method by Haude (1955). These

anthropogenic changes in the water balance due to damming and water management were not considered with the model for the feasiability study according to the present MoRE concept. The impacts of anthropogenic influences are, for example in the dry year 2003, clearly visible (Figure 11 and Figure 12). In the dry year 2003 the calculated discharges are much lower than the measured values. Whereas the model results in this period show the expected typical progress of a recession curve, the measurements stayed at an almost constant level. This effect is caused by the supply of supplemental water (low water concentration) of the dams. In August 2003 alone, the reservoirs in the whole catchment areas had to contribute on 28 days (approx. 15.5 m³/s) to maintain the minimum runoff required by law (e.g. 8.4 m³/s at the gauge at Villigst) (Ruhrverband, 2002b).

So the most important reasons for the discrepancies from the observed hydrograph could be identified and the high calculation quality of the hydrological model for simulating natural water balances could be underlined once more.

Compared to the calculation results by the MONERIS concept so far, the outcome of the new hydrological model approach in the Ruhr catchment area for this period 2003 to 2005 shows a 9 % higher runoff sum. For a better validation of the runoff components further information on the origin of the different water components and loads should be made available for the catchment area.

The derived average daily discharges are subsequently aggregated to monthly average values so they can be transferred to MoRE for the spatial model entities of the analytical units.

3.1.6 Summary and outlook

The example of the Ruhr catchment area showed that it is possible to reproduce spatially distributed water balance and runoff dynamics and with a higher resolution with a conceptional hydrological water balance model such as PRMS. Therefore, an appropriate hydrological modeling basis can be provided for emissions modeling with MoRE on the basis of the available data modeling.

An extension of the hydrological model to large catchment areas or also to the complete MoRE area does demand that on the one side the spatial and temporal data basis (precipitation, discharge, etc.) is available and its continuous recording is assured. On the other hand it is necessary that relevant information is available on water management (e.g. the amount of water extracted) or on infrastructural facilities of urban water management (e.g. volume of storm water overflow basins). The example of the Ruhr shows that the use of water resources can be of great importance and that large dams and major transitions must be considered separately when simulating water balances.

Furthermore, the application of the model in the Ruhr catchment shows that the available data on soil characteristics or land use are suitable for measuring regional runoff behaviour by defining appropriate, homogenous subareas, for example HRUs or land use classes. The number of occurring feature combinations of area characteristics will increase for a larger model area so that for the whole of Germany the intersection of soil information and land use might probably result in 45 different spatial units (e.g. HRUs) with specific hydrologically similar runoff characteristics. It can be supposed that per analytical unit only a limited number of these combinations is influential and actually has to be parameterised in the model.

Future scenarios such as possible changes in land use (Liebert et al., 2011) or climate (Ihringer et al., 2010) can be simulated with hydrological models, e.g. via the adjustable

model parameterisation (land use) as well as via meteorological input data (climate change). But this does require that according scenarios are set with the impact on changed land use and changed meteorological boundary conditions. In the Ruhr catchment area this has already been done with the PRMS model (IWG, 2010). Within the framework of different studies such scenarios are also derived with good success with the help of water balance models (KLIWA, 2009; KHR, 2010).

In the process, based on the global climate calculations (climate projections), high-resolution simulations of regional climates, e.g. for southern Germany, can be made and the results can be used as meteorological input for the hydrological modeling on the catchment scale.

Extending the PRMS model to the large river basins in Germany and Central Europe would imply the need of huge amounts of data and calibration. It therefore seems more sensible and effective to use an existing conceptional water balance model for mapping the runoff characteristics and calculating the water balance in the whole area.

Towards the end of this project it was announced that the German Federal Institute of Hydrology (Bundesanstalt für Gewässerkunde, BfG) is having a water balance model made for Central Europe on the basis of the modeling system mentioned in the section "Analysis of approved water balance models" called LARSIM (LARSIM_ME). In near future LARSIM will be a consistent, spatially (raster size 5 x 5 km²) as well as temporally (daily steps) detailed but especially uniform hydrological model for all Central European river basins (Danube, Rhine, Oder, etc.). The hydrological concept model LARSIM is generally based on computation methods for reproducing individual hydrological processes which are very comparable to those of PRMS. This suggests that with that the individual parts of information (runoff components) that are needed for load flow modeling are also available.

In a first step it shall be tested which further requirements, model adjustments as well as process mappings are needed which haven't been fulfilled and comprised by LARSIM_ME so far, for example for a detailed mapping of runoff characteristics from urban areas as well as covering the emission pathways in urban areas. This could lead to an even better integration with the approaches of load modeling.

3.2 Sewer systems

According to Fuchs et al. (2010) the sewer systems are an important emission pathway for pollutants into surface waters. Within the framework of this report improvements to the input data as well as required adaptations of the modeling approaches on the emission pathway "sewer systems" are presented. The emission pathway sewer system comprises four sub-pathways:

- storm sewers of the separate sewer system,
- combined sewer overflows of the combined sewer system,
- area and inhabitants that are connected to the sewer system but not to wastewater treatment plants,
- areas and inhabitants neither connected to the sewer system nor to wastewater treatment plants.

In Germany, due to the high connection rate of the population to public sewer systems, the two last mentioned sub-pathways are only of importance on a local to regional level. The sub-pathway storm sewers account for approx. 60 % of heavy metal emissions of the sewer

systems, the combined sewer overflows account for 35 % of the emissions (Fuchs et al., 2010). Appendix 6 shows as example an extract of the modeling approach "sewer systems" for the sub-pathways "storm sewers" and "combined sewer overflows". A detailed description of the methodology can be found in Fuchs et al. (2010).

Essential input parameter for all sub-pathways of the emission pathway "sewer systems" is the load from stormwater runoff from sealed (impervious) surfaces. Due to their outstanding role they were focused on in the present project. Key parameters for modeling loads from stormwater runoff are the size of the impervious areas and a substance specific surface load.

So far, due to the available data basis, a derivation of the mentioned key parameters was only possible merely on the basis of empirical approaches (for impervious areas) and as average value for Germany (for surface load), independent from the urbanization intensity. Within the framework of this project, in the sense of a feasibility study for improving the model statements, the data basis was adapted for these key parameters. First a new data set on impervious areas was created on the basis of maps on soil sealing and land use. Then, a regionalized surface load of the impervious areas was determined depending on the anthropogenic activity. This helps to spatially differentiate the emissions via sewer systems.

3.2.1 Data basis on impervious areas

So far the size of the impervious areas were determined by a data set on population density of the European Environment Agency (EEA, 2007) and the urban areas from the land use data set Corine Land Cover 2000 (EEA, 2005) by the empirical approach of Heaney et al. (1976). This empirical approach underestimates the surface areas considerably (Fuchs et al., 2010). Therefore, all model variables that are derived from the impervious areas (urban runoff, urban emissions) are systematically underestimated.

Recently, a data set has been available on the degree of soil sealing with which the size of the impervious areas can be defined more realistically. It is available throughout Europe and called "Fast Track Service Precursor on Land Monitoring" (FTSP, EEA, 2010a).

3.2.1.1 Data set on degree of sealing

FTSP is a raster data set on degree of sealing which maps the share of sealed surfaces per pixel. The satellite basis for FTSP are images from the year 2006 (IMAGE2006) taken by the satellites SPOT-4, SPOT-5 and IRS-P6 LISS-III (ETC/SIA, 2011). The spatial resolution for the survey was approx. 20 m x 20 m and the data set for this project had a computational resolution of 100 m x 100 m (Figure 13).

The degree of sealing was converted into absolute values to calculate the impervious areas, whereas the given degree of sealing was taken as being constant within the whole pixel. In total this results in impervious areas in Germany of 19,062 km². This approach can also be used for the catchment areas outside Germany (e.g. Oder, Rhine) as the data set FTSP in available throughout Europe.


Figure 13: Data set "Fast Track Service Precursor" on the degree of soil sealing (EEA, 2010a)

Not the whole impervious area is needed for modeling the emissions via sewer systems but just those that are within settlements, the so-called urban impervious areas. Outside urban areas that are sealed but are predominantly not connected to a sewer system (e.g. motorways) are not considered. The data set urban impervious areas in Germany was generated by intersecting the FTSP data set with a data set on urban areas. To identify urban areas there were two data sets to choose from: the pan-European Corine Landcover 2006 (CLC2006) (EEA, 2010b) as well as the Digital Basic Landscape Model (Base DLM) (BKG, 2010), which is available for Germany only.

3.2.1.2 Data sets on urban areas

Corine Landcover 2000 (EEA, 2005), the raster data set available throughout Europe, was updated for the year 2006 with a resolution of approx. 20 m x 20 m and published as data set Corine Landcover 2006 (CLC2006) by the European Environment Agency (EEA, 2010b). The satellite data basis for CLC2006 was the data set IMAGE2006 (Keil et al., 2011). This was available in a computational resolution of 100 m x 100 m and identifies artificial areas, agricultural areas, forest and semi natural areas, wetlands and water bodies as land use classes. When extracting the urban areas the sub-classes listed in Table 3 of the land use

class "artificial surfaces" were considered. Figure 14 (on the left) depicts the resulting undifferentiated urban areas.

CLC Code	Level 3 classes of "artificial surfaces"
111	Continuous urban fabric
112	Discontinuous urban fabric
121	Industrial or commercial units
122	Road and rail networks and associated land
123	Port areas
124	Airports
141	Green urban areas
142	Sport and leisure facilities

Table 3: Considered sub-classes (level 3) of the class "artificial surfaces" of CLC2006 (EEA, 2010b)

The Base DLM is based on data from the Authoritative Topographic-Cartographic Information System - (ATKIS) and is therefore only available for Germany. It is available at a scale of 1:25,000 as vector data set for each separate federal state (BKG, 2010). The Base DLM distinguishes between the following land use classes: settlements, traffic zones, vegetation and water bodies. The polygon shape "sie01_F.shp" (settlements) was used to calculate urban areas (Figure 14 on the right).



Figure 14: Comparison of two data sets on urban areas: CLC2006 (EEA, 2010b) and Base DLM (BKG, 2010)

Based on both mentioned data sets, a comparison of the identified total urban areas in Germany showed the following: according to the CLC2006 data set the total urban area is 28,827 km² (corresponds to 8.1 % of the area of Germany) and the Base DLM comes up to an urban area of 30,181 km² (corresponds to 8.5 % of the area of Germany).

The urban area from CLC2006 is in average 4 % lower than the urban area according to the Base DLM. To verify the plausibility of the raster-based data sets the data on the settlement areas of the Federal Statistical Office was used. They state an urban area of about 29,350 km² (StaBu, 2011a). It shows a good compliance to both of the analysed land use data sets. The deviation is about -1.8 % for the CLC2006 data set and +2.8 % for the Base DLM data set.

In contrast to the Base DLM, the data set CLC2006 is available throughout Europe. Therefore this methodical approach can also be transferred to the catchment areas outside Germany. This is why the data set CLC2006 is preferred over the Base DLM data set for updating the input data for the emission pathway sewer systems.

3.2.1.3 Urban impervious areas

To determine the sealed surfaces in settlement areas the data sets FTSP and CLC2006 were intersected. This resulted in a total urban impervious area in Germany of 13,525 km². This correlates to an average degree of sealing of urban areas of 47 %. The determined urban impervious area is depicted in Figure 15 according to the different degrees of sealing. The size retrieved with the described method for sealed surfaces in settlement areas is about 40 % higher than with the methods used previously used for calculating the sealed surfaces in settlement areas by Fuchs et al. (2010).



Figure 15: Urban impervious areas of Germany and their degree of sealing

To verify the plausibility of the data for the year 2006 a further satellite-based data set on soil sealing in Germany was consulted. This was compiled from Landsat images from the year 2000 and also considered the AKTIS data (University of Würzburg, 2010). The ground resolution was 30 m x 30 m, the data set was made available by the University of Würzburg with a computational resolution of 25 m x 25 m (Thiel, 2011). This resulted in an urban impervious area of 12,717 km² for Germany. Considering an increase in urban impervious area in the period of 2000 to 2005 of approx. 780 km² (Frie und Hensel, 2007), this results in an area sized 13,497 km². This confirms the quality of the data set on urban impervious area generated from the data sets FTSP and CLC2006 which are both available throughout Europe.

3.2.2 Regionalizing the surface load

Apart from the size of the sealed surfaces, another elemental input data is their surface load for determining the emissions via sewer systems. The substance specific surface load is an annual average load which is washed off from sealed surfaces. It can be back-calculated from concentration data by considering the average long-term (1983-2005) stormwater runoff amount in urban areas and the impervious areas connected to the sewer system in Germany as well as the runoff coefficient (Fuchs et al., 2010). So far the surface load was used as uniform value for all analytical units. This leads to a lack of differentiation between highly and lowly populated areas. But these areas differ largely in respect to the anthropogenic activities

such as traffic volume and industry. This leads to different direct emissions onto the sealed areas (tire and brake abrasions as well as the corrosion of metal surfaces, atmospheric deposition).

It can be supposed that therefore the substance concentrations in the stormwater runoff in these areas differ. This thesis was tested by analysing the substance concentration in the stormwater runoff and it was examined if representative concentrations could be derived. Within the scope of this project the substances chosen were the heavy metals copper and zinc as there is a relatively good data basis for these. Furthermore zinc is seen as a representative substance for many anthropogenic pollutants (Fuchs et al., 2009).

To regionalize the emissions, the urban impervious areas were split into two settlement classes according to the anthropogenic activity (section 3.2.2.2).

On the basis of the representative substance concentrations and the urban runoff a surface load was then derived for both settlement classes. According to the settlement class a regional surface load was assigned to the sealed areas.

3.2.2.1 Representative concentrations in the stormwater runoff of sealed surfaces

The heavy metal concentrations in stormwater runoff were taken from an existing data pool by Brombach und Fuchs (2002, extended) at the Institute for Water and River Basin Management. This extended data pool is based on a worldwide research for road and stormwater runoff as well as areas drained by a separate sewer system (storm sewers).

On the basis of the available information the attributes "highly urbanized" and "lowly urbanized" was assigned to those measuring points of the data pool that were within settlements and were not located at a motorway. For this allocation information on traffic volume and population figures were consulted. If the traffic volume in the catchment area of the measuring point exceeded 30,000 cars per day the measuring point was allocated to being "highly urbanized". If the information on traffic volume was not available then the population figures for the town that was round the measuring point were taken. All settlements that have more than 20,000 inhabitants were labeled "highly urbanized". The other measuring points were labeled "lowly urbanized".

The available concentrations for copper and zinc were split into two categories according to the measuring points which resulted in four data sets which were statistically analysed. The frequency distribution was determined and interpreted in a histogram (Figure 16 and Figure 17). At first it becomes obvious that all data sets show a right-skewed distribution. Depending on the heavy metal and settlement class between 60 and 70 % of the sample values are below the average. As the median is more robust towards outlier values it was chosen to represent the values for deriving the surface loads.

The median values for copper and zinc concentrations in the stormwater runoff differ with 47 μ g/l and 265 μ g/l resp. in large-town areas a lot from those in small-town areas (29 μ g/l and 165 μ g/l resp.).



Figure 16: Frequency distribution of copper concentrations in stormwater runoff from lowly and highly urbanized areas (Brombach & Fuchs, 2002, extended)



Figure 17: Frequency distribution of zinc concentrations in stormwater runoff from lowly and highly urbanized areas (Brombach & Fuchs, 2002, extended)

In order to consider the differences in substance concentrations of stormwater runoff adequately in the model, the urban impervious area was differentiated into two settlement classes. For this, agglomeration areas were allotted which have a larger substance specific surface potential than small-town areas.

3.2.2.2 Designation of agglomeration areas in Germany

In order to distinguish large- and small-town areas within Germany a database "highly urbanized areas" (agglomerations) was generated. For this a data set of 23 large agglomerations, according to Brinkhoff (2011), as well as all towns with a population over 200,000 inhabitants (StaBu, 2011c) were considered. This information was assigned to the vector database for the administrational borders of municipalities "VG250" (BKG, 2007b) and finally the data basis "highly urbanized areas" was compiled. Then this database was intersected with the urban impervious areas. This resulted in a data set with sealed areas that are given a higher substance specific surface load when modeling the emissions. The other urban impervious areas are given a lower surface load (Figure 18).



Figure 18: Generating input data for modeling emissions via sewer systems – differentiation of the urban impervious areas with the aim of considering usage specific surface loads

3.2.2.3 Regionalized surface load for copper and zinc

Regionalized surface loads for copper and zinc (Table 4) can be calculated after the procedure by Fuchs et al. (2010) using the median of substance concentrations of stormwater runoff in lowly and highly urbanized areas, the stormwater runoff as well as the sealed surface in the separate sewer system. The area-weighted mean values of the surface loads are 120 g/(ha·a) for copper and 806 g/(ha·a) for zinc resp. and therefore significantly lower than the values used by Fuchs et al. (2010).

	Cu [g/(ha₊a)]	Zn [g/(ha₊a)]
lowly urbanized areas	101	584
highly urbanized areas	180	1,501
area-weighted mean	120	806
Fuchs et al. (2010)	204	1,631

Table 4: Regionalized surface loads for copper and zinc [g/(ha·a)]

For the period 1980-2005 Fuchs et al. (2010) calculate the arithmetic mean of the concentrations based on Brombach und Fuchs (2002, extended) for each year and show that in contrast to the other heavy metals there is no temporal trend for copper and zinc. For this reason all concentration values from 1995 onwards are used for the present feasibility study without being allocated to a specific year. This and the continuous extension of the data pool by Brombach and Fuchs (2002, extended) leads to a larger amount of measuring values which allows a statistical analysis. This analysis shows that the median depicts the data

distribution better than the arithmetic mean. As the median is significantly lower than the arithmetic mean (Figure 16 and Figure 17), the surface load derived from the median is lower than for Fuchs et al. (2010).

The regionalized surface load is used in this feasibility study in MoRE parallel to the surface load integrated by Fuchs et al. (2010). A detailed description of the integration follows in the next section.

3.2.3 Implementing the new data basis in MoRE

MoRE enables to store different methodical approaches and input data parallel. These are established in the system as "variants" of an approach or an input data. Due to the transparent presentation and documentation the retrieved results can distinctly be allotted to the approaches and input data used (see chapter 2). With this the results can be traced easily. Also, a quick estimation of the impact of different input data and quantification approaches on the model results can be made. Considering the presented modifications for emission pathway "sewer systems" the calculation of emissions was defined according to two different variants:

- variant 1 (basic variant): results according to Fuchs et al. (2010) and
- variant 2: consideration of the urban impervious areas and the regionalized surface load.

3.2.4 Modeling results and assessment

The new input data (see variant 2) has an immediate effect on the model results. In the following section these effects will be described for the emissions via sewer systems, the individual urban sub-pathways as well as for the total emissions.

3.2.4.1 Emissions via sewer systems

In Figure 19 the emissions via sewer systems are depicted for the chosen heavy metals in the two described variants for Germany. The emissions via sewer systems decrease for copper for variant 2 compared to the basic variant by 15 %, for zinc by 29 %. Even though the values for sealed areas rose by about 40 % (section 3.2.1.3) the emissions decreased due to the significantly lower mean surface load (Table 4). Apart from the decrease in absolute emissions via sewer systems the relevance of the individual sub-pathways did not change.



Figure 19: Copper and zinc emissions into surface waters of Germany via sewer systems for the period 2003-2005 in two variants

3.2.4.2 Total emissions

The decreased emissions via sewer systems in variant 2 also have an effect on the total emissions of copper and zinc when the methodical approach stays the same. Figure 20 shows that the total emissions decrease (ca. 4 % for Cu and ca. 11 % for Zn). The relevance of the emission pathway sewer systems changes for Germany by less than 10 %.



Figure 20: Relevance of emission pathways in the total emissions from Germany for copper (left) and zinc (right) for the period 2003-2005 in two variants

The new input data also lead to a changed spatial distribution of the total emissions. This is reflected in the decrease and increase of emissions in certain analytical units (Figure 21). In

about 30 % (Cu) and 5 % (Zn) of the total German area emissions practically didn't change $(\pm 5 \% \text{ of the basic variant})$. The total area with decreased emissions is clearly larger (67 % and 92 % for Cu resp. Zn) than the area with increased emissions. Figure 21 depicts the relative changes in the Cu- and Zn emissions of variant 2 compared to variant 1 for the individual analytical units. Especially the agglomeration areas in Germany stand out clearly. The increased emissions via sewer systems for copper and zinc are not depicted to the same degree due to the different impact of the new input data on total emissions.



Figure 21: Ratio of variant 2 to variant 1 for the copper (left) and zinc (right) emissions in the analytical units

Within the framework of the feasibility study it was shown that by introducing a regionalized surface load the modeling of emissions into surface waters from urban areas is possible in a higher resolution. Due to the new input data the emissions into surface waters is not exclusively dependent on the size of the sealed areas but also from the intensity of the anthropogenic activities (industry, traffic, etc.). It is therefore a more realistic mapping. With this pollution hotspots can be identified better, leading to better planned target-oriented measures.

3.2.5 Summary and outlook

Within the framework of this project the focus was on improving the data for modeling emissions via sewer systems. Here, the special role of stormwater runoff from sealed areas is to be highlighted. The key parameters for modeling the emissions from sealed areas are the size of these areas and the substance specific pollution potential (surface load).

For both input data significant improvements were made within this project. First of all the size of the sealed areas was calculated based on the soil sealing data set FTSP (EEA,

2010a). Not the complete sealed area is needed for modeling emissions, only those parts that are within settlement areas, the so-called urban impervious areas. This area was identified by intersecting the FTSP data set with a data set on urban areas. For urban areas there were two data sets: Corine Landcover 2006 (EEA, 2010b) available throughout Europe and the Digital Basic Landscape Model (BKG, 2010). A comparison of the two urban data sets showed that they barely differ in the allotted size of the settlement areas. As the data set CLC2006 is available throughout Europe and can therefore also be used for modeling catchment areas outside Germany, it was preferred. The size of the urban impervious areas from this new data set was about 40 % higher than in the previously used data set. Verifying the plausibility of the new data set with a data set on soil sealing, which was made available by the University of Würzburg, confirmed the quality of the data set generated from the FTSP and CLC2006 on urban impervious areas.

Apart from the size of urban impervious areas the surface load is a further elemental input data. So far the surface load was used as uniform value for all analytical units. This made no difference between lowly and highly urbanized areas. But these areas differ greatly in their anthropogenic activities such as traffic volume and industry. This leads to the assumption that there are different loads onto sealed areas and into the sewer system. To check this assumption in a first step representative concentrations for lowly and highly urbanized areas were calculated from an available data pool on concentrations in stormwater runoff at the IWG. In the end this lead to a confirmation of the work hypothesis for copper and zinc for which there was a good database and which also count as guide substance of anthropogenic activities. To regionalize the emissions the urban impervious area was then split into two settlement classes depending on the anthropogenic activity (lowly and highly urbanized areas). On the basis of representative concentrations and the stormwater runoff from sealed areas a surface load was derived for both settlement classes. According to the settlement class a regionalized surface load was allocated to the sealed area. Then the newly created input data was implemented into MoRE as variant 2.

In the results the emissions via sewer systems decrease for copper by 15 %, for zinc by 29 %. This means that even though the sealed area rose by about 40 % the emissions decreased due to a lower mean surface load. The total emissions into surface waters of Germany have decreased by 4 % for copper and by 11 % for zinc. The new input data leads to a better mapping of the spatial distribution of the total emissions. Especially the agglomeration areas and weaker populated areas are depicted better in a map on total loads. Due to the new input data the emissions into surface waters are now not solely dependent on the size of the impervious area but also from the intensity of anthropogenic activities. They are now therefore mapped more realistically. With this pollution hotspots can be identified better, leading to better planned target-oriented measures.

Transferring the shown methods to analytical units outside Germany is in principal possible as the basic data used (FTSP data set for the degree of sealing and CLC2006 for urban areas) is available for the whole European Union. Concerning other substance groups it can be assumed that the method can be transferred if the data situation is as good as for copper and zinc. This is surely given for nutrients such as nitrogen and phosphorus. As far as other pollutants are concerned it can be assumed that the data basis for deriving regionalized surface loads is quite poor.

With regards to the approaches there is further need for adjusting the urban runoff components. Particularly the approach on calculating the discharge rate of combined sewer overflows should be mentioned. The approach used currently was developed for planning

purposes and can only be adapted conditionally for runoff conditions in different settlement areas. Apart from the adjustment of substance specific input data there is space for development in the description of urban runoff components and their distribution.

3.3 Erosion and Retention

For some heavy metals and other particulate transported pollutants erosion is an important emission pathway into the surface waters of Germany. The contaminations due to erosion can hugely vary depending on the morphology, erodability of the soils, land use and the heavy metal concentrations in the soil. Therefore, the spatial resolution of the input data was improved to be able to better predict the heavy metal emissions via the pathway erosion. Based on the new data base, an adapted conceptual model approach was to be developed and implemented into MoRE for estimating sediment delivery into surface waters.

A part of the suspended loads which reach the surface waters from the catchment areas can be deposited in the river system during transportation. This sedimentation process mainly takes place in lakes as well as in the reservoirs. Till now this process cannot be considered adequately in MoRE (Fuchs et al., 2010). This is why an exemplary study in the German catchment area of the Danube should test, whether the consideration of sedimentation rates in retention areas of river systems makes it possible to plausibly estimate the observed transported river loads.

3.3.1 Quantification of sediment input into surface waters

A key variable on quantifying heavy metal emissions via erosion is the sediment input from agricultural land into surface waters. Figure 22 shows the data basis needed and the procedure in MoRE.



Figure 22: Data base for quantifying sediment input in the MoRE model

3.3.1.1 Data base on agricultural land

Till now agricultural land in MoRE was determined based on the CORINE Land Cover 2000. In the meantime there is new CORINE data from the year 2006 (CLC 2006) (EEA, 2010b). There is also data on agricultural land from the Digital Basic Landscape Model (Base DLM) (BKG, 2010). By comparing it with the statistical data it was tested which data set was more suitable for the spatial determination of agricultural land. Statistical data on the total agricultural land is available at the Federal Statistical Office (StaBu, 2011a). In addition, the Federal Ministry of Nutrition, Agriculture and Consumer Protection (BMLEV, 2010) published data on the share of arable land and grassland. In Table 5 the total agricultural land as well as the areas for arable land and grassland from the different sources are illustrated.

Table 5: Agricultural area of Germany according to CLC 2006 (EEA, 2010b), Base DLM (BKG, 2010) and data of the Federal Statistical Office (StaBu, 2011a) as well as the Federal Ministry of Food, Agriculture and Consumer Protection (BMLEV, 2010)

Land use	Area in km² (%)		
	CLC 2006	Base DLM	StaBu/BMLEV
Total agricultural area	212,629 (100 %)	192,823 (100 %)	187,646 ¹ / 167,040 ² (100 %)
Arable land	168,698 (79 %)	129,442 (67 %)	119,933 ² (72 %)
Grassland	43,931 (21 %)	63,381 (33 %)	47,887 ² (28 %)

¹ StaBu: area in terms of use, ² BMLEV: sub-division of cultivated areas for 2008

Table 5 shows that the details for the whole agricultural land as well as the arable land and grassland differ from source to source. Furthermore, the details of the StaBu and BMLEV on the total agricultural land are different, too. Relating to the details from the StaBu the whole agricultural land of CORINE Land Cover is significantly overestimated. The agricultural land of the Base DLM lies also above that of the StaBu, but only by 3 % (Table 5). The same trend is visible for arable land: while CLC 2006 overestimates the arable land of the BMLEV by 41 %, the determined areas from the Base DLM are approx. 10,000 km² (8 %) higher. For all further evaluations the Base DLM was used, as compared to CLC 2006 the agricultural land as well as the share of arable land and grassland comply to the statistical data. Figure 23 shows arable land and grassland of the Base DLM (BKG, 2010). As the Base DLM is not available for the catchment areas outside Germany the CLC data set has to be used for those.



Figure 23: Arable land and grassland in Germany from the Base DLM (BKG, 2010)

3.3.1.2 Soil erosion from agricultural land

In the project "Analysis of the effect of climate change on soil erosion by water" (Wurbs and Steininger, 2011), commissioned by the Federal Environment Agency (UBA), a very detailed estimation was conducted on soil erosion rates of agricultural land using an adapted variant of the Universal Soil Loss Equation (USLE) for Germany which is named ABAG.

The ABAG (Schwertmann et al., 1990) is an empirical equation to estimate long-term soil erosion rates and comprises six factors (precipitation, soil erodability, slope length, slope gradient, soil coverage/tillage and erosion protection) which are multiplied with each other:

Equation 1:

 $\mathsf{B}\mathsf{A} = \mathsf{R} \cdot \mathsf{K} \cdot \mathsf{L}\mathsf{S} \cdot \mathsf{C} \cdot \mathsf{P}$

- BA average long-term soil erosion rate [t/(ha·a)]
- R rainfall erosivity index $[(kJ \cdot m)/(m^2 \cdot h)]$
- K soil erodability factor $[(t \cdot m)/(ha \cdot a \cdot kJ \cdot h)]$
- LS topographical factor (slope length and slope gradient) [-]
- C plant cover and tillage factor [-]
- P specific erosion control practices [-]

The ABAG factors were derived by Wurbs and Steininger (2011) as follows:

- The R-factors were derived from the long-term average summer precipitation on the basis of precipitation data from the DWD in a 1 km x 1 km grid for the period 1971-2000 and updated regression equations.
- The K-factors were derived by the Federal Institute for Geosciences and Natural Resources (Bundesamt für Geowissenschaften und Rohstoffe, BGR) according to Hennings (2000) differentiated according to land use for each of the 68 guidance soil units of the BÜK 1000 (BGR, 1998) depending on the position in one of the four climate zones in Germany.
- The determination of the LS-factor was conducted on the basis of the Digital Elevation Model (DEM) for Germany with a grid width of 50 m (BKG, 2007). The slope length was derived by including utilisation structures, field borders and further landscape elements which serve as barriers such as streets and rivers.
- The C-factors were determined by the technological approach of additive calculation according to Schwertmann et al. (1990). 502 nature regions of the Federal Agency of Nature Conservation (Bundesamtes für Naturschutz, BfN) were chosen as spatial assessment level as it is assumed that concerning the agricultural use the range and systems of cultivation are similar or equal. The C-factors were derived from conventional tillage. Furthermore, three scenarios for 25 %, 50 % and 100 % conservation tillage were compiled.

The digital maps for the ABAG factors were made available by the Federal Environment Agency for this project. Using the program ArcGIS Spatial Analyst the soil erosion on agricultural areas was calculated for a 50 m x 50 m grid. Figure 24 shows the result for the soil erosion for 100 % conventional tillage in Germany.



Figure 24: Soil erosion rates for conventional tillage in t/(ha-a) on agricultural areas in Germany, calculated using the ABAG factors given by Wurbs and Steininger (2011)

Comparison of different data sets for soil erosion

On the basis of the data set for the ABAG factors the soil erosion in the analytical units was calculated. Then the erosion rates were compared to the present data base on soil erosion. (Venohr et al., 2008). For quantifying the present soil erosion rates the following input data was used:

- CLC 2000 was used for the land use,
- the calculation of the R-factors was based on the long-term average summer precipitation according to the approach of Deumlich and Frielinghaus (1993),
- the basis for the K-factors was the European Soil Map (European Soil Bureau, 2007),
- the LS-factors were derived from the digital elevation model NASA-SRTM (NASA, 2005) and
- the C-factors were determined by literature research (Auerswald and Schmidt, 1986; Schwertmann et al., 1990; Deumlich and Frielinghaus, 1993; Strauss and Wolkersdorfer, 2004) and average factors at a federal state level.

Figure 25 shows the comparison of the average soil erosion rates in t/(ha·a) in the analytical units. Both data sets encompass the whole agricultural area (arable land and grassland) and assume conventional tillage.



Figure 25: Mean erosion rates from agricultural areas in the analytical units of Germany. Left side: erosion rates according to Venohr et al. (2008). Right side: erosion rates calculated using the ABAG-factors of Wurbs and Steininger (2011)

From Figure 25 it is obvious that the previous erosion rates on agricultural areas (Venohr et al., 2008) are higher than the soil erosion based on the factors of Wurbs and Steininger (2011). This is also confirmed by comparing the cumulative soil loss for all German analytical units (Figure 26). While according to Venohr et al. (2008) the total soil loss calculates to 44 million t for the whole of Germany, the sum calculated on the basis of the data from Wurbs and Steininger (2011) only comes up to 31 million t. Furthermore, spatial differences can be found for the soil erosion rates (Figure 25). The reason for the different erosion rates in both data sets lies mainly in the different consideration of land use and the C-factors. While Venohr et al. (2008) dwells on the agricultural area according to CLC 2000, Wurbs and Steininger (2011) used the data of the Base DLM. In Table 5 it has already been shown that the arable land of CLC is significantly overestimated. A further reason for the different erosion rates lies in the differentiated view of the C-factors for the crop type shares in the nature regions in Germany. Venohr et al. (2008) used the average C-factors at a federal state level. Furthermore, erosion barriers were considered when Wurbs and Steininger (2011) determined the LS-factors. It can be assumed that the calculated soil erosion rates based on the ABAG factors according to Wurbs and Steininger (2011) lead to a more realistic estimation as the input data used is more detailed.



Figure 26: Comparison of cumulative soil loss in t from agricultural areas in the analytical units according to Venohr at al. (2008) and calculated using the ABAG factors of Wurbs and Steininger (2011)

Processing the soil erosion data

For calculating soil erosion in the model system MoRE it is distinguished between the kind of use on agricultural areas – arable land or grassland. This is why the soil erosion was calculated separately for arable land and grassland. From the 31 million t of soil eroded from agricultural land in Germany, 1 million t are from grassland.

Furthermore, soil erosion from arable land was differentiated into gradient classes according to Fuchs et al. (2010). The following classes were considered: < 1 %, 1-2 %, 2-4 %, 4-8 % and > 8 %. For this, first the arable areas was extracted from the DEM. Then the grid data sets of the arable land were derived for each gradient class. The resulting 5 grid data sets were intersected with the soil erosion map (Figure 24). Table 6 shows the shares of arable land in the 5 gradient classes as well as the resulting average values of the specific soil erosion rates on arable land in the classes. The average soil erosion increases in a non-linear way with the rising gradient class.

	Gradient class								
	<1%	1-2 %	2-4 %	4-8 %	> 8 %				
Share of arable land [%]	34.4	16.1	18.4	17.7	13.4				
Mean erosion rates [t/ha·a]*	0.049	0.261	0.785	2.68	9.27				

Table 6: Share of arable land for different gradient classes in Germany and calculated mean erosion rates in t/(ha•a) from arable land in the gradient classes

^{*} For a 100 % conventional tillage

For the model system MoRE only the "potential" soil erosion on the gradient classes is needed. The potential soil erosion results from the multiplication of the R-, K- and LS-factors of the ABAG (Equation 1). The C-factor is deposited separately in the data base so that different C-factors can be considered in the model calculations (comp. section 3.3.1.3). To be able to consider the different precipitation situations of the individual years from 1983-2007, a weighting factor by Venohr et al. (2008) was introduced on the basis of the summer precipitation in the observed year and the long-term average for summer precipitation. (Equation 2).

Equation 2:

 $PR_F = \frac{0.152 \cdot PR_{Y_F} - 6.88}{0.152 \cdot PR_{LT} - 6.88}$

 PR_F factor for correcting the precipitation [-] PR_{Yr} summer precipitation in the observed year [mm/a]

*PR*_{LT} long term average in summer precipitation [mm/a]

3.3.1.3 The consideration of conservation tillage techniques

The term "conservation soil tillage" comprises non-turning (ploughless) tillage methods. The main character being the reduced tillage intensity concerning type and depth of the mechanical intrusion as well as leaving the crop residues on the surface (mulch). A distinction is made between techniques with and without loosening the soil.

The primary soil tillage is either done with a cultivator or similar machines, which also allows a deeper loosening of the soil if needed. Or the primary soil tillage is left out whereas the seedbed preparation is done e.g. with milling machines, rotary harrows or spike drums, mainly combined with mulch sowing procedures (Loibl, 2006). In contrast to the conservation procedures the direct sowing methods completely do without any soil tillage and the seeds are planted in small furrows between the stubbles of the previous crop

A reduction of soil erosion with conservation soil tillage is mainly due to the crop residue and soil consolidation. The higher soil coverage protects the soil surface against the impact of rain drops and absorbs a large amount of the flow impulse in the surface runoff. Furthermore, the infiltration capacity increases for the conservation tillage, which leads to reduction of the surface runoff and with that a reduction of erosion on sloped arable land (Köller, 2005).

Farming systems without ploughing are commonly used by farmers in the meantime. The distribution of conservation soil tillage across Germany differs from region to region. The operational range of fluctuation is quite high. Where some farmers only use one system, others even switch tillage methods on the same area within the crop sequence. At the moment there is no federal statistic on the proportion of conservation tillage available. Details on the type and extent of tillage in farming are mainly from surveys within the frame of special analyses and consider either crop or country (Wurbs and Steininger, 2011).

Wurbs and Steininger (2011) could only derive scenarios for C-factors, whereby they supposed a steady proportion of 25 %, 50 % and 100 % resp. of conservation soil tillage in the whole of Germany. Therefore, in the framework of this study research was made on the proportion of conservation soil tillage in the federal states.

Proportion of conservational soil tillage processes

In the current agricultural census of 2010 (StaBu, 2011b) data was collected on soil tillage methods for the first time. The agricultural census is part of the agricultural census taken in all countries of the EU. A representative choice of farms is questioned to make comparable data on agriculture available to enable to make statements on the effect of past agricultural policy measures. At the moment preliminary results are available on the percentage of soil

tillage methods for the whole of Germany. Regional results are not available yet. According to this 57 % of agricultural land in Germany is conventionally tilled with ploughs, 37 % are tilled using conservative methods (e.g. cultivators, harrows), 1.3 % are tilled with the direct sowing method and on 4.7 % of the area there is no crop rotation of the annual plants. This survey included agricultural land which was tilled during the harvesting year. Areas with crops that remained on the land for longer than one year were not considered (StaBu, 2011b).

A further possibility of obtaining information on the range of conservation soil tillage is via offering sponsorship for erosion or water protection measures. In some federal states (e.g. Baden-Wuerttemberg, Hessen, Saxony and Saxony-Anhalt) conservation soil tillage is sponsored within the framework of agricultural environmental programs. In the level of the federal states there is more information about the size of the area. Often only those areas are sponsored which are within a strictly defined area setting. Therefore only a certain amount of the agricultural area of the federal states is included.

As there can be large regional differences in the distribution of different tillage methods the agriculture ministries in the federal states were asked directly¹. Figure 27 shows the results of the percentage of conservative methods on a federal state level. These results are, too, only conditional as the results are mainly preliminary. Mecklenburg-Western Pomerania delivered no results so the average result of all federal states was used.

¹ the Brandenburg Ministry for Agriculture, Conservation and Development; the Baden-Wuerttemberg Department of Nutrition and Rural Space and the Agricultural Technology Centre Augustenberg; Bavarian State Ministry of Agriculture and Forestry; Hessian Ministry of the Environment, Rural Affairs and Consumer Protection; Ministry of Food, Agriculture, Forestry and Fishing of Mecklenburg-Western Pomerania; the Ministry of Rural Areas, Food, Agriculture and Consumer Protection Lower Saxony; Ministry of the Environment and Nature Conservation, Agriculture and Consumer Protection of North Rhine-Westphalia; Ministry of Economic Affairs, Transport, Agriculture and Viticulture of Rhineland-Palatinate; Ministry for the Environment in Saarland; Saxon State Ministry of the Environment and Agriculture; Ministry of Agriculture and Environment of Saxony-Anhalt; Schleswig-Holstein Ministry of Agriculture, the Environment and Rural Areas; Thuringian Ministry of Agriculture, Nature Management and Environment



Figure 27: Share of conservation soil tillage in the federal states following a survey of federal state authorities (as of April 2011)

The percentage of conservation tillage methods is at least 20 % in all federal states. The highest percentage of erosion-decreasing tillage methods was found in Saxony with 50 %. 30 % of which are permanently tilled conservationally (SMUL, 2011). The weighted average by the size of the arable land for Germany gives a percentage of 28.7 % for conservation tillage. This value is below the preliminary values of the agricultural census (StaBu, 2011b). In the agricultural census the respondents pointed out that giving up ploughing depended on many criteria such as crop rotation, region, climate, weather and soil conditions as well as financial considerations. Therefore, the agricultural census is only a snapshot of the situation at the moment which only conditionally allows the results to be transferred to long term trends. In addition, the agricultural census does not consider all businesses (e.g. those with arable areas < 5 ha).

C-factors for considering conservation tilling methods

With a growing percentage of conservation tillage systems the C-factor decreases for the crops. Figure 28 (left) shows the calculated C-factors of Wurbs and Steininger (2011) for the present use structure on arable land in the natural areas of Germany supposing a 100 % use of conventional cultivation.

Based on the C-factors by Wurbs and Steininger (2011) the C-factors for the present cultivation structure were derived according to the research results on the percentage of conservationally tilled arable land in Figure 27. The results of the regionalized C-factors is depicted in Figure 28 (right) for the nature regions in Germany. C-factors over 0.1 are mainly found in the eastern hilly area of Bavaria, in the western hilly area of Allgäu, in the Upper Rhine, in the west of North-Rhine Westphalia and Lower Saxony as well as in Schleswig-Holstein. In the last mentioned federal states the higher C-factors do not lead to higher soil erosion rates as the slope gradients are lower in these regions.



Figure 28: C-factors in the nature regions of Germany. Left: for 100 % conservational tillage (Wurbs and Steininger, 2011). Right: for the current percentage of conservation tillage in the federal states according to Figure 27

Based on the current C-factors in the nature regions the soil erosion was calculated again for arable land. Figure 29 shows the average erosion rates in the federal states for 100 % conventional tillage as well as the current percentage of conservation tillage methods in the federal states. Furthermore, the soil erosion for the scenario of an even percentage of 50 % conservation tillage (according to Wurbs and Steininger, 2011) was calculated.



Figure 29: Mean soil loss on arable land in the federal states for 100 % conventional tillage, the current percentage of conservation tillage (according to Figure 27) and a scenario of 50 % conservation tillage (Wurbs and Steininger, 2011)

Figure 30 shows the soil erosion on arable land for a 100 % conventional soil tillage as well as for the current percentage of conservational tillage. Compared to a 100 % conventional

tillage the erosion of arable area in Germany increases in average by 23 % from 30 million t to 23 million t if the current percentage of conservational methods are considered for the calculation.



Figure 30: Soil loss on arable land for different C-factors. Left: for 100 % conventional tillage (Wurbs and Steininger, 2011). Right: for the current percentage of conservation tillage in the federal states according to Figure 27

3.3.1.4 Determination of the sediment delivery ratio

The ABAG (Equation 1) estimates the long term average soil erosion on arable areas. But not all eroded soil material is delivered into the surface water as a part is deposited temporarily or permanently in flatter sloping regions, floodplains or in the surface water itself (Walling, 1983). A connection between the soil material that is eroded on the hill slopes and the percentage that reaches the surface waters can be made by the sediment delivery ratio (SDR) (Figure 22, Equation 3) (Walling, 1983; Boardman, 1996).

Equation 3:

$$SDR = \frac{\sum_{i=1}^{n} BA_i \cdot A_i}{SL} \cdot 100$$

SDR sediment delivery ratio [%]

 BA_i average long term soil erosion rate on the area i [t/(ha·a)]

A_i size of the area i [ha]

SL average long term sediment load in the surface water [t]

Sediment delivery into surface waters is influenced by many morphological influential factors and environmental factors such as the type and location of the sediment source areas, the relief and stream network, land use, soil characteristics and climate (Walling, 1983; Verstraeten and Poesen, 2001; de Vente et al., 2007).

Approaches on determining the sediment delivery ratio

There are different approaches on determining the sediment delivery ratio which differ hugely concerning the complexity and data demand (Lu et al., 2005). Process-based models implement detailed process approaches on detachment, transport and deposition of soil particles. As the processes are described along the flow paths to the surface waters these model approaches can represent the spatial variability of the influence parameters. But the process-based models can only be used in very small catchment areas (Boardman and Favis-Mortlock, 1998; Harmon and Doe, 2001; Jetten and Favis-Mortlock, 2006; Scherer, 2008). This is why mainly simplified conceptual approaches are used on a larger scale which estimate the sediment delivery ratio from catchment characteristics (Walling, 1983; Verstraeten and Poesen, 2001; Lu et al., 2005).

In current literature the catchment area is commonly identified as the dominant reference value for sediment delivery ratios. The relation is explained by saying that with increasing size the gradient decreases on the slopes and surface waters and there is therefore more potential deposition surface available (Walling, 1983; Osterkamp and Toy, 1997) or the flow pathway to the catchment outlet is longer (Parsons et al., 2006). On the other hand, other authors found an increase of the SDR for larger catchment areas (e.g. Faran Ali and De Boer, 2010). The variable association between the size of the catchment area and the SDR can be explained by a variously intense dominance of the process chain on the slopes or in the waterway resp. as well as the predominant land use in the catchment areas (intensive farming compared to natural vegetation) (De Vente et al., 2007). Furthermore, a high spatial variability of the sediment sources and depressions (erodability of the soil, morphology, land use, precipitation, etc.) can lead to there no being any link between the SDR and the catchment area (Lu et al., 2005; de Vente et al., 2007. Verstraeten and Poesen (2001) conclude that the size of the catchment area is no suitable parameter to determine the sediment delivery as the process is mainly determined by the morphology. This leads to the problem that the spatially variable morphology of the catchment areas has to be determined by individual representative parameters (Walling, 1983; Verstraeten and Poesen, 2001).

Simple approaches use the average elevation (Diodato and Grauso, 2009) or the gradient in the catchment areas (Behrendt et al., 1999; Verstraeten and Poesen, 2001), whereby it is assumed that for higher elevations or higher gradients a higher share of eroded soil reaches the surface water. Further, as example, the percentage of the catchment area with a gradient less than 2 % is taken as measure for the percentage of potential deposition surface or drainage density, to be able to estimate the connectivity till the outlet of the catchment (Delmas et al., 2009). A further parameter on the integral description of the morphology is the hypsometric integral (HI) (Equation 4). The HI is derived from the hypsometric curve which depicts the relative percentage of the catchment area that is situated below a certain altitude. Catchment areas with a high HI have large differences in altitude near the outlet of the area which is connected to a high erosion risk and short flow paths. With a low HI the high altitudinal gradients are in regions far away from the area outlet and it is possible that more is deposited there (Verstraeten and Poesen, 2001).

Equation 4:

$$HI = \frac{H_{mean} - H_{min}}{H_{max} - H_{min}}$$

HIhypsometric integral [-] $H_{mean}, H_{min}, H_{max}$ mean, minimum and maximum altitude in the catchment area [m]

Whether the eroded soil material is deposited in the catchment area or not depends on length and characteristics of the flow path. Lenhart et al. (2005) therefore identified the distance between the sediment source areas and the river as one of the main influences on the SDR. They developed a method to determine the weighted average distance factor D_w of the source area to the water in a catchment (Equation 5). For each sediment source area a weighting factor is assigned along the length of the flow path which depends on the gradient of the source area.

Equation 5:

$$W_i = \frac{1}{S_i} \longrightarrow D_w = \frac{\sum_{i=1}^n W_i \cdot D_i}{\sum_{i=1}^n W_i} \longrightarrow SDR = k \cdot \frac{1}{D_w}$$

- *W_i* weighting factor for the sediment source area i [-]
- S_i gradient of the sediment sour area i [-]
- *D_i* the length of the flow path of the sediment source area i to the water [m]
- n number of sediment source areas [-]
- *D_w* weighted average distance of all sediment source areas to the water in a catchment area [*m*]
- *k* catchment area-specific factor for calibrating [*m*]

Apart from the morphological influence factors spatially lumped model approaches consider further catchment area-specific factors such as land use (e.g. the percentage of arable land), annual precipitation or soil texture (Behrendt et al., 1999; Verstraeten and Poesen, 2001; Diodato and Grauso, 2009).

The depicted approaches on estimating the SDR in the literature differ in reference to the relevant influence factors, the kind of regression (linear or non-linear), and the empirical factors. Walling (1983) ascribed the absence of universal spatially-lumped model approaches to the complexity of the sediment delivery process and the interaction with variable catchment characteristics. The spatial structure of the topography, land use and further relevant influence factors are therefore insufficiently grasped if they are combined as one lumped parameter (Lenhart et al., 2005). This is why a conceptual model approaches were developed that allow for a spatially differentiated representation of the SDR in river basins (Ferro and Minacapilli, 1995; Ferro et al., 1998; Halbfass and Grunewald, 2008; Jain et al., 2009; Faran Ali and De Boer, 2010). Ferro and Minacapilli (1995), for example, suggest a model approach which calculates the SDR for each sediment source area on the basis of the length and gradient of the flow path to the next surface water:

Equation 6:

$$SDR_i = \exp\left[-\beta \frac{D_i}{\sqrt{S_{p,i}}}\right]$$

 SDR_i Sediment delivery ratio of the sediment source area i [-] $S_{p,i}$ gradient of the flow path of the sediment source area i to the water [-] β catchment-specific factor [1/m]

Further spatially-distributed models are based on the calculation of the transport capacity in the surface water runoff with a simple empirical method such as e.g. the model WATEM/SEDEM (Van Rompaey et al., 2001; Verstraeten et al., 2007; Alatorre et al., 2010). But this model is mainly used for modeling individual events.

All approaches presented so far from literature estimate the SDR as part of the potential soil loss. This is often done on the basis of the ABAG (Equation 1) or the USLE (Universal Soil Loss Equation) developed in the USA, which is the basis for the ABAG (Wischmeier and Smith, 1978) or a modification of the USLE (Williams and Berndt, 1977; Renard et al., 1994). In the past years the model PESERA (Pan-European Soil Erosion Risk Assessment) is being used to estimate soil erosion (Kirkby et al., 2008). Some authors criticize the combined SDR approaches as the soil erosion estimated by the USLE or the other models cannot be validated on larger scales (Kinnell, 2004; Parsons et al., 2006). To avoid the problems of a combined approach, conceptual model approaches were developed, which directly estimate the sediment delivery into surface waters (Parsons et al., 2004; Lu et al., 2005).

Sediment delivery from arable areas

In the following a spatially lumped model approach will be derived for SDR, to be able to determine the percentage of soil loss from arable areas that reaches surface waters for the analytical units. Until now the sediment discharge ratio (SDR) was determined in MoRE according to Venohr et al. (2008) on the basis of the percentage of arable land and the average gradient in the analytical units:

Equation 7:

$$SDR = 0.006684 \cdot (S - 0.25)^{0.3} \cdot (20 + A_{AL})^{1.5}$$

SDR sediment delivery ratio [%]

S average gradient (determined from DEM with a 1000 m grid) [%]

A_{AL} share of arable land [%]

However, the approach can only be used in combination with the soil erosion rates determined by Venohr et al. (2008) (section 3.3.1.2.) as this data was used to calibrate the empirical factors in Equation 7. Within the framework of this project the approach therefore has to be adapted and overhauled resp. to be able to estimate the sediment delivery ratio in the analytical units for the soil erosion rates derived on the basis of the ABAG-factors calculated by Wurbs and Steininger (2011) (section 3.3.1.2).

First of all, test catchments were chosen which had long term data in suspended sediment concentrations (SS) to be able to quantify the sediment delivery ratio. Suspended sediment

loads from long term measurements (preferably 30 years) are available in water-resources yearbooks. For the choice of catchments the following criteria were defined:

- The analytical units are in average 130 km² in MoRE. It is therefore preferable that the areas of the test catchments are within the same size range. However, long term suspended sediment loads are generally not available for small catchment areas. Therefore it was set that the catchment areas should be below 10,000 km² if possible.
- The SDR approach should be adapted for the soil erosion rates from arable areas as arable areas potentially show the highest soil erosion rates. The percentage of arable land in the test areas should therefore be at least 25 %. Furthermore, it was set that the potential soil loss from natural areas (woodland, meadows and open mountain areas) should only play a minor role (less than 10 % in relation to the total potential soil loss)
- As last criterion a minimum gradient was defined for the test catchments to be able to rule out the influence of in-stream retention processes as far as possible. It was therefore defined that the average gradient should preferably be 1 % (derived from the DEM with a grid width of 1,000 m).

Considering the defined criteria 13 catchments were chosen. In Figure 31 and Table 7 the 13 catchments, their location within Germany and the most important characteristics (size of the catchment area, area of arable land, gradient and long term average suspended sediment concentration) are listed.

Catch- ment	Monitoring station	Area [km²]	Dis- charge [m³/s]	SS ⁶ [mg/l]	Arable area [%]	Grass- land [%]	Gra- dient [%]	SDR [%]
Spree ¹	Cottbus	2,328	21.7	11	32	7	1.22	4.8
Leine ²	Herrenhausen	5,151	52.4	39	45	31	3.27	11.6
Fulda ²	HannMünden	6,915	63.4	25	29	9	3.78	7.3
Werra ²	HannMünden	5,457	51.6	56	27	12	4.47	17.0
Lahn ³	Kalkofen	5,298	45.6	24	25	23	3.38	10.8
Regnitz ⁴	Pettstadt	6,980	53.7	43	37	4	2.12	10.4
Main ⁴	Kemmern	4,424	45.0	41	32	29	3.49	9.3
Main ⁴	Marktbreit	13,974	117.0	29	38	9	2.55	7.7
Naab⁵	Duggendorf	5,487	51.2	24	32	15	2.75	5.3
Gr. Laber⁵	Schönach	419	2.5	48	59	12	1.20	2.6
Gr. Vils ⁵	Vilsbiburg	347	2.8	80	53	13	0.99	4.6
Rott ⁵	Ruhstorf	1,195	9.5	91	56	10	1.64	5.3
Amper⁵	Inkhofen	3,204	47.0	26	27	24	2.55	10.1

 Table 7: Characteristics of the 13 catchments selected to adapt the sediment delivery ratio approach for arable land

German water-resources yearbook: ¹ Elbe basin, part II (BfG 1996); ² Weser basin (BfG 2007c); ³ Rhine basin, part III (BfG 2006a); ⁴ Rhine basin, part II, Main (LfU 2002a); ⁵ Danube basin (LfU 2002b), ⁶ SS: Suspended sediment.

Deviating from the mentioned criteria for the choice of catchments the Main catchment area (till Marktbreit) was considered even though the area is bigger than 10,000 km². But a large part of the area is covered by the Main catchments (till Kemmern) and the Regnitz. It can

therefore be assumed that the large Main area reacts like the partial areas. The Große Vils catchment was selected, too, as the average gradient of 0.99 % only just lies below the proposed limit of 1 %. The sizes of the 13 catchment areas lie between 347 km² (Große Vils) and 13,974 km² (Main till Marktbreit). The average gradient (derived from the DEM with a grid width of 1000 m) varies between 0.99 % (Große Vils) and 4.47 % (Werra). The percentage of arable land lies between 25 % (Lahn) and 59 % (Große Laber). The long term average suspended sediment concentrations also show a high variability. In the Spree the lowest values were measured (11 mg/l), whereas the Rott with 91 mg/l showed the highest concentrations (Table 7). The soil erosion rates were summed up in ArcGIS for the test catchments. Then the sediment delivery ratio was calculated on the basis of the long term average suspended sediment loads (Equation 3). The Große Laber with 2.6 % has the lowest and the Werra with 17 % has the highest SDR (Table 7).



Figure 31: Location of the 13 test catchments and monitoring stations used to adapt the SDR approach for agricultural land

In the next step the calculated SDRs for the 13 test catchments were correlated to the catchment area characteristics to derive a model approach that can then be transferred to all analytical units. Figure 32 and Table 8 show the relation to the size of the catchment areas and to the gradient. As expected the calculated SDR in the test catchments rises with the increasing gradient. For the non-linear regression based on a power function the correlation coefficient (R^2) is 0.65 (Figure 32, right).

There was also a correlation to the size of the catchment area (Figure 32, left), however, the SDR does rise with the increasing area. The reason for this lies in the geographic location of

the 13 test catchments (Figure 31): catchments with a larger area have a higher average gradient. Both parameters have an R^2 of 0.64 and do not correlate linearly with each other. Therefore the gradient has a more significant influence on the SDR.



Figure 32: Correlation between the SDR and the catchment area (left) as well as the average gradient (right) for the 13 test catchments

It was subsequently tested whether there is a relation between the SDR and further spatiallylumped morphological catchment characteristics (comp. literature review). Taken into account were:

- the amount of area with a gradient of less than 2 % (Delmas et al., 2009), calculated from the DEM in a 50 m grid (BKG, 2007);
- the amount of depressions, determined from the digital map on geomorphological relief parameters (GMK 1000) (BGR, 2006);
- the drainage density of the stream network, calculated by the length of the waterway in a catchment divided by the area of the catchment;
- the hypsometric integral (HI, Equation 4), derived from the DEM in a 50 m grid (BKG, 2007);
- and the weighted average distance of all sediment source areas to the water D_w (Equation 5) according to Lenhart et al. (2005), calculated from the DEM in a 50 m grid (BKG, 2007).

Both parameters for estimating potential deposition areas "amount of area with a gradient of less than 2 %" and "amount of depressions" only delivered a significant correlation for the parameter "amount of depression areas" to the SDR with an R² of 0.49 (Figure 33, left).

For the parameter "drainage density" no relation was found to the SDR. But the calculated values for the drainage density of the test catchments were very similar and only had a low variation coefficient (< 10 %). The hypsometric integral (Equation 4) correlated to the SDR of the test areas with an R² of 0.24. However, the SDR decreases with a rising HI which is opposed to the hypothesis of Verstraeten and Poesen (2001). One reason for the vague relation could be that different hypsometric curves can lead to the same values for the HI (Hurtrez et al., 1999). Furthermore, the HI of the test catchments correlates with the area of the catchment (R² = 0.29) so that the positive correlation between area and SDR depicted in Figure 32 (left) is transferred to the relation between the HI and the SDR.



Figure 33: Correlation between the SDR and the amount of depressions (left) as well as the hypsometric integral (right) for the 13 test catchments

As last integral morphological parameter the weighted average distance D_w (Equation 5) according to Lenhart et al. (2005) was calculated for the test catchments. However, no relation was found between D_w and the SDR. A relation to the SDR can only be found if the catchment area-specific factors k in Equation 5 are calibrated in each individual test catchment. An approach adapted like this would not be transferable to other catchments though, as k is not known for the other areas.

Following the morphological parameters further catchment area characteristics such as land use and the long term average precipitation were examined for relations to the SDR. For the long term average precipitation there is no correlation to the SDR (R² = 0.03, Table 8). As land use parameter following Equation 7 the share of arable area of the land use was observed. The share of arable land correlates with an R² of 0.43 to the SDR (Figure 34, left, and Table 8). However, against expectations, the SDR decreases for a rising share of arable area in the test areas. For partial catchment areas of the Spree and Salza (tributary of the Saale) Behrendt et al. (1999) found a positive correlation between the percentage of arable land which was in the direct vicinity to surface water and the percentage of arable in a catchment (comp. Equation 7). Figure 35 shows the location of the arable land in the 13 test catchments. Areas with a high percentage of arable area such as the Große Laber, Rott and Große Vils show an even distribution of arable land, however, there are no such catchments in the mid-mountain areas (e.g. Harz, Upper Palatinate Forest and Thuringian Forest) as well as at the foot of the Alps. Especially in the mountainous catchment areas that have a comparably low percentage of agriculture the arable land lies mainly in the flatter regions and is therefore in the vicinity of surface waters. The percentage of arable land in land use is therefore not suitable to derive the SDR for catchments in different landscapes.







Figure 35: Location of arable land in the 13 test catchments

Therefore, in the next step, the distance between the sediment source area to the surface water was analysed. As flow paths can significantly differ from the beeline due to the topography the length of the flow paths were calculated for each grid cell on the basis of the DEM (50 m grid, BKG, 2007). For this the flow directions were defined in the DEM along the largest gradient (Jenson and Domingue, 1988). Then a water network was generated from the depression lines of the DEM with the help of an algorithm for calculating flow accumulations, whereby the generated waterway denseness in the test catchments was adapted to the actually existing flow water network. Then the flow lengths were calculated for each cell to the generated water network. As example Figure 36 shows the results of the flow length calculation for the Werra. In the figure the flow length grid was superimposed with a map of the actual water network of the Werra. It shows that the generated water network coincides well with the actual flow.

After this a grid data set was created which only contains the flow lengths for the arable land and determines the percentage of arable land which has a given distance to the water. The distances 300, 500 and 1000 m were tested.



Figure 36: Calculated flow distances from each grid cell to the next surface water for the Werra catchment

The determined percentages of arable land within in the given distances were then recalculated on correlations to the SDR in the test areas. For all three arable land percentages there was a negative correlation to the SDR. The flow length of 500 m had the highest correlation with an R² of 0.42 (Figure 34, right). Figure 37 shows the percentage of arable land in the Werra with a flow length of below 500 m to the next surface water.



Figure 37: Arable land in the Werra catchment area located in a flow distance below and above 500 m to the next surface water body

In Table 8 the correlations and measures of determination between the SDR and the most important catchment characteristics are compiled.

Of all parameters

- the "average gradient",
- the "amount of depressions" and
- the "percentage of arable land with a flow distance below 500 m"

proved suitable to derive the SDR for arable areas.

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Parameter	Equation	R²
Catchment area, A [km ²]	$SDR = 0.54 \cdot A^{0.32}$	0.50
Average gradient, S [%]	$SDR = 3.61 \cdot S^{0.84}$	0.65
Amount of depressions, <i>sink</i> [%]	$SDR = 34.2 \cdot sink^{-0.60}$	0.49
Hypsometric integral, <i>HI</i> [-]	$SDR = 3.60 \cdot HI^{-0.59}$	0.24
Precipitation, <i>P</i> [mm/a]	$SDR = 1000.2 \cdot P^{-0.74}$	0.03
Share of arable land, A _{AL} [%]	$SDR = 433.5 \cdot A_{AL}^{-1.14}$	0.43
Share of arable land < 500 m flow distance, A_{AL500} [%]	$SDR = 0.057 \cdot A_{AL500}^{1.56}$	0.42

A non-linear correlation according to Equation 7 was used and the empirical factors were adapted with the method of the smallest squared difference. This showed that the measure of determination R² is not improved by if the "amount of depressions" is considered in addition, to the parameters "average gradient" and "share of arable land with a flow distance below 500 m". The amount of depressions correlates non-linearly with an R² of 0.63 with the

average gradient (for small gradients the amount of depressions is larger, as expected). Therefore, the parameter does not explain any additional variance and was therefore not considered. Equation 8 shows the resulting approach for calculating the SDR for all analytical units:

Equation 8:

$$SDR = 2.27 \cdot S^{0.86} \cdot A_{41500}^{0.16}$$

 A_{AL500} Share of arable land with a flow distance to the next surface water below 500 m [%]

First Equation 8 was used on the 13 test catchments to define the model efficiency according to Nash and Sutcliffe (1970) (Appendix 1). Figure 38 shows the comparison between sediment load observed at the monitoring stations and the predicted values calculated using the SDR approach (Equation 8). It is found that the observed sediment load is equally over and underestimated. The model efficiency was determined as 0.80 for the 13 test catchments which confirms the good connection visible. The measure of determination of the linear correlation between observed and calculated sediment load is 0.81.



Figure 38: Comparison between the observed and calculated sediment loads at the monitoring stations of the 13 test catchment areas. The solid line represents the 1:1 line, the dotted lines represent a deviation of \pm 30 %, ME = model efficiency, R² = coefficient of determination

Sediment delivery from areas not used for agriculture

Apart from erosion from agriculturally used areas it must be considered that there is sediment eroded from woodland, natural grass and shrubland as well as from open mountainous areas. Soil erosion from woodland and grass areas was calculated on the basis of the R, K and LS-factors of the ABAG and the C-factors according to Venohr et al. (2008). The average soil erosion is 0.1 t/(ha·a). It was supposed that half of the potentially eroded soil material from areas with natural vegetation is transported into surface waters.

The sediment delivery from mountainous areas can be calculated by multiplying the open area in a height above 1000 m with an area-specific erosion rate. Behrendt et al. (1999) suggested a value of 4 t/(ha·a) for the area-specific erosion rate. This value was tested and adapted according to long term suspended sediment loads of catchment with alpine character. For this 8 water bodies were chosen from the Danube region for which suspended sediment load measurements were available (LfU, 2002b) and which catchment areas feature open mountainous area (min. 10 % of the area). In table 1 of Appendix 2 the areas and their characteristics are given. The catchment area size lies between 903 km² (Saalach) and 9,522 km² (Inn). First, the sediment load from arable land, woodlands and other areas with natural vegetation coverage was calculated. Sediment delivery from open mountainous areas was added to these loads. In the process the area-specific erosion rates were varied till the model efficiency (ME) (determined from the differences between observed and calculated sediment load (table 1 of Appendix 2) reached a maximum of 0.78. With 3.5 t/(ha·a) the adapted value for the area-specific erosion rate deviates slightly from the suggested value by Behrendt et al. (1999). Figure 39 shows the comparison of the observed and calculated sediment loads in the 8 catchments.



Figure 39: Observed and calculated sediment load at 8 alpine monitoring stations in the Danube basin. The solid line represents the 1:1 line, ME = model efficiency

From Figure 39 it becomes obvious that the suspended sediment loads for Inn, Isar, Lech, Salzach, Iller and Loisach are equally over and underestimated resp., whereas the loads for both of the smaller areas Saalach and Tirolean Achen are strongly underestimated. A good compliance for these areas can only be achieved if the area-specific erosion rate is increased considerably. In this case the sediment loads in the other areas would be strongly overestimated. A comparison of the water areas shows that the Saalach and Tirolean Achen only have a small percentage of water area and therefore do not have any larger lakes (table 1 of Appendix 2). It can therefore be concluded that the retention in the water system is low during the transportation to the catchment outlet. However it can be assumed that retention processes take place in the other catchments, either through sedimentation in lakes and dams or through a low gradient of the main waterway, for example like in the Inn valley. But at the moment local retention processes cannot be represented for the whole of Germany in

MoRE. For the calculated sediment load for catchments with alpine character the local retention processes are therefore implicitly represented, as the adaptation of sediment load was optimized for the outlet of larger catchments (Figure 39). To be able to consider retention processes better in the future, section 3.3.4 shows the tests exemplary for the Danube basin, whether considering local retention processes in lakes and dams allows for a realistic figure of observed suspended sediment loads.

Validation of calculated sediment loads

In the next step the sediment load from all German analytical units were calculated and validated with the help of long term sediment discharge, which were not used for calibrating. For this the sediment load of the analytical units were summed up with an algorithm along the flow direction in the river basins. For validating suspended sediment loads, monitoring stations with large catchment areas, such as the Rhine, Elbe and Danube were considered, too.

As mainly the data basis for the German catchment areas is to be validated, differences between suspended sediment load monitoring stations were generated for catchments with a large proportion of catchment area outside Germany (Rhine and Elbe) so that predominantly German areas were covered (Rhine: Maxau to St. Goar and St. Goar to Düsseldorf, Elbe: Torgau to Hitzfeld). In table 2 of Appendix 2 the monitoring stations as well as a comparison of the catchment areas and suspended sediment loads from water-resources yearbooks with the data of the model system MoRE are depicted.

Figure 40 presents the comparison between the sediment load observed at the monitoring stations and the sediment load calculated in MoRE. All in all it can be seen that there is a good compliance between the observed and calculated loads. The model efficiency according to Nash-Sutcliffe (equation in Appendix 1) is 0.92, the coefficient of determination of the linear correlation lies at 0.93. The sediment loads were predicted at most gauges with a deviation of less than 30 %.

For most catchments the loads are slightly overestimated, as expected, as sediments can be deposited due to slower flow velocities with increasing catchment area or due to damming. A good example is the Danube between the monitoring stations at Ingolstadt and Vilshofen (comp. section 3.3.4) or the Elbe. An overestimation of the loads in large catchment areas is therefore plausible and is considered within retention calculations in MoRE (comp. section 3.3.4). Whereas an underestimation points to the fact that the complete sediment input have not been completely covered or that it was not considered that internal water retention processes could play a role. The load was strongly underestimated for the Ems and, to a lesser extent, for the Neckar (Figure 40).



Figure 40: Comparison between observed and calculated sediment loads at the monitoring stations for 20 monitoring stations in Germany. The solid line represents the 1:1 line, the dotted lines represent a deviation of \pm 30 %, ME = model efficiency, R² = coefficient of determination

In the long term average the Ems shows comparably high suspended sediment concentrations of 30 mg/l at Rheine and 20 mg/l at Lathen (BfG, 2007c), even though the average gradient in the catchment area is very low with only 0.57 % (comp. Table 7)

In the Water Framework Directive (WFD) reports on surface water quality of the Ems (NLWK, 2005a, b) high suspended sediment loads are lead to the use of the Ems as shipping lane which distorts the suspended matter content considerably. In the lower Ems a changed tide dynamic and expansion measures lead to a multiplication of suspended sediments and an upstream offset and expansion of the turbidity zone at the border between the sea water and freshwater (Talke and De Swart, 2006). Furthermore, the Ems is strongly eutrophicated due to its intensive agricultural use (NLWK 2005a). This can lead to an increase in phytoplankton growth which is included in the suspended matter load measurements. It can therefore be concluded that the high suspended matter concentrations in the Ems are not exclusively due to surface erosion, which is why they could not be represented completely in MoRE.

Based on both mentioned data sets, a comparison of the identified total urban areas in Germany showed the following: according to the CLC2006 data set the total urban area is 28,827 km² (corresponds to 8.1 % of the area of Germany) and the Base DLM comes up to an urban area of 30,181 km² (corresponds to 8.5 % of the area of Germany).

The urban area from CLC2006 is in average 4 % lower than the urban area according to the Base DLM. To verify the plausibility of the raster-based data sets the data on the settlement areas of the Federal Statistical Office was used. They state an urban area of about 29,350 km² (StaBu, 2011a). It shows a good compliance to both of the analysed land use data sets. The deviation is about -1.8 % for the CLC2006 data set and +2.8 % for the Base DLM data set.

In contrast to the Base DLM, the data set CLC2006 is available throughout Europe. Therefore this methodical approach can also be transferred to the catchment areas outside Germany. This is why the data set CLC2006 is preferred over the Base DLM data set for updating the input data for the emission pathway sewer systems.
Figure 41 shows the suspended sediment loads and discharge in the Neckar at the monitoring station Rockenau from 1978–2007 (BfG, 1978–2007a). The linear trend line signals a decrease in suspended sediment loads. Discharge also decreases slightly but not in the same range as for the suspended matter. There is indeed no linear connection between the discharge and suspended sediment load and in the end the erosion in the catchment area does not depend on the discharge but on the precipitation intensity and the time of the heavy rain events, but it is questionable if the changed precipitation/discharge situation can completely explain the decrease in suspended sediment loads.

Further reasons for the observed decrease could be the change of land use and/or due to a change in cultivation. The estimation of the sediment load in MoRE is based on the current land use data (section 3.3.1.1). If only the suspended sediment loads at Rockenau in the past ten years are used for the comparison, the sediment load in MoRE is even only slightly underestimated (16 %). For the Neckar, furthermore, it can be assumed that the sediments can be whirled up by shipping traffic and the measured suspended sediment concentrations are therefore not just due to erosion in the catchment area.



Figure 41: Suspended sediment load (top) and discharge (bottom) in the Neckar at Rockenau for the period of 1978-2007 (Water Resources Yearbook: Rhine basin, Part I 1978-2007)

3.3.2 Regionalizing the heavy metal content in soils

For quantifying the heavy metal emission by the emission pathway erosion it is distinguished between cultivation-caused erosion on arable land and the erosion of surfaces with natural vegetation coverage and open mountainous areas resp. Up until now the heavy metal concentrations for arable land in MoRE are available as average values for the federal states. The quantification of the emissions by natural erosion are based on an average geogenous background level for Germany (Fuchs et al., 2010). Within the scope of this project heavy metal contents in the top soil were regionalized to be able to spatially differentiate the emissions in the analytical units.

3.3.2.1 Heavy metal contents in the top soil of arable land

For the top soils of arable land background values for heavy metals were put together by the LABO, the German Federal States' Working Group on Soil (LABO, 2003), on the level of the federal states which are based on federal state specific research. First of all national background values were derived from this data. The background value describes the matter content of a soil which is made up of the basic geogenous content and the ubiquitous matter dissemination as a result of diffuse loads into the soil. The measured values were mainly taken in the 1990's and are therefore used for the reference year 1995 in MoRE. The heavy metal compilation is available at a federal state level differentiated into different soil parent material, land use (arable area, grassland and woodland) as well as settlement area types (urban and rural areas) and are given as 50 or 90 percentile. For the regionalization the federal state values were used as these allow a high regional differentiation due to the regional reference. First of all the 50-percentile-values for arable land and the most common soil parent materials were compiled for each federal state. If there was no value for a parent material for arable land then it was reverted to values of other land uses. Gaps in the data of the federal states were completed with values from neighbouring states with similar geological conditions or with nationwide derived background values resp. In few cases the measured values were below the determination limit. These values were replaced by half of the determination limit. The used background values are depicted on the level of federal states for the soil parent material in tables 3 to 18 of Appendix 3 (Schenk, 2009).

In the next step the rock formations of the digital geological map GK 1000 (BGR, 2001) were summarized as the most common parent materials on a federal state level for when data was available on heavy metals (tables 3 to 18 of Appendix 3).

The grouped rock formation units were assigned to the heavy metal loads of the federal states. Then a unified data set was created for Germany. On the basis of this data the heavy metal contents were calculated for arable land in the analytical units. It is important that only the areas that actually are used for agriculture are included in the averaging. For example especially the southern and central German solid rock regions show high heavy metal contents, however, these areas are hardly used for agriculture in higher altitudes. Therefore, in the next step the map for heavy metal contents was crossed with the arable land in Germany of the Base DLM (BKG, 2010). Figure 42 shows the maps for the regionalized heavy metal contents in the top soil of arable land in Germany. The lowest heavy metal contents are featured in the sandy soils of the north German lowlands. High contents are found in the low mountain ranges such as the Rhenish Slate Mountains, Ore Mountains, Thuringian, Upper Palatinate and Bavarian Forest as well as the basaltic rock formation of the Vogelsberg. Regions with low agricultural use such as the Alps, the Black Forest and the Harz as well as the urban centers of the Ruhr area, Berlin Hamburg and Bremen are depicted colourless.



Figure 42: Heavy metal content in the topsoil of arable land in mg/kg

Temporal accumulation of heavy metals

As already shown at the beginning of this section the regionalized heavy metal contents based on the data from the LABO (2003) can be seen as representative for the reference year 1995. Heavy metal balances for the arable land on a federal state level was generated (Neuß, 2010) to be able to map the temporal trend for the whole observed period (1983-2007). Atmospheric deposition and the use of fertilisers (mineral and organic fertiliser, sewage sludge and compost) were considered as loads. Data on the atmospheric deposition from 1983-2007 were taken from the MoRE data base (Fuchs et al., 2010). The application rates of mineral fertiliser (N, P, K, Ca, multiple element fertiliser) were made available on a federal state level by the Federal Statistical Office (StaBu, 1986a, 1998b, 2000, 2006a). The organic fertiliser amounts were defined from livestock (StaBu, 1986b, 1996, 1999, 2006b) and the specific production of pig and cow manure as well as solid and poultry dung (Fuchs et al., 2002). The agricultural use of sewage sludge is compiled in the statistic on "public water supply and sanitation services" (StaBu, 1983, 1987, 1991, 1995, 1998a, 2001, 2004, 2007). To be able to calculate the heavy metal loads the application rates were multiplied at federal state level with the heavy metal loads which Fuchs et al. (2002) compiled in the framework of literature research. Then the specific loads were calculated for each federal state for the arable land.

On the discharge side the losses from surface runoff, seepage water and the extraction due to harvesting were balanced. Discharges through erosion were not considered as these are negligible compared to the other discharge pathways (Bannick et al., 2001). If when ploughing, less contaminated subsoil is incorporated, this can lead to a decrease of heavy metal contents in the topsoil. The net discharge through erosion would be made up of the difference between a possibly higher heavy metal content of the eroded topsoil and the lower content of the subsoil incorporated into the plough horizon.

Heavy metal extraction by harvested material was compiled by Bannick et al. (2001) and Knappe et al. (2008). For estimating discharge with the seepage water the concentrations measured by Bielert et al. (1999) from lysimeter analysis in 2 m depth were used. The seepage water rate was calculated for each federal state with the model system MoRE (comp. Appendix 4) and multiplied by the area of arable land of the respective federal state. Discharge from surface runoff was also taken from the model system MoRE. The heavy metal loads from the runoff of precipitation on arable land and the surface wash of fertilisers was considered.

At first a discharge and load balance was compiled for each federal state per ha of arable land. For converting the heavy metal contents (μ g/kg and mg/kg resp.) the first 30 cm of the arable land (corresponds in general to the ploughing depth) was chosen as reference value as well as assuming a soil density of 1,3 g/cm³ (Bannick et al., 2001). The accumulation from 1983 to 1994 and from 1996 to 2007 for all heavy metals and federal states is depicted in Appendix 5. Figure 43 shows the average accumulation in arable land for Germany from 1983 to 2007.

The highest percentaged accumulation rates from 1995 to 2007 show Cu (3%) and Zn (2.9%) which is due to the high content of both metals in organic fertilisers. The discharge for nickel in seepage water in many cases exceeds the calculated matter loads from atmospheric deposition and land management (comp. Appendix 5). The amount of Ni (and Cr) in topsoil is strongly reasoned to the geogenous conditions, anthropogenic play a minor role. Research on permanent monitoring plots have shown that the concentrations of nickel

in soil seepage water increase with increasing soil depth. Consequently, especially in the subsoil nickel reserves are available for mobilising (Knappe et al., 2008). It is possible that the concentrations from soil depths of up to 2 m according to Bielert et al. (1999) for unifying discharge with seepage lead to an overestimation of discharge. In the cases of a calculated negative Ni-balance a harmonious balance was assumed and the accumulation was set to 0.

On the basis of accumulation rates at a federal state level the heavy metal contents in arable land for the analytical units were calculated for MoRE for the period 1983-2007 based on the regionalized heavy metal contents in the reference year 1995.



Figure 43: Average accumulation of heavy metals in the topsoil of arable land in Germany in mg/kg (the values of Zn have been divided by 5 for a better presentation in the figure)

3.3.2.2 Geogenous background values for heavy metals

Apart from the erosion from arable land erosion takes place on areas with natural vegetation and especially on areas without protective vegetation coverage such as mountainous areas. As there are no agriculturally related loads the geogenous contents were used for quantifying heavy metal emissions by natural erosion. Hindel and Fleige (1991) determined the heavy metal contents in the most common rock formations in Germany, depicted in Table 9.

According to the procedure for arable land (section 3.3.2.1) the rock formation units of the digital geological map GK 1000 (BGR, 2001) were grouped according to the rock formation unit in Table 9 where heavy metal contents were available (Figure 44). This grouped data set was then linked to the heavy metal contents from Table 9. On the basis of the generated maps the average geogenous heavy metal contents were calculated for the analytical units of MoRE.



Figure 44: Grouping of rock formation units of the geological map of Germany GK 1000 (BGR, 2001) as a basis for the regionalization of geogenic heavy metal contents

Rock	Area	Heavy metal content							
unit	[%]	Cd [mg/kg]	Cr [mg/kg]	Cu [mg/kg]	Hg [mg/kg]	Ni [mg/kg]	Pb [mg/kg]	Zn [mg/kg]	
Sand/ gravel	38.5	< 0.3	1.5	1.5	0.005	5	10	11	
Loam	10.3	< 0.3	20	9.0	0.024	15	20	36	
Clay	11.5	< 0.3	103	22.0	0.044	60	39	98	
Turf	3.8	0.4	k.A.	10.0	0.056	12	17	29	
Sand stone	8.7	< 0.3	17	8.0	0.019	14	20	30	
Lime stone	10.6	< 0.3	5	9.0	0.018	16	38	35	
Schist	8.5	< 0.3	65	28.0	0.015	39	35	124	
Basalt	2.2	< 0.3	317	50.0	0.027	207	31	103	
Crystalline rocks	4.5	< 0.3	2	4.0	0.019	8	25	31	

Table 9: Geogenic heavy metal contents in rock formation units of Germany in mg/kg (Hindel und Fleige 1991 and GK 1000)

3.3.3 Implementing the new data base and calculation approaches in MoRE

All new data on soil erosion rates, heavy metal contents and constants as well as the new approach on calculating sediment delivery was implemented into the MoRE system. Like the procedure for the sewerage systems (section 3.2) variants were created in MoRE to be able to test the impact of changed input data and approaches compared to the existing model variant. The variants were implemented for Germany and the period 2003-2005. The following variants were defined:

- variant 1 (basic variant): results according to Fuchs et al. (2010);
- variant 2: with consideration of the newly calculated soil erosion rates according to the gradient class of arable land (based on the ABAG factors according to Wurbs and Steininger, 2011) for conventional tillage (section 3.3.1.2), the approach on estimating sediment delivery (section 3.3.1.4) as well as the regionalized heavy metal contents in the top soil (section 3.3.2);
- variant 3: input data and approaches according to variant 2, but compared to variant 2 the current percentage of conservation tillage was considered for the calculation of soil erosion from arable land (section 3.3.1.3).

Variant 2 is directly comparable to variant 1 as both variants assume that the soils are tilled 100% conventionally. Variant 3 considers the current percentage of conservation tillage in the federal states and enables the quantification of the current sediment input from arable land in Germany. The consideration of conservation tillage techniques in MoRE results from the C factor. Apart from the C factor for conventional tillage (variable ER_ABAG_factor_C_v2_conv) and for the current state of conservation tillage techniques (variable ER_ABAG_factor_C_v2_cons_act) scenarios for C factors with an average percentage of conservation tillage techniques of 50% and 100% (variable ER_ABAG_factor_C_v2_cons_50P and ER_ABAG_factor_C_v2_cons_100P) according to Wurbs and Steininger (2011) were implemented into the MoRE system.

In the following the calculation results are illustrated for the different variants for Germany and the period 2003-2005. Figure 44 shows the comparison of the heavy metal emissions by erosion for the three variants. It shows that the total loads for all three variants are within a similar order. The variation coefficients lie between 5.0 % (Cr) and 11.7 % (Pb).

Variant 1 and 2 are based on conventional tillage on arable land. For all metals an increase of emissions is detected from variant 1 to variant 2. This increase is between 1.6 % (Ni) and 33.6 % for (Pb). Figure 45 shows the changes in the analytical units as ratio of variant 2 to 1 for the example of the metal chromium. Factors < 1 mean that the emission by erosion has decreased in an analytical unit, factors > 1 show an increase in emissions.



Figure 45: Heavy metal emissions via erosion in Germany for the period of 2003-2005 and the variants 1-3. (Variant 1: according to Fuchs et al. (2010), Variant 2: calculation with new input data and calculation approaches assuming conventional tillage, Variant 3: calculation with new input data and calculation approaches assuming the current share of conservation tillage)



Figure 46: Ratio of variant 2 to variant 1 in the analytical units for chromium and the period 2003-2005. (Variant 1: according to Fuchs et al. (2010), Variant 2: Calculation with new input data and calculation approaches)

From Figure 46 it becomes obvious that the observed increase in total emissions by erosion is not spread out evenly across the analytical units, but especially in the low mountain range there is an increase in emissions, whereas other areas record decreases. The decrease in emissions compared to the results calculated by Fuchs et al. (2010) is due to the low sediment input to surface waters which was determined on the basis of changed input data for the ABAG factors and the revision of the approaches on sediment delivery ratios. In contrast, the increase of emissions is lead back to the regionalization of heavy metal contents in the soils according to the geological boundary conditions. Especially the lower

mountain ranges in Germany show geogenously related higher heavy metal contents. The increases in these regions are therefore seen as plausible.

Compared to variant 2, variant 3 considers the current situation of conservation tillage. Accordingly it shows a decrease in total emissions for all metals from variant 2 to 3 between 11.1 % (Ni) and 13.9 % (Hg) (Figure 45). In Figure 47 the changes in the analytical units are depicted as ratio of variant 3 to 2 for the example of the metal chromium.

For most of the analytical units the emissions decrease. The highest reductions are in Saxony, Thuringia, Brandenburg and in parts of Lower Saxony, corresponding to the higher percentages of conservation tillage in these federal states. For the Alpine area, the Black Forest and the Harz and part of the Rhenish Slate Mountains no decreases were calculated. In these areas there is generally no agriculture and the sediment discharge predominantly has natural causes.



Figure 47: Ratio of variant 3 to variant 2 in the analytical units for chromium and the period 2003-2005. (Variant 2: conventional tillage, variant 3: current situation of conservation tillage)

Figure 48 shows the impact of the three calculation variants on the relative meaning of the emission pathways and the total emissions in Germany. According to Figure 45 there are no significant changes, if the whole of Germany is considered. However, due to the large spatial variation, local changes can be severe in the river areas, as depicted in Figure 46 for the example of chromium.



Figure 48: Effect of the three erosion calculation variants on the relative importance of the emission pathways and the total heavy metal emissions (Cd, Cr, Cu, Hg, Ni, Pb, Zn) into the surface waters of Germany for the period 2003-2005

3.3.4 Estimating the retention of suspended sediments in river systems

The plausibility of the modeled heavy metal emissions can be checked with the observed river loads, which are balanced from quality and discharge measurements. However, for this comparison the in-stream retention has to be taken into consideration, as the river systems can retain particulate transported heavy metals. The retention of heavy metals mainly takes place by the process of sedimentation of suspended matter. From Fuchs et al. (2002, 2010) the retention was estimated by adapting a power function of the basis of the specific runoff rate in the river basins. This procedure is based on the hypothesis that rivers with a low runoff rate have a high retention of particulate transported heavy metals. The relation was parameterised for each metal by adapting the empirical factors according to the modeled and observed heavy metal emissions. For some river basins the observed river loads were clearly underestimated with this procedure, e.g. when the quality monitoring station was behind a lake or dam, as the retention within lakes and reservoirs is underestimated when assuming the same relation that was derived for rivers. Furthermore, river systems with canals and barrages (e.g. Spree, Große Röder) cannot be mapped with an approach based on the specific runoff rate. The aim of the following study was therefore to test for an exemplary river basin whether considering sedimentation in lakes and river structures can lead to realistically mapped suspended matter loads.

The basin of the Danube was chosen for the analysis, as it was discovered in section 3.3.1.4 that the suspended matter loads of the Danube were highly overestimated if sediment retention in the river system was not explicitly considered (Figure 40). Figure 49 shows the catchment area of the Danube up to Passau, in Table 10 the characteristics of chosen suspended matter monitoring stations within the basin are listed (LfU, 2002b). If the transported suspended matter loads in Table 10 are compared then losses can be seen for some flow stretches, for example in the Danube between Ingolstadt and Vilshofen. Even though the catchment area doubles between the measuring points the long term average sediment load from Ingolstadt with 458,884 t/a till Vilshofen only rises by about 20 % to 555,776 t/a. The Isar alone, which flows into the Danube shortly before Vilshofen, transports a load of 195,180 t/a, which is significantly more than the increase in the Danube from Ingolstadt to Vilshofen (Table 10). Unfortunately there are no more suspended matter measuring points after the Inn flows into the Danube at Passau. The measuring point in Engelhartszell along the Danube, shortly behind the German border in Austria, can be used for the comparison (Lebensministerium Österreich, 2004). At approx. 3,500,000 t/a the average suspended matter load at that measuring point is significantly higher as the loads at Vilshofen but the Inn alone transports a load of 3,555,768 t/a into the Danube at Passau-Ingling. These differences in the balance can only be explained with a retention of sediment in the river systems, e.g. by dams as they exist along the Danube.

Between Kehlheim and Jochenstein the Danube is used as a federal waterway for 203 km. In this section there are 6 barrages with locks and hydropower use. Further river structures are located up and downstream (BfG, 2010, Table 10).

Table 10: Characteristics of selected suspended sediment monitoring stations in the Danube basin till Passau (LfU, 2002b). Monitoring stations located in the main water course of the Danube are marked in bold

Catchment	Monitoring station	Area [km²]	Suspended matter load [t/a]	Lakes, reservoirs and river structures	
Neu Ulm	Danube	5,460	77,402	-	
Kempten	Iller	955	170,760	1 reservoir	
Füssen	Lech	1,422	384,692	5 reservoirs	
Ingolstadt	Danube	20,008	458,884	11 river structures	
Duggendorf	Naab	5,432	40,109	4 reservoirs	
Schönach	Große Laber	406	3,797	-	
Inkofen	Amper	3,076	39,316	Lakes Ammersee, Starnberg	
Schlehdorf	Loisach	639	53,934	-	
München	Isar	2,855	112,417	1 reservoir	
Plattling	Isar	8,839	195,180	-	
Vilshofen	Danube	47,677	555,776	5 river structures	
Ruhstorf	Rott	1,052	27,542	1 reservoir	
Burghausen	Salzach	6,649	1,413,036	Several small lakes	
Oberaudorf	Inn	9,715	1,690,385	Several small lakes	
Passau-Ingling	Inn	26,063	3,555,768	Lakes Tegernsee, Chiemsee	



Figure 49: Location of the 22 suspended sediment monitoring stations in the Danube basin (till Passau)

Furthermore, the Danube basin has many natural lakes and reservoirs. The two largest reservoirs are Lake Forggen in the catchment areas of the Lech just after Füssen and the Sylvenstein reservoir in the catchment of the Isar (Table 10 and Figure 49). In addition, there are many small barrages in the tributaries of the Danube which were not explicitly considered.

The sediment input into the Danube was calculated according to the described procedure in section 3.3.1.4 for all analytical areas and summed up along the flow path of the river system. In contrast to the described procedure for alpine catchments the natural erosion rate from mountainous regions was increased, as now local retention processes in lakes were to be explicitly considered. For both of the small catchment areas of the Saalach and Tirolean Aachen is was shown in section 3.3.1.4 that the sediment discharge is significantly higher if there are no sedimentation areas such as lakes in the catchment (comp. Figure 39). The area-specific erosion rate from alpine areas was therefore assumed to be 10 t/(ha·a) for all analysis areas. Figure 50 shows the resulting calculated suspended matter loads for all 22 suspended matter measuring points in the Danube basin compared to the observed loads (LfU, 2002b). As expected the observed loads at the measuring points were overestimated due to the increased erosion rates from the mountainous areas. Significantly higher sediment loads were calculated especially for both measuring points along the lsar, for the Danube at Vilshofen after the Isar flows into the Danube and for the measuring points along the Inn. For the three smaller catchment areas (Mindel, Traun and the Ammer at Weilheim) the sediment input is underestimated. For these areas the local characteristics cannot be deduced and represented adequately using the approaches developed for large river basins.



Figure 50: Comparison between observed and calculated sediment loads for all 22 monitoring stations in the German Danube basin without considering local retention processes (modified after Neuss, 2012). The solid line represents the 1:1 line, the dotted lines represent a deviation of \pm 30 %

In the next step the local retention rates were adapted for lakes and large river structures. For this it was assumed that the average sedimentation rate for natural lakes and reservoirs are similar. For barrages in the main course of the Danube it was assumed that the sedimentation rate was lower than for lakes as flood events and ships passing through the

locks transport much of the suspended matter loads downstream in a long term average. To adapt the calculated to the observed loads the model efficiency according to Nash-Sutcliffe (1970, Appendix 1) was used. The highest model efficiency of 0.93 was retrieved for a retention rate of 50 % for lakes and for 10 % for river structures (Neuß, 2012). Figure 51 shows the comparison between observed and measured sediment load for the monitoring stations in the Danube basin after considering the local sedimentation rates. For all suspended matter monitoring stations that encompass a large catchment area, such as the Isar, the Inn and the measuring points along the Danube at Ingolstadt and Vilshofen, a good adaptation of the observed and calculated loads which is due to local characteristics that cannot be represented adequately using the approaches derived for large river basins.



Figure 51: Comparison between observed and calculated sediment loads for all 22 monitoring stations in the German Danube basin with considering local retention processes (modified after Neuss, 2012). The solid line represents the 1:1 line, the dotted lines represent a deviation of \pm 30 %, ME = model efficiency, R² = coefficient of determination

3.3.5 Summary and outlook

Within the framework of this study a detailed data set on the quantification of soil erosion from arable land (based on the derived factors of the ABAG by Wurbs and Steininger (2011) as well as research on the percentage of conservation tillage) was implemented into the model system MoRE.

Based on the new data set a consistent spatially lumped approach for quantifying sediment input into surface waters was developed and validated with the help of long term suspended matter loads at monitoring stations. It showed that the sediment input significantly depends on the large scale gradient in the catchment areas and the percentage of arable land that lies in close vicinity to surface waters. But it was also shown that spatially lumped parameters describing the morphological characteristics are only of limited value to represent the influence factors on sediment transportation on a large scale. The sediment delivery is

significantly controlled by the location of the sediment source areas in the catchment and the morphology along the flow path to the surface water bodies. This complex interaction of spatially varied physiographic characteristics cannot be adequately represented by lumped morphological parameters which explains the malfunction of promising approaches such as that of Lenhart et al. (2005) for example. Based on this insight the length of the flow paths from the sediment source areas to the surface waters was considered. This approach can be further improved by characterizing the morphological conditions along the flow paths and by identifying the sediment depressions. Such a procedure was suggested for example by Ferro and Minacapilli (1995) where each source area has its own calculated specific sediment delivery ratio. But this calculation approach to determine the sediment delivery ratio does need preprocessing and cannot only be directly implemented into MoRE on the basis of lumped chatchment characteristics. Bearing in mind that the aim is to increase the simulation of scenarios with the model system (e.g. for changes in land use and cultivation) such a spatially explicit procedure is indispensable as the specific characteristics of the source areas as well as the length and morphology of the flow paths to the surface water play a decisive role for the emission pathway erosion.

To be able to map the suspended matter loads into the river systems the in-stream retention has to be considered in addition, to the sediment input from the catchment areas. The example of the Danube showed that considering local sedimentation rates in lakes and reservoirs leads to a good adaptation of the transported suspended matter loads in the river system for larger catchment areas. This approach still has yet to be tested and adapted for other river basins in Germany.

Furthermore, within the frame of this project, the top soil concentrations for heavy metals in arable land as well as natural areas (areas with natural coverage and mountainous areas) were regionalized based on data on a federal state level. The comparison calculations in the model system MoRE with the results of Fuchs et al. (2010) show an increase of heavy metal loads in the lower mountain regions in Germany (variant 1 and 2). This increase is plausible as these regions have geogenously caused higher heavy metal contents in the top soil. Considering local characteristics is indispensable for adequately estimating the emissions on a regional scale. For example the comparison between the calculated and observed heavy metal emissions by Fuchs et al. (2010) showed a good compliance for the large river areas (Rhine, Elbe, Weser) but also some very high deviations for small to medium sized catchment areas, which was due to the fact that the data base was not sufficient enough to map local characteristics.

Especially areas with geogenously increased heavy metal concentrations show large deviations (e.g. catchment areas in the Erz mountains). The regionalization of top soil concentrations on the basis of federal state data therefore contributes to the improvement of the local data base. However, up till now only data was used that was available uniformly for Germany on a federal state level (LABO, 2003). In the last years federal state specific data sets on top soil concentrations were increasingly collected (e.g. in Saxony, Rhineland Palatinate, Baden-Württemberg) which are significantly more detailed as the data sets which are made available by the German Working Group of the Federal States on Soil. Due to the emission calculations for erosion is was therefore sensible to implement federal state specific data. In addition, the balances for the temporal changes of the top soil concentrations can be validated and adapted where necessary based on the data from the permanent monitoring plots (Kaufmann-Boll et al., 2011; Schilli et al., 2011; LfL, 2005).

3.4 Optimized measuring concept for recording transported matter during flood events

When modeling emissions uncertainties naturally occur concerning the emissions that reach surface waters due to the state of input data and empirical approaches. To be able to validate the plausibility of the modeled emissions into surface waters, the river loads are often derived from the modeled emissions and compared to the observed river loads.

Due to the set measuring cycles (generally every 7, 14 or 28 days) standardized measuring programs only coincidentally detect flood events, whereas these are the events that massively lead to a high mobilisation of matter. This results in the necessity to develop specific flood event measuring programs that examine apart from suspended solids also nutrients and pollutants. Yet they are very expensive and are therefore seldom used.

In the frame of this project an approach was developed which on the one hand leads to an improved understanding of the role of flood events for sediment transportation and with that the transportation of particulately bound priority substances such as heavy metals and organic pollutants as well as nutrients (phosphor). On the other hand it serves to validate the plausibility of the corresponding mass balances from substance flow models used across Germany as well as to expand the existing database. The focus was on the feasibility of the sampling techniques in the frame of a measuring campaign.

3.4.1 Planning and preparation of the measuring campaign

During the preparation of this measuring program different possibilities were explored for the coordination, supervision and selecting the location. For this purpose possible locations and responsibilities were discussed in meetings with representatives from the environmental authorities of Baden-Württemberg and Bavaria. During these exploratory talks it became clear that the planned measuring program would need an intensive supervision. For this the choice of possible locations was confined to the Karlsruhe area. Criteria for the choice of the flowing water apart from the minimum size of the catchment area (1,000 km²) were the accessibility and the existing infrastructure (gauge signal, electricity and measuring hut) at the measuring point. Taking these criteria into consideration and after consulting with the representatives of the federal state government in Stuttgart, the Jagst (third largest tributary of the Neckar) was chosen as location for the test measurements (Figure 52). Representative measurement values are expected for comparable natural areas as the Jagst can be classified as medium sized with regard to the length of the river course (189 km) and the size of the catchment area (1,826 km²).



Figure 52: Location of the monitoring station Untergriesheim (Jagst) and analytical units of the Jagst river

In addition, the Jagst is suited as location because there is already considerable information on the hydrological characteristics of the Neckar catchment area at the Institute for Water and River Basin Management of the KIT. Due to the location near the catchment outlet of the Jagst into the Neckar the gauging stations in Untergriesheim offers good conditions for assembling a sediment collector and therefore a representative data collection for the complete catchment area of the Jagst is possible. The sampling was scheduled for one year.

3.4.2 Methodology

Sediment collectors were set up for sampling along the Jagst and were operated for the period of one year.

3.4.2.1 Assembling the sediment collectors

The sediment collectors were made of three units (Figure 53). The first is a collecting tank in which the withdrawn water in pumped. The tank has a capacity of 1 m³ and is made out of a reaction-stable fiberglass composite. The stored sample is protected from evaporation, direct sunlight and falling leaves etc. by a lid. In the upper area of the collector there is a floating switch which switches the pump off to prevent the tank to overflow.

The second unit is the control unit. It is connected to the gauge signal of the measuring station by an isolating amplifier and thereby receives the water level in real-time. The gauge height is equivalent to a certain current from the measuring sensor (0-20 mA) and is directly converted into a virtual digits-value (between 195 and 975). The digits therefore match a gauge height and are used to clock and configure the measuring intervals which are directly set via the input interface of the control unit. In the control unit the h/Q relation is deposited for the specific section of the river.

The third unit is a pump and its mounting bracket. The pump is in a pipe fastened to a chain. The height of the pump is balanced so that the pump doesn't run dry at low water levels and has enough space to the inner wall of the pipe so the water can freely flow around it. The pipe protects the pump from floating debris during flood events and against strong currents.



Figure 53: Design of the sediment collector

3.4.2.2 Gauge information

The average water level (mean value) at the gauge at Untergriesheim (Jagst) for the period 1980-2003 was 124 cm which corresponds to a discharge of 18.6 m³/s. Further master data on this gauge location can be found in Table 11. To be able to measure sufficient events in the chosen period of one year, the minimum level to initiate the measuring was set to 182 cm (51.5 m³/s). This is about three times as much as mean-flow conditions. For comparison, biennial flood events at this gauge reach a water level of 3.58 m (183 m³/s). This corresponds to ten times the amount of water than mean-flow conditions. As the sampling period was only restricted to one year the minimum level of sampling was set below the biennial flood level.

Table 11: Master data of the gauge in Untergriesheim (Jagst)

	figures
Catchment area	1,826 km²
Northing	3516082 m
Easting	5459077 m
Gauge datum altitude	148,68 m above sea level
Flood report level	4.00 m

With the developed approach for sampling a volume dependent sampling is carried out which leads to the mixed samples for the individual results.

3.4.2.3 Configuring the sediment collectors

The control unit regulates the pump and processes the incoming gauge signals. The signal (in 0-24 mV) is converted into a digit value using a stored formula (h/Q relation). This value corresponds to an exact water level and therefore to a specific discharge.

Pump intervals are defined for the sampling to retrieve a representative volume-specific mixed sample of a flood event. As the pump and tube to the tank run dry between the intervals the pumping intervals should be at least long enough that the minimum time is not shorter that the time the water needs from the pump to the container. Otherwise the sampling material will not reach the collector. The maximum interval length depends on the annuality (discharge volume) and the potential duration of the flood. The longer the flood event lasts and the higher the runoff is at the gauge, the shorter the intervals are set to sample the complete flood event if possible. In the control unit the interval boundaries are defined according to the location-specific runoff characteristics.

The duration of the pumping intervals was set to 120 s which corresponds to an amount of 48 l of extracted water. This pumping duration allows the volume of 20 pumping intervals to be collected in the container (1 m³ volume) during one flood event. The distance between the intervals was set to the discharge amount of 360,000 m³. This allows a sampling of events (from 51.35 m³/s) with a duration of up to 40 h. The interval was set high to be able to sample longer flood events or flood events with higher discharge peaks from start to beginning.

3.4.3 Results and evaluation

The following will analyse the results of the measuring and put them in the context of standardized collected long term data quality.

3.4.3.1 Measuring program for flood events

In the time from September 2010 to June 2011 one flood event was sampled. On the 23rd and 24th November 2010 a sampling volume of 70 I was taken in two pumping intervals. As the taken sample volume was not the full volume of two intervals (96 I) it was concluded that during the pump sequence the water level must have fallen below the threshold limit or that



the pump was delivering less water than measured earlier. At this flood event the threshold value (51.5 m³/s) was exceeded for only a few hours for the sampling (see Figure 54).

Figure 54: Discharge curve during the sampling period

For this analysis a sediment load (79.4 g) was analyzed. The solids content from the sampling volume was filtered and then sieved into five grain fractions (> 0.5 mm, 0.500 - 0.250 mm, 0.250 - 0.125 mm, 0.125 - 0.063 mm, < 0.063 mm). It was assumed that the fluid phase had no relevant amounts of heavy metals compared to the solid phase. The heavy metal amounts were measured with the help of atom absorption spectroscopy (AAS), whereas for determining the amount of phosphor the sampling material was solubilised with the help of perchloric acid and then photometrically determined.

Figure 55 shows the results of the analyses of the dried and fractioned samples. About 92 % of the AFS were allotted to the fraction < 0.063 mm, approx. 5 % to the fraction 0.063 - 0.125 mm and the remaining 3 % of the weight proportion to the three larger grain size fractions.

In Figure 56 the contents of the measured heavy metals (Cd, Cu, Cr, Ni, Pb, Zn) and of the total phosphor (P) are set in contrast to the loss on ignition (LOI) for each grain size fraction. The LOI represents the percentage of organic substance in the sample.



Figure 55: Weight of the grain size fractions in [%] and [g]

Figure 56 shows the LOI-shares for all five fractions. The LOI especially in the smaller fractions is striking. If the LOI for comparable samples is generally in the range of 6 %, the percentage measured in the finer fractions was 19 %. The presence of a lot of organic material additionally to the high percentage of clay and silt causes an excess of ion exchange spaces in the solid phase. As consequence, not all spaces can be taken up by dissolved ions. The large amount of exchange spaces has a levelling effect on the distribution of bound heavy metals and phosphor on the different fractions. A significantly higher contamination of the finer fractions would have been expected, which had not been shown significantly in the analyses (Figure 56 and Figure 57). The highest heavy metal loads were measured in the middle-sized fraction.

For P, Cu and Zn the trend is visible, that the highest contaminations were measured in the fraction between 0.250 and 0.500 mm. The contamination of the solid matter decreases with smaller grains sizes. This correlates to the lower organic share in the finer fractions.

It can therefore be concluded that a large amount of the three mentioned substances were bound to organic matter. In the fraction > 0.5 mm the LOI is the highest but the contamination is lower than in the next smaller fraction. It is assumed that the surface of the larger particles in relation to the mass has fewer binding points for adsorption. The distribution of the loading by Ni, Pb and Cr in the different fractions follows no clear trend and fluctuates slightly from fraction to fraction (Figure 57 and Table 12).



Figure 56: Heavy metal content and loss on ignition



Figure 57: Detailed view on heavy metal contents

Fraction	Weight	LOI	Ptot	Cu	Cd	Cr	Ni	Pb	Zn
mm	g	%	mg/kg						
total	79.4								
> 0,500	0.5	64.1	161	32.8	0.274	15.1	23.9	15.2	167
0,250 - 0,500	0.4	50.8	173	51.2	0.308	23.8	29.2	22.4	259
0,125 - 0,250	1.5	38.8	210	42.9	0.416	17.8	34.0	24.1	97
0,063 - 0,125	3.7	14.5	146	35.6	0.323	19.1	34.4	16.8	88
< 0,063	73.4	18.9	144	25.1	0.266	19.8	34.7	18.3	58

Table 12: Heavy metal contents of various grain size fractions

3.4.3.2 The comparison of the results with the quality data of a standardized measuring program

To validate the measurement values the results will be compared with data from a standardized measurement program of the federal state of Baden-Württemberg. Unfortunately there were no substance contents available for suspended solids in the Jagst. This is why a concentration for the sampled flood event was calculated back from the measurement results. This can then be compared to the quality data from the annual data catalogue of watercourses in Baden-Württemberg (LUBW, 2011). The measuring point Jagstfeld (CJA 903) is suitable for the comparison as this is in close vicinity (approx. 3 km) to the measuring point in Untergriesheim (see Figure 58)



Figure 58: Location of the monitoring stations (source: Google Earth)

The measured concentration during the flood event was 1,130 mg/l of suspended solids. At the measuring point Jagstfeld a suspended solids concentration of 14.8 mg/l was found as average value for the years 1997 - 2008 from 155 samples, whereas the concentrations varied between 4.62 mg/l and 34 mg/l (Table 13). According to this, during the flood event 80 times as much solid matter was transported than during an average discharge.

In Table 13 the converted back phosphor and heavy metal concentrations are shown alongside the data from the annual data catalogue. Similarly to the solid matter the heavy metal concentrations are significantly higher during the flood event: 4 times for cadmium and up to 30 times for lead. In contrary to the heavy metals, the phosphorus concentration during the event was similar to those of the average concentrations at mean water. This leads to the conclusion that there is only a limited phosphorus storage in the system in which phosphorus can be enriched and then remobilised during flood events.

It must be said that the comparison between a unique event and long term measurements is not fully plausible. Nevertheless, the comparison of the results illustrates the effect that flood events have on the transportation of solid matter and the attached substances.

The sampled flood event statistically occurs more often than every two years, the discharge was 2.7 times higher than the average discharge. But still the substance contents, apart for phosphor, rose by clearly more than a factor of 2.7.

Table 13: Concentrations of suspended solids (SS), phosphorus and heavy metals in the Jagst river at the monitoring station Jagstfeld (LUBW, 2011)

parameter	average concentration [µg/l]	number of recordings	concentration in Jagst river at flood event [µg/l]	factor
SS [mg/l]	14.8	155	1,134	76
Cd	0.07	173	0.31	4
Cr	1.62	173	22.4	14
Cu	2.12	169	29.6	14
Ni	1.63	169	39.3	24
Р	170	173	165	1
Pb	0.78	173	20.8	27
Zn	9.33	173	70.3	7

3.4.4 Problem analysis

Due to different problems the implementation of the approach within the given period proved to be difficult. For one the positioning of the solid matter containers taking into consideration the infrastructure needed (electrification gauge signal, fortified terrain, weather shield, etc.) and the usability of the content of the data concerning the position of the catchment area were very time-consuming. And the assembly was delayed due to technical complications at the integration of the solid matter container (control unit) into the existing infrastructure (connection to the gauge signal). The decisive point that limited the amount of event samplings was the fact that the during time the system was ready there were only two flood events with relevant measurements. One of which was sampled successfully, the second unfortunately couldn't due to technical reasons (loss of electricity). The installed solid matter collector will continue to operate and will continue to deliver data sets. The assembly and functionality of the solid matter container were able to be tested in the described measuring campaign successfully.

3.4.5 Summary and outlook

To check the plausibility of modeled river loads these are often compared to river loads that are calculated from monitoring data (observed river loads). The role of flood events is only insufficiently understood in the context of river loads from monitoring data, as due to the set measuring cycles (generally every 7, 14 or 28 days) standardized measuring programs only cover flood events by chance.

An approach to improve the data is to determine the role of flood events for sediment transportation and therefore for the transportation of particulately bound priority substances such as heavy metals and organic pollutants as well as phosphor. On this account there is a long term volume-proportioned sampling of flood events at the Jagst, a tributary to the Neckar.

Sediment collectors were set up along the Jagst for sampling and were operated for the duration of one year.

A sediment collector is made up out of a collecting tank, a control units as well as a pump. It is connected to a gauge station and receives the gauge measuring values in real-time. The system can be configured via the control unit so that it starts sampling at a certain level. In volume-dependent intervals (discharge) samples are automatically taken from the river, for the duration of a flood event and are stored in a collecting tank as a mixed sample. This way the transported solid matter amount and the bound pollutants and nutrients can be quantified afterwards.

Only one flood event could be sampled during the operation period. The solid matter load obtained this way was filtered out and split into five grain fractions. The heavy metal and phosphor contents were determined for each fraction. The main share of the solid matter load (92 %) was in the finest grain fraction (< 0.063 mm), the other 8 % were spread across the other fractions. By determining the loss on ignition (LOI) the percentage of organic material within the fractions was determined. With 19 % the finest fraction showed an above-average value. The highest contaminations with e.g. P, Cu and Zn were measured in the middle fraction (0.250 – 0.500 mm), whereas the loads with Ni, Pb and Cr followed no clear trend.

The measured concentrations were compared to the data from the standardized measuring program of the federal state of Baden-Württemberg at a monitoring station in close vicinity. According to this, during the flood event 80 times as much solid matter was transported than during an average discharge. Similar as for solid matter the heavy metal concentrations were significantly higher during the flood event: 4 times for cadmium, up to 30 times for lead. Other than for the heavy metals the phosphor concentrations during the flood event came up to the concentration at mean water.

The sampling is continued after the end of the project and the results continue to be evaluated.

4 Conclusions and further procedure

The aim of this research project was to methodically develop existing approaches on modeling pollutant emissions and to test them on their ability to model on the scale of large river basins as well as integrate spatially and temporally higher resolved input data sets. The initial point of this project was a project of the German Federal Environment Agency completed in the year 2010 (Fuchs et al., 2010; Venohr et al., 2008) in which homogenous data bases and model approaches were developed for all relevant substance groups (nutrients, heavy metals, PAH).

Furthermore, in the frame of this project the flexible and transparent Open Source Model system MoRE for quantifying and visualizing emissions into surface waters was developed in which all modeling bases on pollutants of the preceded project (Fuchs et al., 2010) were implemented as basic variant. The architecture of MoRE lets users without any knowledge of programing supplement the basic variant with other input data and quantification approaches as well as add new substance groups. This way different variants of input data and modeling approaches can be applied parallel to the basic variant and the results obtained can be compared to each other. On the one hand this allows to assess the quality of the input data. On the other hand the implementation of different variants allows the sensitivities to be analysed in a model. Both points are of great importance for priority pollutants as for most of these substances there are no consistent data sets and hardly any established modeling approaches. In addition, the possibility to create variants in MoRE set the technical requirements to consider scenarios for modeling emissions.

Based on the results of Fuchs et al. (2010) on relevant emission pathways for pollutant emissions the following model approaches were chosen and developed in the framework of a feasibility study:

- the model approach for water balancing and runoff components,
- the data basis and model approach on the quantification of emissions via sewer systems,
- the data basis and model approaches on erosion and sediment delivery into surface waters,
- the in-stream retention of particulately transported pollutants
- and the metrological recording of river loads at flood events.

In the following section the most important results will be outlined and the possibilities of developing the approaches as well as the transferability to all river areas in Germany will be shown.

Water balance and runoff components

The amounts of water from the different runoff components (surface, intermediate and base runoff) are an important database for the modeling of emissions from diffuse sources. Till now the hydrology in MoRE is mapped by simple empirical approaches on an annual basis. But this procedure does not adequately show regional characteristics such as the dynamics of runoff events (Fuchs et al., 2010).Therefore, as example the conceptional water balance model PRMS (Precipitation Runoff Modeling System) was used for the Ruhr catchment area (4,485 km²) to test whether the water balance and runoff characteristics can be used as model basis to quantify emissions. Special attention was given to the characterisation of

heterogenic area structures in the analytical units as well as a high temporal resolution for measuring the runoff dynamics. For this the analytical units of MoRE were split into hydrological units (land use and soil type) which are assumed have a homogenous runoff behaviour. The example simulating the Ruhr catchment area showed that a land use specific survey of the runoff pathways with the help of a water balance model enables regionally differentiated data bases for matter load modeling from diffuse sources,

However, an adaptation of the model system PRMS for the complete research area came with a very high effort which is why it is better to revert to an existing model system if possible. At the moment the water balance model LARSIM (Bremicker, 2000) is being built up on behalf of the German Federal Institute for Hydrology for Central Europe (LARSIM_ME). The spatial coverage of LARSIM_ME includes all river areas in Germany as well as the catchment areas outside Germany and therefore covers the complete relevant research area. The model is made up out of single models for the river area units with a grid length of 5 x 5 km and for daily steps. The simulation period comprises the years 1974 - 2006, a continuation of the model is intended by the BfG (German Federal Institute for Hydrology). The completion of LARSIM_ME (predicted for the summer of 2012) will offer a consistent hydrological model basis which can be used for modeling emissions in MoRE. Before implementing the results in MoRE the output of simulation results by LARSIM_ME has to be adapted to the requirements of emissions modeling, e.g. the land use specific differentiation of runoff components.

Furthermore, the runoff pathways in urban areas need to be considered separately for the different sewer systems as it is only of little interest to the water balance modeling via which runoff components (storm sewers, combined sewer overflows, sewage treatment plants) the stormwater runoff from sealed areas is discharged into surface waters. In contrast, when modeling emissions the different urban runoff components play an important role. Furthermore, it was shown with the example of the Ruhr catchment area that the use of water resources can be of importance and that large reservoirs and transfer lines should be considered separately when simulating the water balance.

The use of a water balance model as hydrological basis for modeling emissions enables the consideration of scenarios on land use or climate change in the future. The impact of climate scenarios on the water balance is also examined in LARSIM_ME so that synergy effects can be used for this problem, too.

Data base and model approaches for quantifying emissions via sewer systems

Pollutant emissions via sewer systems contribute considerably to water pollution according to Fuchs et al. (2010). Within the framework of this current project the modeling basis was improved to get a better regional resolution of the emissions. This especially concerns the part of stormwater runoff from sealed areas. For this a new data base was created for the size of the sealed areas. In addition, two settlement classes were designated depending on the anthropogenic activities, and the pollution potential (surface potential) was calculated for each class. The changes were implemented for the analytical units in Germany so far. In principle it is possible to transfer the procedures to analytical units outside Germany, as the basic data used (FTSP data set on sealing degrees and CLC2006 on urban areas) is available for the whole European Union. The vector data of the "Urban Atlas" (EEA, 2010c) of the European Environmental Agency could be used as data set on agglomerations. As part of a unified data basis it has to be checked how far this data set is suitable for mapping agglomerations in Germany.

The surface load was regionalized for copper and zinc as for these substances there was a good data basis available on concentrations in stormwater runoff from sealed areas. Furthermore, zinc is seen as a guide substance of anthropogenic activities. In principle, this procedure can be used for other substances or substance groups as far as there is an adequate data basis available. This could surely work for nutrients such as nitrogen and phosphor. For further pollutants the data basis for deriving differentiated surface loads is rather poor. Selective measuring campaigns on measuring concentrations in stormwater runoff from sealed areas would be of help.

As already explained in the conclusions on "water balance and runoff components", there is a need for adjustment concerning the approaches on urban runoff components. This is especially true for the approach on calculating the discharge coefficient and discharge ratio of combined sewer overflows. So far the discharge coefficient is calculated depending on the degree of sealing of urban areas and is 46 % based on the new input data in average for Germany. This is significantly lower than the generally assumed value of at least 70 % (ATV-A 128). Currently, the discharge rate of combined sewer overflows is estimated on an annual basis by an approach which was originally developed for planning. In future, the LARSIM_ME daily precipitation data could be used to adapt the approach in order to quantify the discharge rates from combined sewer overflows depending on the actual precipitation dynamic and the storage volumes of the tanks.

The results of the project consolidate the statement by Fuchs et al. (2010) whereby the sewer systems play a large role in water pollution due to pollutants. Due to the new input data the emissions into surface waters are not solely dependent on the size of the sealed area but also from the intensity of anthropogenic activities. The examples for copper and zinc showed that the better data basis lead to a changed spatial distribution of emissions. Consequently, regionally, the share of individual emission pathways within the total emissions changes towards a more realistic picture of the actual source of those emissions. It is especially relevant for the choice of measures to reduce the emissions into surface waters as well as for the resulting investments and therefore for the compliance with European law.

Data base and model approaches on quantifying emissions from erosion

Emissions via erosion can strongly vary depending on land use, morphology, erodibility of the soils and the heavy metal content in the soil. Therefore, the spatial resolution of the input data should be improved for estimating the pollutant emissions by erosion.

For this reason a detailed data set on the quantification of soil erosion from arable areas (based on the derived factors from the ABAG by Wurbs and Steininger (2011) as well as research on the share of conservation tillage) was implemented into the model system MoRE. Based on this data set a spatially lumped approach on the quantification of sediment delivery into surface waters was developed and validated with the help of long term sediment loads at monitoring stations. It was shown that the sediment delivery strongly depends on the large scale gradients in the catchment areas and the share of agricultural land which lies within immediate vicinity to surface waters. However, spatially lumped model approaches, which are currently used in MoRE for all emission pathways, can only reach a limited characterisation of catchment properties that strongly vary in their landscape. The sediment delivery depends on the location and characteristics of the sediment source area as well as the morphology and land use along the flow path to the next surface water. This complex interaction of spatially distributed catchment characteristics cannot be mapped sufficiently by lumped morphological parameters. It is therefore recommended to determine the sediment

load based on a spatially distributed procedure such as e.g. the approach by Ferro and Minacapilli (1995) which determines a specific sediment delivery ratio for each source area depending on the length and gradient of the flow path. With such a spatially explicit procedure future advanced scenarios on land use and cultivation procedures can be simulated as the land use and cultivation can be locally changed and the consequences of these changes can be determined for the sediment delivery ratio.

Apart from the improved data basis in sediment delivery the top soil concentrations for heavy metals based on the data from the German Federal States' Working Group on Soil was regionalized for the different parent materials. However, in the last years more federal state collected specific data sets on top soil concentrations (e.g. in Saxony, Rhineland Palatinate, Baden-Württemberg) which are significantly more detailed than the data sets that were made available by the Federal States' Working Group on Soil. Due to the significance of top soil concentrations for calculating the emissions by erosion the detailed data of the federal states should be implemented in future.

Compared to the results of Fuchs et al. (2010) there are no significant changes for the total heavy metal emissions by erosion in Germany. However, the area-specific emissions in the analytical units show strong regional deviations. Therefore, local pollution hotspots are mapped more realistically due to the detailed input data.

Consideration of in-stream retention processes

A part of the suspended sediments which reach the surface waters from the catchment areas can be deposited during transportation in the river system. This retention process must be included for comparing modeled and observed sediment loads in surface waters. Fuchs et al. (2002, 2010) estimated the retention by adapting a power function based on the specific runoff in the river basins. For some basins this procedure lead to modeled sediment loads which were significantly higher than the observed loads, e.g. when the quality measuring point was behind a lake or dam, as the retention cannot be considered adequately in such cases. In the frame of a feasibility study for the example of the Danube basin specific sedimentation rates were adapted for natural lakes and reservoirs as well as river structures. The location of the lakes and structures were mapped along the flow path in the river system. It showed that the observed suspended matter loads were mapped realistically if local sedimentation rates were considered. This approach still has yet to be transferred to other river areas in Germany and tested.

Based on the adapted sediment loads in the river area of the Danube the heavy metal loads were modeled from Neuß (2012) and then compared with the observed loads. For Cu and Zn the modeled and observed loads corresponded well. For metals that mainly reach the surface waters by erosion, such as Cr, Pb and Ni the observed loads were strongly overestimated, even though the calculation was carried out with validated suspended matter loads. Therefore, the question must be asked whether the measurements really measure the transported loads in a realistic way. If, for example, the measurements do not take place during a flood event, during which a large amount of the erosion-caused loads are transported, it can lead to a severe underestimation of the loads. Apart from considering local retention processes, the metrological determination of the actually transported pollutant loads are of importance for validating the calculated pollutant loads.

The metrological determination of river loads in the case of a flood event

As already mentioned in the section on in-stream retention processes the metrological determination of the actually transported river loads is of central concern for improving the

data basis. An optimized measuring concept was developed for an improved recording of the transportation of solid matter and the attached nutrients and pollutants. One important uncertainty when calculating the transported river loads results from the insufficient recording during flood events. The measuring concept plans an exemplarily sampling from a medium sized river (catchment area approx. 1,000 km²) during a flood event (approx. biennial event). The results from the sampling were compared to long term standardized measurements. These showed large differences between the transportation at average water levels and the transportation during flood events. In case of a flood event about 80 times more solid matter was transported than at an average discharge. Similarly to the solid matter, the heavy metal concentrations rose significantly during a flood event: four times for cadmium and up to 30 times for lead. The phosphor concentrations during the event were, in contrast to the heavy metals, about the same as the concentration at mean water.

With the help of the strongly deviating transportation during a flood event this targeted sampling shows that further measurements are urgently needed to validate the transported sediment loads and the attached substances. The prototype of the solid matter collector will continue to sample flood events and contribute to an improvement of the estimation of sediment loads transportation. This measuring concept illustrates a sensible supplement to continuous standardized sampling.

In the presented feasibility study the methodological approaches on modeling the emissions into surface waters via the emission pathways of the sewer systems and erosion were developed and implemented into the model system MoRE. In addition, new approaches for modeling the water balance as well as the recording of river loads during flood events was recommended and tested. This established the basis to guarantee an optimal adaptation of the complete model in a subsequent phase of model development and to transfer the approaches to the whole of Germany.

In the framework of an international conference the project results and the model system MoRE were introduced to an audience of federal state representatives and German as well as European research colleagues and discussed.

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Appendices

Appendix 1: Modeling efficiency according to Nash and Sutcliffe (1970)

$$ME = 1 - \frac{\sum_{i=1}^{n} (sim_i - obs_i)^2}{\sum_{i=1}^{n} (obs_i - \overline{obs})^2}$$

ME modeling efficiency sim simulated values obs observed values

obs average of the observed values

Appendix 2: Characteristics of the catchments used to adapt and validate the sediment input

Catchment	Monitoring station	Area MoRE [km²]	Open moun- tainous area [%]	Suspended solid load (observed) [t/a]	Fracht angepasst [t/a]	Water surface area [%]
Iller	Kempten	1,333	19.6	170,760	130,841	1.97
Lech	Füssen	1,406	54.8	384,692	296,101	0.93
Loisach	Schlehdorf	928	13.4	53,934	61,443	1.71
Tiroler Achen	Staudach	939	22.2	283,510	91,630	0.68
Salzach	Burghausen	6,648	28.7	1,413,036	766,363	1.23
Saalach	Unterjettenberg	903	28.4	312,001	108,998	0.51
Isar	München	3,208	17.2	112,417	245,075	1.90
Inn	Oberaudorf	9,522	57.7	1,690,385	2,007,792	0.82

Annexed table 1: Characteristics of the 8 alpine catchments used to adapt the specific erosion rate from open mountainous areas

German water-resources yearbook (DGJ): Danube basin (LfU 2002b).

Annexed table 2:	Characteristics	of the 18 catchmen	ts used to validate	e sediment input to	surface waters
of Germany					

Catchment	Monitoring station	Area DGJ [km²]	Area MoRE [km²]	Suspended solid load (observed) [t/a]	Suspended solid load (calculated) [t/a]
Rhein ^{1,3}	Maxau bis St. Goar	53,646	53,528	628,356	802,402
Rhein ³	St. Goar bis Düsseldorf	43,838	43,772	517,621	574,440
Neckar ¹	Rockenau	12,676	12,622	382,947	209,160
Main ²	Kleinheubach	21,505	21,575	260,824	332,887
Weser ⁴	Bodenwerder	15,924	15,848	224,515	328,037
Weser ⁴	Nienburg	21,815	22,079	298,711	398,646
Weser ⁴	Intschede	37,720	37,874	521,191	539,165
Aller ⁴	Marklendorf	7,209	7,412	22,527	17,892
Aller ⁴	Rethem	14,730	14,817	90,679	140,239
Ems ⁴	Lathen	8,686	8,618	59,510	9,159
Donau⁵	Neu Ulm	5,460	5,415	77,402	73,940
Donau⁵	Ingolstadt	20,008	20,024	458,884	590,634
Donau⁵	Vilshofen	47,677	47,738	555,776	1,233,513
lsar ⁵	Plattling	8,839	9,059	195,180	320,692
Inn⁵	Passau-Ingling	26,063	25,821	355,768	3,055,118
Elbe ^{6,8}	Torgau bis Hitzfeld	74,666	74,159	239,217	444,927
Saale ⁶	Calbe	23,719	23,644	126,668	313,848
Spree ⁷	Lübben	4,492	4,527	8,015	8,154

German water-resources yearbook (DGJ): 1 Rhine basin, Part I (BfG 2007a); 2 Rhine basin, Part II; Main (LfU 2002a); 3 Rhine basin, Part III (BfG 2006a); 4 Weser-Ems (BfG 2007c); 5 Danube basin (LfU 2002b); 6 Elbe basin, Part I (BfG 2007b); 7 Elbe basin, Part II (BfG 1996); 8 Elbe basin, Part III (BfG 2006b)

Appendix 3: Heavy metal content in different parent materials in the federal states of Germany (LABO, 2003)

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Granite, gneis	0.24	17.0	7.0	0.13	7.0	25.0	45.0
Clay schist, mica schist, phyllite	0.30	52.0	26.0	0.09	26.0	38.0	85.0
Sand stone	0.20	18.0	5.0	0.08	11.0	20.0	30.0
Mud stone – Triassic period	0.30	52.0	39.0	0.09	43.0	23.0	50.0
Mud stone – Jurassic period	0.30	47.0	32.0	0.09	88.0	33.0	120.0
Lime stone – Triassic period	0.31	44.0	33.0	0.08	44.0	50.0	85.0
Lime stone - Jurassic period	0.31	66.0	27.0	0.08	60.0	31.0	97.0
Marl stone	0.18	34.0	10.0	0.08	24.0	20.0	46.0
Loess	0.36	37.0	17.0	0.09	29.0	26.0	57.0
Sand, gravel	0.16	17.0	8.0	0.08	12.0	11.0	31.0
Detrital marl	0.18	34.0	16.0	0.08	26.0	19.0	52.0
Turf	0.23	12.0	9.5	0.025	5.1	26.0	23.0
Basic rocks	0.23	142.0	42.0	0.09	148.0	37.0	126.0

Annexed table 3: Heavy metal content in different parent materials in the federal state of Baden-Wuerttemberg in mg/kg

Annexed table 4: Heavy metal content in different parent materials in the federal state of Bavaria in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Loess, loess loam	0.22	62.0	18.0	0.090	31.0	28.0	62.0
Sand stone	0.15	21.0	6.7	0.080	7.8	27.0	32.0
Clay, mud stone	0.31	64.0	26.0	0.090	43.0	49.0	89.0
Granite, gneis	0.24	48.0	16.0	0.130	21.0	71.0	110.0
Lime stone	0.76	54.0	18.0	0.080	38.0	68.0	120.0
Turf	0.23	12.0	9.5	0.025	5.1	26.0	23.0
Basic rocks	0.23	142.0	42.0	0.090	148.0	37.0	126.0

Annexed table 5: Heav	y metal content in	different parent material	s in the federal state of	of Berlin in mg/kg
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Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Without differenciation of bedrock	0.15	2.2	10.0	0.05	0.8	22.0	16.0

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Sand	0.10	4.0	4.0	0.025	2.0	12.0	15.0
Loam (except for meadow loam)	0.10	4.0	5.0	0.025	2.0	11.0	16.0
Fen turf	0.05	12.0	9.5	0.025	5.1	20.0	23.0

Annexed table 6: Heavy metal content in different parent materials in the federal state of Brandenburg in mg/kg

Annexed table 7: Heavy metal content in different parent materials in the federal state of Bremen in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Sand	0.10	8.0	6.0	0.04	2.0	17.0	17.0

Annexed table 8: Heavy metal content in different parent materials in the federal state of Hamburg in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Pleistocene sand and sandy loam	0.30	26.0	28.0	0.20	11.0	51.0	48.0
Holocene fluviatile loam and clay of the intertidal zone	0.30	42.0	24.0	0.20	16.0	39.0	90.0
Turf	0.23	12.0	9.5	0.025	5.1	26.0	23.0
Mud stone	0.30	37.0	23.0	0.09	37.0	39.0	99.0

Annexed table 9: Heavy metal content in different parent materials in the federal state of Hesse in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Sand (wind-borne sand, valley sand etc.) and teraces	0.20	12.0	11.0	0.02	12.0	29.5	53.5
Loess, Loess loam, Colluvium	0.40	18.0	17.0	0.04	25.0	29.0	64.0
Meadow loam	0.10	40.5	18.5	0.05	32.0	40.5	87.5
Flood loam	0.50	14.0	16.0	0.05	17.0	34.0	66.0
Mud stone, clay schist, phyllite	0.30	37.0	15.0	0.09	16.5	41.0	73.0
Sand stone, quarzite, greywacke	0.05	29.0	13.0	0.02	28.0	37.0	86.0
Basalt, green stone, diabase etc.	0.50	142.0	52.0	0.07	207.	42.0	144.0

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Detrital marl	0.10	17.0	13.0	0.06	10.0	13.0	37.0
Sand	0.10	12.0	13.0	0.05	7.0	13.0	27.0
Clay	0.20	39.0	23.0	0.09	21.0	24.0	72.0
Turf	0.23	12.0	9.5	0.025	5.1	26.0	23.0

Annexed table 10: Heavy metal content in different parent materials in the federal state of Mecklenburg-Western Pomerania in mg/kg

Annexed table 11: Heavy metal content in different parent materials in the federal state of Lower Saxony in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Sediments of the tidal zone	0.16	32.0	12.0	0.06	18.0	26.0	73.0
Sand	0.10	7.0	7.0	0.06	2.0	15.0	19.0
Sand loess	0.20	13.0	8.0	0.08	4.0	15.0	30.0
Loess	0.22	24.0	12.0	0.06	15.0	19.0	48.0
Detrital loam	0.10	12.0	8.0	0.08	3.0	15.0	25.0
Sand stone	0.20	24.0	11.0	0.06	15.0	18.0	48.0
Turf, bog	0.90	35.0	15.0	0.26	7.0	70.0	84.0
Mud stone	0.20	24.0	15.0	0.09	11.0	39.0	40.0
Lime stone	0.06	36.0	15.0	0.08	20.0	73.0	87.0
Basic rocks	0.80	72.0	51.0	0.09	37.0	37.0	134.0
Acidic rocks	0.20	6.0	12.0	0.13	3.0	71.0	34.0

Annexed table 12: Heavy metal content in different parent materials in the federal state of North Rhine-Westphalia in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Air-borne sand, sand loess	0.30	17.0	8.0	0.06	6.0	21.0	46.0
(Alluvial-)Loess	0.43	26.0	12.0	0.08	16.0	27.0	64.0
Fluviatile deposits	0.40	27.0	12.0	0.07	17.0	27.0	67.0
Carbonic bedrock	0.38	32.0	16.0	0.08	21.0	26.0	60.0
Fluvioglacial deposits	0.24	11.0	5.0	0.05	3.0	15.0	27.0
Moraine	0.35	24.0	9.0	0.07	12.0	24.0	59.0
Bog	0.43	21.0	10.0	0.10	8.0	25.0	54.0
Solifluidally reworked and weathered material	0.49	28.0	13.0	0.08	19.0	32.0	82.0
Without differenciation of bedrock	0.61	31.0	20.0	0.14	18.0	51.0	124.0

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Meadow sand, terrace sand	0.23	15.0	11.0	0.10	11.0	24.0	42.0
Meadow sand, terrace sand (free from carbonate)	0.20	12.0	9.0	0.10	8.0	20.0	35.0
Meadow sand, terrace sand (carbonic)	0.40	23.0	20.0	0.11	19.0	36.0	100.0
Meadow silt, terrace silt (free from carbonate)	0.41	37.0	26.0	0.13	39.0	55.0	127.0
Meadow sand, terrace sand (carbonic)	0.27	27.0	19.0	0.13	27.0	31.0	62.0
Meadow clay	0.62	45.0	31.0	0.17	43.0	34.0	79.0
Air-borne sand (free from carbonate)	0.12	4.0	9.0	0.11	5.0	23.0	21.0
Loess, fluvial loess, solifluidally reworked loess, loess rich solum sediment	0.26	30.0	18.0	0.13	29.0	29.0	60.0
Loess loam, solifluidally reworked loess loam, loess loam rich solum sediment	0.23	31.0	13.0	0.11	23.0	26.0	68.0
Unconsolidated sediment: sand stones/arkoses/conglomerates/ brecchias (percentage of loess < 1/3)	0.17	21.0	8.0	0.07	16.0	16.0	50.0
Unconsolidated sediment: sand stones/arkoses/conglomerates/ brecchias (percentage of loess > 1/3)	0.19	22.0	11.0	0.12	22.0	31.0	53.0
Unconsolidated sediment: pelites (mud stones, silt stones) (percentage of loess < 1/3)	0.32	38.0	16.0	0.13	31.0	26.0	66.0
Unconsolidated sediment: schists (clay schist, flaser schist, etc.) (percentage of loess < 1/3)	0.25	42.0	25.0	0.11	55.0	43.0	130.0
Unconsolidated sediment: schists (clay schist, flaser schist, etc.) (percentage of loess > 1/3)	0.23	42.0	22.0	0.09	52.0	39.0	121.0
Unconsolidated sediment: pelite- carbonate-rocks (silt marl, clay marl etc.) (percentage of loess < 1/3)	0.26	40.0	25.0	0.09	35.0	32.0	71.0
Unconsolidated sediment: pelite- carbonate-rocks (silt marl, clay marl etc.) (percentage of loess > 1/3)	0.22	28.0	22.0	0.11	29.0	34.0	62.0
Unconsolidated sediment: basic magmatic bedrock (vulcanites, plutonites, tuffs) (percentage of loess < 1/3)	0.49	69.0	32.0	0.13	57.0	47.0	136.0
Unconsolidated sediment: basic magmatic bedrock (vulcanites, plutonites, tuffs) (percentage of loess > 1/3)	0.43	73.0	23.0	0.15	51.0	56.0	129.0
Unconsolidated sediment: intermediate magmatic unconsolidated sediments (ash layers) (percentage of loess < 1/3)	0.40	18.0	15.0	0.19	25.0	89.0	113.0
Unconsolidated sediment: intermediate magmatic unconsolidated sediment (ash layers) (percentage of loess > 1/3)	0.39	25.0	16.0	0.21	29.0	86.0	110.0
Turf	0.23	12.0	9.5	0.02 5	5.1	26.0	23.00

Annexed table 13: Heavy metal content in different parent materials in the federal state of Rhineland-Palatinate in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Valley infill of rivers (Quaternary)	0.28	14.20	16.50	0.08	16.5	37.0	91.5
Meadow terraces (Quaternary)	0.32	8.50	8.90	0.01	9.3	26.0	66.9
Middle and Upper Buntsandstein	0.21	11.90	7.70	0.06	6.7	23.3	53.0
Rotliegend	0.20	27.00	10.00	0.06	18.0	22.5	69.0
Upper Carboniferous period - Stefan	0.25	32.00	11.30	0.07	20.6	23.5	73.0
Upper Carboniferous period - Westfal	0.30	19.90	24.00	0.18	27.4	59.9	104.0
Mean heavy metal contents of Upper	0.28	25.95	17.65	0.13	24.0	41.7	88.5

13.30

49.00

36.50

19.00

37.00

7.70

19.00

22.20

15.00

23.00

0.15

0.06

0.09

0.09

0.09

8.8

41.5

31.0

20.0

37.0

57.0

33.0

36.0

31.0

39.0

61.0

99.0

84.0

54.0

99.0

Carboniferous period

Muschelkalk

Mud stone

Loess

Acitic magmatites (rhyolithe)

Intermediate and basic magmatites

Annexed table 14: Heavy metal content in different parent materials in the federal state of Saarland in mg/kg

Annexed table 15: Heavy metal content in different parent materials in the federal state of Saxony in mg/kg

0.22

0.28

0.50

0.36

0.30

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Periglacial relocation layer above clay moderately acidic magmatites, metamorphites	0.68	46.0	21.0	0.110	16.0	79.0	100.0
Periglacial relocation layer above clay schist, phyllite, mica schist, greywacke	0.63	70.0	30.0	0.160	28.0	71.0	140.0
Periglacial relocation layer above basic magmatites, metamorphites	0.44	79.0	32.0	0.110	49.0	43.0	100.0
Periglacial relocation layer above Rotliegend sediments	0.59	50.0	18.0	0.120	28.0	46.0	110.0
Aeolian sediment, sand loess	0.33	28.0	12.0	0.100	11.0	40.0	49.0
Aeolian sediment, loess	0.40	39.0	14.0	0.090	14.0	44.0	55.0
Periglacial sediment, (sand-)loam	0.25	20.0	10.0	0.080	8.0	35.0	39.0
Periglacial sediment, sand	0.21	18.0	7.0	0.070	5.5	32.0	30.0
Lime stone	0.31	34.0	21.0	0.080	32.0	30.0	70.0
Turf	0.23	12.0	9.5	0.025	5.1	26.0	23.0

Annexed table 16: Heavy metal content in different parent materials in the federal state of Saxony-Anhalt in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Moraine sand	0.10	10.0	6.0	0.06	5.0	15.0	25.0
Loess loam	0.20	25.0	12.0	0.10	20.0	25.0	55.0
Weathering loam (silt- and mud stone with loess)	-	29.0	20.0	0.09	28.0	47.0	94.0
Meadow loam (exept for flood plains)	0.15	25.0	12.0	0.10	16.0	20.0	52.0
Lime stone	0.31	34.0	21.0	0.08	32.0	30.0	70.0
Mud stone	0.30	37.0	23.0	0.09	37.0	39.0	99.0
Turf	0.23	12.0	9.5	0.025	5.1	26.0	23.0
Acidic rocks	0.55	22.0	21.0	0.13	15.0	71.0	88.0
Basic rocks	0.53	142.0	42.0	0.09	148.0	37.00	126.0

Annexed table 17: Heavy metal content in different parent materials in the federal state of Schleswig-Holstein in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Sand	0.10	8.0	6.8	0.040	4.0	13.0	25.0
Loam	0.10	17.0	9.2	0.040	11.0	14.0	43.0
Turf	0.23	12.0	9.5	0.025	5.1	26.0	23.0
Lime stone	0.31	34.0	21.0	0.080	32.0	30.0	70.0

Annexed table 18: Heavy metal content in different parent materials in the federal state of Thuringia in mg/kg

Parent material	Cd	Cr	Cu	Hg	Ni	Pb	Zn
Loess	0.19	43.0	17.0	0.07	22.0	26.0	54.0
Mud stone, clayey marl, marl, solifluidally reworked material of Keuper and Roet	0.18	58.0	23.0	0.06	36.0	24.0	67.0
Clay stone, clay marl, solifluidally reworked material of Upper Muschelkalk	0.16	80.0	33.0	0.07	52.0	28.0	81.0
Lime stone, lime marl and dolomite of Middle and Lower Muschelkalk	0.37	48.0	21.0	0.07	28.0	43.0	99.0
Sand stone and sandy-clayey alternations of Middle and Lower Buntsandstein	0.14	20.0	9.3	0.06	6.4	28.0	30.0
Acidic and intermediate vulcanite and granite	0.14	28.0	10.0	0.21	7.4	78.0	49.0
Clay schists and greywacke-clay schist alternations of Thuringian Slate Mountains	0.32	76.0	28.0	0.17	32.0	42.0	126.0
Basic rocks	0.53	142.0	42.0	0.09	148.0	37.0	126.0

Appendix 4: Seepage water rate in the federal states of Germany

Annexed table 19:	Seepage water	r rate in the fede	al states of	i Germany ir	n mm/(m²-a),	extracted	from the
MoRE database				-			

Federal state	1985	1995	2000	2005
Brandenburg	161.80	149.40	165.18	137.31
Berlin	159.45	144.95	159.02	134.03
Baden-Wuerttemberg	257.02	242.18	285.96	201.44
Bavaria	228.83	214.64	248.88	192.50
Bremen	223.41	204.97	235.81	194.64
Hesse	237.66	222.68	258.03	203.61
Hamburg	219.37	198.23	224.08	179.43
Mecklenburg-Western Pomerania	171.46	157.07	177.50	142.33
Lower Saxony	221.45	204.32	231.21	190.87
North Rhine-Westphalia	252.63	230.15	267.38	218.35
Rhineland-Palatinate	243.00	231.94	275.12	195.46
Schleswig-Holstein	208.44	184.03	211.41	168.65
Saarland	265.22	246.31	297.10	191.03
Saxony	180.88	170.46	183.00	154.35
Saxony-Anhalt	171.27	170.45	184.45	152.47
Thuringia	205.53	200.75	222.15	180.27

Appendix 5: Calculated heavy metal accumulation in the federal states of Germany

Land	Cd [µg/kg]	Cr [µg/kg]	Cu [µg/kg]	Hg [µg/kg]	Ni [µg/kg]	Pb [µg/kg]	Zn [µg/kg]
Baden-Wuerttemberg	-11.8	-229.9	-590.9	-1.6	0.0	-354.0	-2490.5
Bavaria	-14.3	-373.1	-641.7	-2.8	-45.0	-351.8	-2935.0
Berlin	-152.1	-339.0	-601.8	-4.5	-89.0	-361.1	-2671.9
Brandenburg	-80.5	-339.0	-601.8	-4.5	-89.0	-361.1	-2671.9
Bremen	-14.6	-266.5	-876.4	-2.4	-21.4	-367.2	-3435.0
Hamburg	-21.5	-315.9	-288.7	-1.9	-14.6	-363.0	-1571.1
Hessen	-11.6	-176.0	-516.5	-2.4	-0.4	-344.8	-2180.7
Mecklenburg-Western Pomerania.	-81.4	-434.9	-663.5	-4.5	-99.9	-370.9	-2857.7
Lower Saxony	-14.6	-266.5	-876.4	-2.4	-21.4	-367.2	-3435.0
NorthRhine- Westphalia	-12.7	-293.1	-927.2	-2.3	-11.8	-358.4	-3395.8
Rhineland-Palatinate	-11.4	-111.7	-380.1	-2.3	0.0	-327.4	-1785.4
Saarland	-7.8	-73.3	-315.2	-2.2	0.0	-318.4	-1560.7
Saxony	-80.9	-376.8	-647.4	-4.5	-93.9	-370.6	-2904.6
Saxony-Anhalt	-80.3	-312.7	-595.8	-4.4	-83.0	-358.5	-2571.9
Schleswig-Holstein	-18.9	-295.4	-796.0	-2.4	-40.8	-385.6	-3559.7
Thuringia	-12.0	-291.4	-561.1	-3.8	-34.9	-486.1	-2443.6

Annexed table 20: Heavy metal accumulation on arable land from 1983 to 1994 in μ g/kg

Annexed table 21: Heavy metal accumulation on arable land from 1996 to 2007 in μ g/kg

Land	Cd [µg/kg]	Cr [µg/kg]	Cu [µg/kg]	Hg [μg/kg]	Ni [µg/kg]	Pb [μg/kg]	Zn [µg/kg]
Baden-Wuerttemberg	2.7	44.2	378.5	0.0	0.0	105.2	1433.9
Bavaria	5.3	139.4	810.6	0.5	36.1	134.9	3404.4
Berlin	12.2	40.0	167.0	0.2	0.1	99.6	785.8
Brandenburg	2.5	40.0	167.0	0.2	0.1	99.6	785.8
Bremen	5.6	127.8	799.5	0.1	1.0	145.8	2384.4
Hamburg	16.9	232.5	176.6	0.0	15.9	178.7	858.5
Hessen	3.0	66.9	342.5	0.1	0.0	118.8	1354.0
Mecklenburg-Western Pomerania	3.8	62.0	159.1	0.2	0.0	87.2	777.9
Lower Saxony	5.6	127.8	799.5	0.1	1.0	145.8	2857.1
NorthRhine- Westphalia	4.8	104.5	838.5	0.2	0.0	151.4	2744.8
Rhineland-Palatinate	2.5	55.4	215.0	0.1	0.0	101.3	950.1
Saarland	0.7	29.5	142.8	0.1	0.0	80.6	732.5
Saxony	2.8	45.1	178.4	0.3	0.0	99.7	858.0
Saxony-Anhalt	2.4	33.2	155.9	0.2	0.0	86.1	661.7
Schleswig-Holstein	8.3	188.4	704.2	0.4	23.3	178.2	2924.0
Thuringia	1.0	18.1	188.8	0.2	6.5	77.0	787.1

Appendix 6: Flowcharts for the improved algorithm stacks

A6.1: Algorithms stack "Heavy metal emissions via sewer systems, variant 2"

Areas > Impervious areas > Impervious areas that are connected to the combined sewer system (variant 2)



Areas > Impervious areas > Impervious areas that are connected to the separate sewer system (variant 2)



Areas > Impervious areas > Impervious areas that are connected to sewer system but not to a wastewater treatment plant (variant 2)





Areas > Impervious areas > Impervious areas that are not connected (variant 2)

Emissions > Heavy metal emissions via sewer systems > Emissions from combined sewer overflows (variant 2)



Emissions > Heavy metal emissions via sewer systems > Emissions from combined sewer overflows (variant 2)



Emissions > Heavy metal emissions via sewer systems > Emissions via separate sewer system (variant 2)



Emissions > Heavy metal emissions via sewer systems > Emissions from areas and inhabitants that are connected to sewer system but not to a wastewater treatment plant (variant 2)



Emissions > Heavy metal emissions via sewer systems > Emissions from areas and inhabitants that are not connected (variant 2)



Emissions > Heavy metal emissions via sewer systems > Emissions from sewer systems, total (variant 2)



A6.2: Algorithms stack "Heavy metal emissions via erosion, variant 2"

Emissions > Emissions via erosion > Soil loss on agricultural areas (variant 2)





Emissions > Emissions via loss > Soil loss on agricultural areas (variant 2)

Emissions > Emissions via loss > Soil loss on natural covered areas (variant 2)



Emissions > Emissions via erosion > Sediment delivery ratio (variant 2)



Emissions > Emissions via erosion > Enrichment ratio (variant 2)



Emissions > Heavy metal emissions via erosion > Emissions via erosion (variant 2)

