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Abstract: In Europe and world-wide, adequate water quality is one of the most eminent concerns for future generations. Diffuse pollution inputs such as agriculture, as well as local sources in terms of industrial, military and mining sites pose considerable stress on water quality. For the design of sustainable management strategies, decision makers need appropriate planning tools to assist them in the assessment, selection and optimisation of possible alternatives. Recent policies set a focus on the management of existing risks to human health and ecosystems within a tiered assessment and decision making approach giving increased emphasis to modelling. We propose a novel system dynamics modelling approach that quickly provides estimates of current and future risks originating from soil and groundwater contamination, as well as of the costs of possible risk reduction strategies. The use of analytical approaches for contaminant fate and transport modelling, as well as for risk assessment, enables a fast and effective "screening" method that is particularly qualified for large-scale applications. Results from a pilot case study in Germany illustrate the large potential of the proposed method for the preliminary assessment of management scenarios involving individual treatment technologies, as well as combinations of those.

Keywords: Risk-based land management, modelling, system dynamics, cost-effectiveness

1. INTRODUCTION

In Europe and world-wide, adequate water quality is one of the most eminent concerns for future generations. This is recognized by recent EU policies including the Water Framework Directive (WFD), the associated Groundwater Directive (GWD), and the EU communication on a Thematic Strategy for Soil Protection. Stress on water quality comes from a range of diffuse pollution inputs such as agriculture, as well as from local sources. The latter stem predominantly from industrial, military and mining activities during the past century, which have led to a vast contamination of soil, ground-water and surface waters. In many cases a complete restoration of the subsurface is both technically and economically infeasible, and remedial actions have to be focused on the management of existing risks to human health and ecosystems.

For the design of sustainable management strategies, decision makers need appropriate planning tools to assist them in the assessment, selection and optimisation of possible alternatives. Complexity and scale of the situation at these sites (in terms of contamination extent, boundary conditions/limitations, stakeholders, etc.) has led to the proposal of a tiered framework for site investigation, risk assessment and management [e.g. UK Environment Agency, 1999; ASTM, 2002]. Recent policies request an increased emphasis on modelling (e.g. EU Water Framework Directive).

A methodological gap exists particularly with respect to preliminary assessment methodologies to support early decisions on prioritising hot spots and preselection of mitigation options to streamline the further planning process. To fill this gap, we propose a novel system dynamics modelling approach utilising a multiple source-pathway-receptor concept. The model quickly provides reasonable estimates of current and future risks originating from soil and groundwater contamination, as well as of the costs of possible remediation (risk reduction) strategies for integration into the planning process.

2. THE MODEL CONCEPT

2.1 System Dynamics Approach

System dynamics (SD) is a methodology for representing complex systems and analysing their dynamic behaviour and dates to the work of Forrester [1961]. The focus of SD is to study and analyse the behaviour of complex system changes through time. The SD approach has been widely applied to water related issues, including water balance simulation [Khan et al., 2008] and world water dynamics modelling [Simonovic, 2002]. In this study, an SD model is used to assess the risks originating from contaminations in soil and groundwater, as well as possible risk mitigation options. The model describes the dynamic system of soil, water and contaminants in the subsurface and is implemented in the decision support tool (DSS) CARO-plus [McKnight & Finkel, 2008a and 2008b]. The dynamics of the system are dominated by contaminant release from long-term source zones and contaminant flux along the pathway to the receptor(s). The contaminant mass flux model, the risk assessment module and all other parts of the model framework, including technological performance and cost models for various remediation options, were developed using the off-the-shelf software platform Vensim [Ventana Systems, 2007]. The Vensim platform and other similar SD tools, e.g. STELLA [isee systems, 2007], particularly simplify the conceptualisation and set-up of models of dynamic systems. The modelling process starts with sketching the relevant variables and input constants of a model and its relationships (causal connections). The variables are then further distinguished into stocks (e.g., 'Compound Mass i at Source'; see Figure 2), flows (e.g., 'Mass Release Rate Compound i') and auxiliaries (e.g., 'Mole Fraction Compound i'). Model building is completed by specifying equations for each of the relationships and numerical quantities for input parameters. This kind of "visual" icon-based model building does not only ease model building but also facilitates the communication of the model to the stakeholders. The computation of a model run includes an automatic ordering of the network of equations and time step-wise calculation of auxiliaries, flows, and finally, stocks by integration of previously calculated flows going in and out of the particular stock.

2.2 Assessment Tool CARO-plus

The utilisation of a source-pathway-receptor (SPR) concept implies a considerable simplification of reality in the model. Mass transport is conceptualised via two SPR sequences for source zones in soil and groundwater (Figure 1). This simplification is, on the one hand, an adequate measure since the data that is available for early preliminary assessment is typically scarce and so does not allow for sophisticated modelling. On the other hand, the simplification is a necessary means to use analytical models and to establish a computationally efficient model-based assessment tool. The undisturbed natural system, as well as the effects of possible remediation options may be analysed with CARO-plus in terms of contaminant mass flux and concentration, and risk indices (carcinogenic/non-carcinogenic). Using either of these three metrics, compliance with environmental targets can be controlled at various lines or points of compliance. Following the MEPAS approach developed by Strenge & Smith [2006], the risk assessment considers various transfer paths that are specific to the particular land use type. Simulation of the effects of potential risk mitigation actions includes partial source removal and plume treatment options. To give an example of the model structure, Figure 2 sketches the major structural elements of the source release model. Contaminant release from NAPL is modelled according to Raoult's
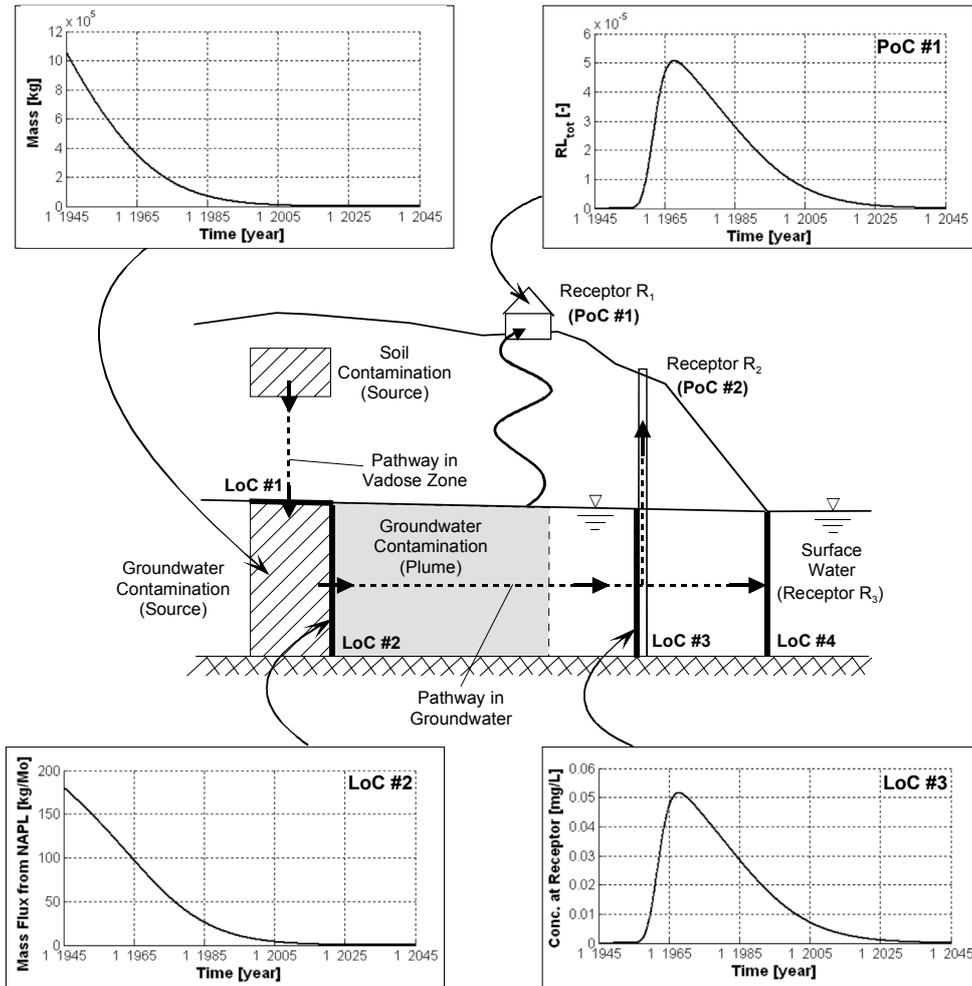
Figure 1. Source-pathway-receptor scheme with receptors R_i and options to set lines and points of compliance (LoC and PoC). Data plots show exemplary results for compound mass at source and selected LoCs or PoCs.
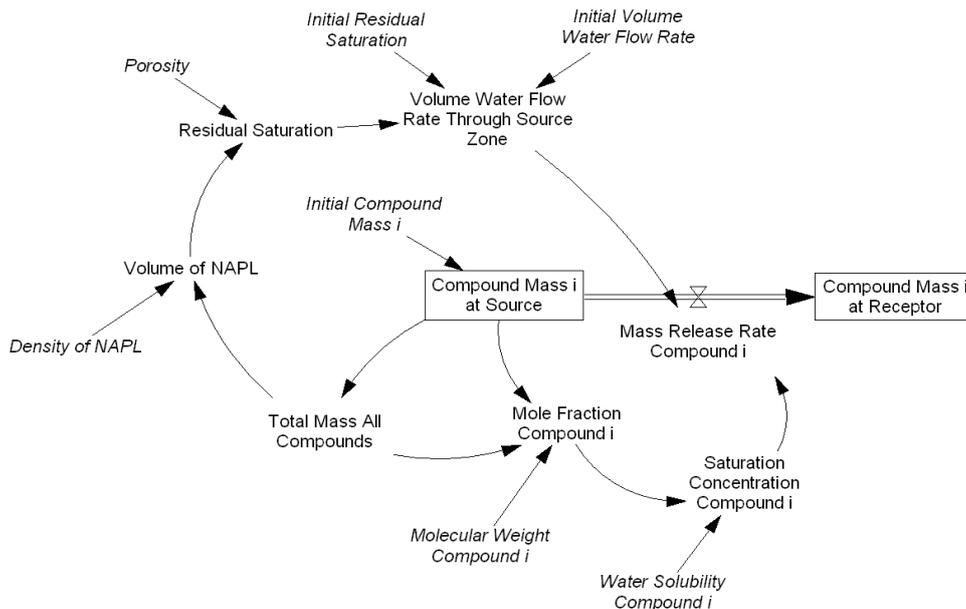

Figure 2. Major structure of contaminant release model according to Raoult's law.

law and features two feedback loops. A positive feedback loop reinforces contaminant release via a reduction of residual saturation, a negative feedback loop counteracts contaminant release via a lesser saturation concentration due to a reduced mole fraction. Several extensions to this "natural" contaminant release model quantify the effect of source remediation technologies, e.g. through an enhancement of the saturation concentration by surfactant application or thermal treatment.

2.3 Linking to Existing Models

The core module of CARO-plus, as shown in Figure 1, may be linked to an existing ordinary flow model in two ways. A straightforward option is to transfer key descriptive effective parameters of hydrogeology and source zone characteristics, as well as travel times between source zone(s) and receptor(s), from the flow model (incl. particle tracking) to CARO-plus. Figure 3 illustrates how larger areas can be structured into smaller units in the form of SPR sequences. Output data (e.g. contaminant flux, risk and cost profiles over time) may be communicated back to the flow model (or to a controlling GIS system if available). A second option is to integrate the core module as a real part of the existing model, i.e. to replicate it in each cell of the host model [e.g. Voinov et al., 1999].
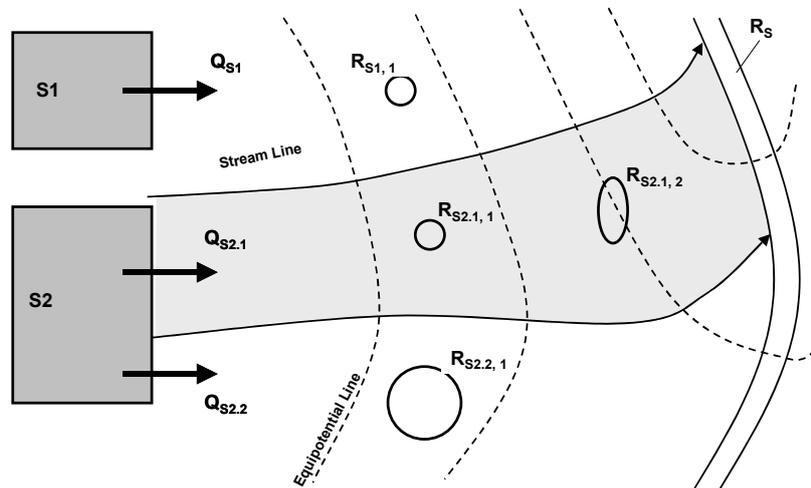

Figure 3. Structuring of a large-scale area into source-pathway-receptor sequences (one sequence shaded in grey). Concerned receptors may correspond to individual sequences (e.g. a domestic well $R_{S2.1,1}$) or to multiple sequences (e.g. surface water R_S).

3. CASE STUDY

The case study features the site of a former coking plant, located in Germany. The site exhibits an extensive contamination of both soil and groundwater, dominated by BTEX and PAH. The contaminations are mainly due to destruction during world war II. Figure 4 illustrates the situation at the site. The contamination is also vertically spread within the source zone, which is an LNAPL pool dominated by benzene, and a DNAPL pool, dominated by naphthalene. Starting from this source zone, one SPR sequence, considering the downgradient groundwater pathway to the residential area, was examined. Best guess parameter values and exposure pathways considered are listed in Table 1. The given best guess estimates are believed to best describe prevailing conditions on average or in terms of an effective parameter value. The estimates were derived based on expert knowledge rather than on statistics, since the limited available site data did not allow otherwise. This also applies to the type and parameters of the input parameter distributions used in the probabilistic analysis, which are listed in Table 2. These kind of rather rudimentary (e.g. uniform, triangular, etc) distribution assumptions are adequate if the analysis is primarily of an exploratory nature [e.g. Helton, 1993], as is the case in preliminary assessment. Note that uncertainty may also refer to performance or cost parameters of risk reduction

technologies, but were not considered in the scenarios presented here. We used Monte Carlo (MC) simulation to analyse the combined effect of variations in the inputs (Table 2). The Latin Hypercube sampling technique was selected to reduce computational time, and to produce more stable analysis outcomes than pure random sampling [Helton & Davis, 2003].
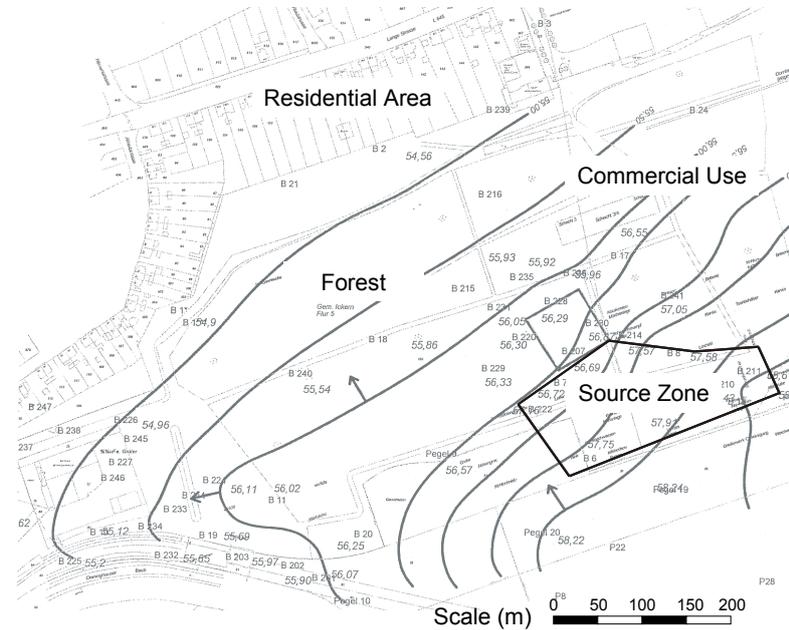

Figure 4. Map of the case study area with locations of potential receptors, labelled residential area, industrial forest and commercial use.

Table 1. Best guess values ("Estimate") of major model input parameters, considered pathways and target values for scenario "residential area".

Parameters	Estimate	Exposure pathways	Targets
Plume aquifer thickness [m]	5	Drinking water ingestion	Risk:
kf [m month^{-1}]	129.6	Leafy vegetable ingestion	$HQ_{tot} < 1$
i [-]	0.00625	Soil ingestion	$RL_{tot} < 1E-5$
NA rate GW [month^{-1}]	0.058	Inhalation of resuspended soil	Concentration:
Retardation [-]	4.3	Outdoor air inhalation	C < 0.01 mg/l
Today's average concentration in source zone [mg L^{-1}]	79	Indoor air inhalation	
Plume width receptor [m]	250		
Distance source/receptor [m]	300		

Table 2. Probabilistic model input parameters.

Parameters	Estimate	Distribution	Min	Max	Start	Peak	Stop
Plume aquifer thickness [m]	5	Uniform	4	6			
Conductivity K [m month^{-1}]	129.6	Uniform	100	160			
Hydr. Gradient i [-]	0.00625	Uniform	0.004	0.008			
NA rate GW [month^{-1}]	0.058	Triangular	0.0024	0.114	0.0024	0.058	0.114
Retardation factor R [-]	4.3	Uniform	1.8	6			
Today's average concentration in source zone [mg L^{-1}]	79	Triangular	14.32	272	14	142	670
Distance source/receptor [m]	300	uniform	200	300			

4.   RESULTS

The results from a first deterministic screening analysis based on best guess values of all model input parameters indicate that the risk peak has already passed. The predicted values of both concentration and risk level do slightly exceed the target values (Figure 5). The preliminary assessment therefore suggests to conduct further and more detailed investigations to obtain more data and information. Depending on what the new data will reveal, a second screening-level assessment or a more sophisticated modelling should then be performed. The planning of new investigation campaigns may be supported by an early assessment of risk mitigation options in order to get a first idea of feasible options. This may help to set the focus of new investigations on gaining knowledge specifically regarding the most feasible technological options. As an example, Figure 5 shows the effects we may expect from e.g. a pump-and-treat measure. Here, an operation time of 21 years (from 1/2000 until 12/2020) is assumed. Since the pump-and-treat system is hypothetically considered to be a protection measure, the system's location is set to 50 m upgradient of the receptor. As an addition to the deterministic analysis, risk and risk mitigation options were also assessed using a probabilistic method, as described above. Some example results are shown in Figure 6 for the "natural" system (no action scenario) as well as with respect to the effects of the abovementioned pump-and-treat measure.
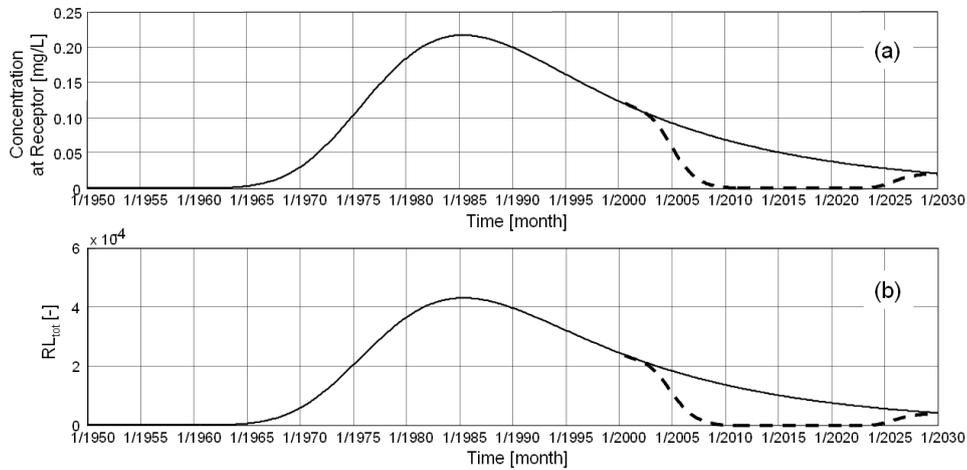
Figure 5. Deterministic results for receptor "residential area": (a) concentration in groundwater at the receptor, (b) risk level at the receptor. Dashed lines indicate the effect of a pump-and-treat measure between 1/2000 and 12/2020.
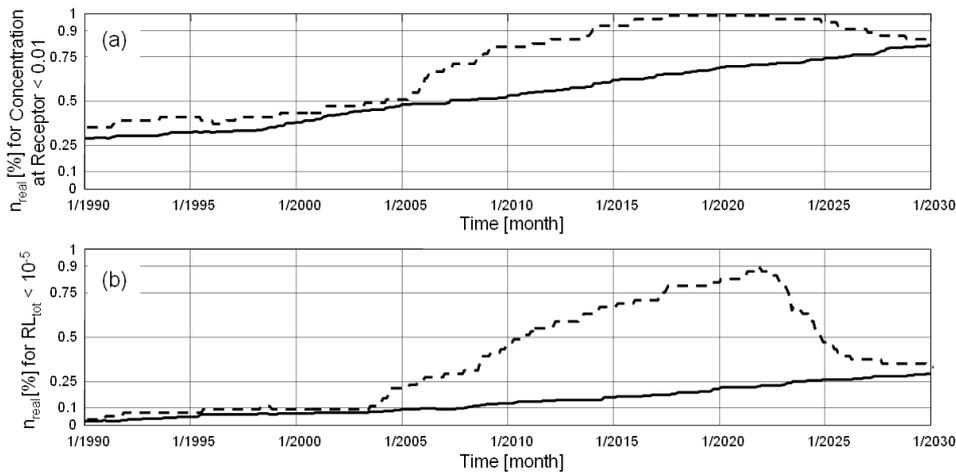
Figure 6. Probabilistic results for receptor "residential area": (a) probability to reach the groundwater concentration target at the receptor, (b) probability to reach the target level of risk at the receptor. Dashed lines indicate the effect of a pump-and-treat measure between 1/2000 and 12/2020.

5. CONCLUSIONS

It is has been shown for a pilot case study in Germany that there is a large potential of preliminary assessment for contaminated land management. The presented assessment tool CARO-plus is capable of analysing the existing and future situation at a site with respect to risks, as well as regarding the effects of possible risk mitigation options in terms of contaminant mass flux, concentration and risk indices. Costs of mitigation options are also estimated, but haven't been shown here. A special emphasis is given to the uncertainty of predictions using Monte Carlo simulations.

ACKNOWLEDGEMENTS

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