Development of an Integrated Decision Support System for Brownfield Restoration

Dissertation
der Mathematisch-Naturwissenschaftlichen Fakultät
der Eberhard Karls Universität Tübingen
zur Erlangung des Grades eines
Doktors der Naturwissenschaften
(Dr. rer. nat.)

vorgelegt von
Maximilian Morio
aus Annweiler am Trifels

Tübingen
2012

Tag der mündlichen Qualifikation:	12.03.2012
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Betrachte immer die helle Seite der Dinge!
Und wenn sie keine haben, dann reibe die Dunkle, bis sie glänzt.

Norman Vincent Peale

Acknowledgments

I would like to thank Dr. Michael Finkel, who as supervisor provided me the possibilty to work on this topic. The fruitful discussions in and outside office are invaluable. I kindly thank Prof. Peter Grathwohl and Dr. Michael Finkel for examining this thesis.

I also like to thank the colleques and alumni of the D-site working group and all others who gave support and endured me for the last couple of years: Sebastian Schädler, Peter Bayer, Ursula McKnight, Andreas Justen, Fernando Mazo D'Affonseca, Uli Mayer and Claudius Bürger. The numerous Coffee-break discussions and after office beers gave me insights to different ways of thinking about science, nature, and the earth.

Thanks also go to Ksenia Voronina and Noah Stern for language editing of the manuscripts.

Finally, I'd like to thank Sylvia without whom I had not made it so far.

This work was funded by the German Ministry of Education and Research (BMBF) under grant 0330757C as a part of the Refina priority program and additional funding Helmholtz Centre for Environmental Research – UFZ in Leipzig (contracts no. 4500029698 & 4500050981). Additional funding has been provided by TASK - Centre of Competence and the EU-research project TIMBRE (Project no. 265364, FP7-ENV-2010).

Abstract

The re-use of underused or abandoned contaminated land, so-called brownfields, is increasingly seen as an important means for the reduction of land consumption. But brownfield redevelopment often fails during early project stages due to complex decisions that stakeholder with potentially different interest have to make, based on typically very scarce data. Seeking sustainable re-use solutions, many existing decision support systems are not appropriate as they focus mainly on environmental or economic aspects, and neglect sustainability issues. To fill this gap, this thesis presents a framework for spatially explicit integrated planning and assessment of brownfield redevelopment options. Aiming to support efficient and sustainable revitalization and communication between stakeholders, the presented assessment framework integrates three pinnacles of brownfield revitalization: (i) the identification of required subsurface remediation and associated site preparation costs, (ii) market-oriented economic appraisal, and (iii) the expected contribution of planned future land use to sustainable urban and regional development. For the assessment, focus is set on the early stage of the brownfield redevelopment process, which is characterized by limited data availability and by flexibility in land use planning and scope of development.

A convenient starting point for the planning of different land uses and respective remediation measures is the early identification of focal areas with respect to groundwater contamination. Therefore, a flow guided interpolation method (FGI) was developed, which has been tailored to the type, scale and information basis that are typically available at the early stages of revitalization projects at contaminated sites. As a second step, a spatially explicit procedure is introduced, which compares the previously characterized subsurface contamination to land-use specific requirements regarding subsurface quality in order to identify remedial measures that are required for the implementation of specific re-use scenarios. This GIS-based conflict analysis is coupled to spatial remediation cost estimation models. A market oriented value appraisal approach, which includes value reducing factors like stigma effects caused by former use, present or suspected contamination, and liability completes the economical assessment. Furthermore, an indicator based sustainability assessment methodology is integrated into this assessment framework by utilizing spatial metrics to assess the contribution of a brownfield re-use scenario to sustainable development in the region.

To further improve planning and decision making, a multi-criteria genetic algorithm is adapted to the assessment framework aiming to find optimal mixed land-use configurations with respect to one or more assessment criteria and given constraints on the composition of land-use classes. The framework is applied to a case study at a former military site near Potsdam, Germany. Emphasis is given on the trade-off between economic goals and the need for sustainable development in the regional context of the brownfield site. Results from the case study application indicate that the integrated assessment provides help in the identification of land use options beneficial in both a sustainable and an economical sense. Although brownfield redevelopment is shown to be not automatically in line with sustainable regional development, it can be demonstrated that additional contributions to sustainability are not intrinsically tied to increased costs.

The methods presented in this thesis also are embedded into a user-friendly computer based, integrated decision support system.

Keywords: brownfields revitalization, megasite, market value, contamination, groundwater, remediation costs, sustainability, optimization, genetic algorithms, GIS

Kurzfassung

Ehemals genutzte, brach liegende, kontaminierte Flächen werden zunehmend zu einem Problem angesichts des weltweit zunehmendem Flächenverbrauchs. Die nachhaltige Revitalisierung solcher Brachflächen, sogenannter 'brownfields', kann daher einen wertvollen Beitrag leisten, den fortschreitenden Flächenverbrauch zu verringern. Brachflächenrevitalisierung scheitert jedoch häufig schon in frühen Entwicklungsphase aufgrund der komplexen Entscheidungen, welche von Akteuren mit potentiell unterschiedlichen Sichtweisen und Interessen zu fällen sind. Entscheidungsunterstützungssysteme können bei der Suche nach Nachnutzungsszenarien helfen, die meisten existierenden Systeme sind hierfür jedoch nicht umfassend geeignet, da sie in der Regel auf die Bewertung entweder ökologischer oder ökonomischer Aspekte abzielen und Fragen der nachhaltigen Entwicklung vernachlässigen. Um eine effiziente und nachhaltige Brachflächenrevitalisierung mit dem Ziel einer verbesserten Kommunikation und Entscheidungsfindung der beteiligen Akteure zu fördern, präsentiert die vorliegende Arbeit ein Bewertungs- und Entscheidungsunterstützungsmodell welches drei Kernelemente der Revitalisierung berücksichtigt: (i) die Ermittlung von Sanierungs- und Flächenaufbereitungskosten, (ii) eine marktorientierte Grundstückswertermittlung und (iii) der Beitrag einer geplanten Nachnutzungsvariante zur nachhaltigen Entwicklung in der Region. Das Bewertungssystem zielt auf eine frühe Planungsphase ab, welche durch geringe Informationsdichte bezüglich der Standortbeschaffenheit gekennzeichnet ist, andererseits aber noch Spielräume hinsichtlich möglicher Nachnutzungen bietet.

Die Komplexität und der Umfang von Grundwasserverunreinigung großer Brachflächen bedingt eine Priorisierung bestehender Risiken und Probleme, um weitere Entscheidungen und Maßnahmen bezüglich Standortuntersuchung und Sanierung fokussieren zu können. Es besteht insbesondere Bedarf an Methoden zum Umgang mit häufig spärlich vorhandenen Schadstoffkonzentrationsdaten. Daher wurde eine Methode entwickelt, welche Informationen über Grundwasserströmung berücksichtigt um die Schadstoffverteilung im Grundwasser bei geringer Datenlage zu interpolieren. Zur Ermittlung des Sanierungsbedarfs für die Umsetzung einer Nachnutzungsvision wird eine GIS-basierte Konfliktanalyse vorgestellt, welche das bestehende Schadstoffinventar mit den Anforderungen zukünftiger Nutzungsarten an die Boden- und Grundwasserqualität abgleicht und den Sanierungsbedarf visualisiert. Die Konfliktanalyse ist mit räumlichen Modellen zur Schätzung der Sanierungskosten verknüpft. Die ökonomische Bewertung wird durch ein marktorientiertes Wertermittlungsmodul vervollständigt, welches Wert mindernde Faktoren, wie Stigmaeffekte durch vorherige Nutzung oder befürchtete Restrisiken, und Risikoüberwälzbarkeit, berücksichtigt. Die Nachhaltigkeit einer Nutzungsvariante wird mittels eines indikatorenbasiertes Bewertungssystems bewertet, welches in das Bewertungssystem mittels räumlich expliziter Metriken eingebunden wurde.

Zur weiteren Unterstützung der Nachnutzungsplanung wurde ein multikriterielles Optimierungssystem, basierend auf genetischen Algorithmen, weiterentwickelt und den Bedürfnissen der Brachflächenbewertung angepasst. Die Optimierung generiert bestmögliche Nachnutzungskonfigurationen in Bezug auf ein oder mehrere Kriterien und gegebenen Randbedingungen bezüglich der Flächenanteile eines

Nutzungstyps. Das Bewertungssystem wurde an einem Modellstandort, einer ehemals militärisch genutzten Fläche bei Potsdam, nahe Berlin, angewandt. Im Vordergrund stand die Abwägung ökonomischer Ziele und dem Ziel der nachhaltigen Entwicklung. Die Ergebnisse zeigen, dass eine integrierte Brachflächenbewertung das Auffinden sowohl ökonomisch attraktiver als auch nachhaltiger Nachnutzungsvarianten effektiv unterstützen kann. Es konnte zudem aufgezeigt werden, dass bei einer Nachnutzung der Beitrag zur nachhaltigen Entwicklung in der Region nicht zwangsläufig mit höheren Entwicklungskosten einhergeht.

Die in dieser Arbeit vorgestellten Methoden wurden in ein integriertes, computerbasiertes Entscheidungshilfesystem integriert.

Schlagwörter: Brachflächenrevitalisierung, Megasite, Flächenbewertung, Kontamination, Grundwasser, Sanierungskosten, Nachhaltigkeit, Optimierung, Genetische Algorithmen, GIS

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Chapter 1

Introduction

Uncontaminated and undeveloped land has become a scarce resource in the densely populated and highly industrialized parts of the world. Due to this fact, brownfields, variably defined as abandoned, underutilized, and contaminated land [e.g. Alker et al., 2000, U.S.EPA, 2002, Dasgupta and Tam, 2009], are gaining more attention, especially in urban and peri-urban regions. Restoring brownfields (BF) to developable land in terms of establishing economically favorable and sustainable re-use options, can provide a valuable contribution to reduction of land consumption [e.g. Umweltbundesamt, 2005, REFINA, 2007, also see Figure 1.1]. For example, one of the major priorities of the German sustainability strategy is the reduction of land consumption for human settlements and transport, from ca. 80 ha/day in 2010 to 30 ha/day by 2020 (cf. Figure 1.2). This is seen as one of the major challenges for Germany to meet its sustainable development goals [German Federal Government, 2011]. While large amounts of green land are being consumed, it should be noted that at the same time the amount of land being abandoned or turning fallow in the cities and communities increases about 10 ha/day (for the years 1997–2000) [Kälberer et al., 2005].

Several problems may hinder the re-use of BF and therefore have to be addressed. Environmental hazards may exist that cause a threat to ecological and human health. Depending on the intended future use, in order to mitigate environmental threats, different remediation measures may be needed for site revitalization. Therefore, the extent of required remediation has to be identified and associated costs must be determined. Suspected contamination, whether present or not, can cause an obstruction to investors because of stigma effects or risks, which are difficult to predict [Mundy, 1992]. On the other hand, economical benefits of a particular re-use scenario can be highlighted by monetary assessment. Therefore, a market value appraisal of BF re-use scenarios has to include all factors that may affect the mercantile value [Syms and Weber, 2003]. Future land-use scenarios also have to be assessed regarding their influence on the sustainable development within the regional context of the site. Within a BF revitalization process, different stakeholders are affected, e.g. investors, rural communities, neighbors, etc., with each of them having different goals and perspectives [e.g. Altherr et al., 2007, Pediaditi et al.,

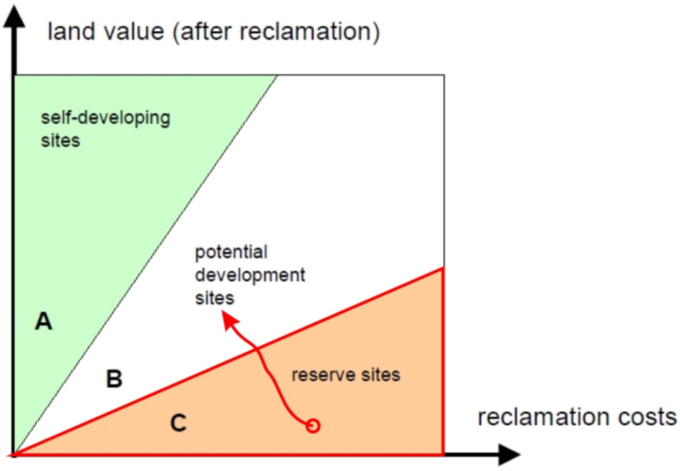


Figure 1.1: Cabernet's ABC model [changed acc. to CABERNET, 2005].

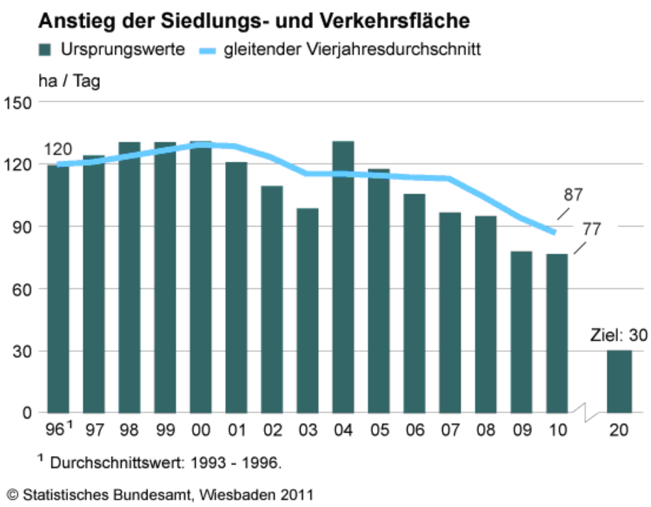


Figure 1.2: Land consumption in Germany (ha/day) in the years 1996 to 2010. Blue line indicates four-year moving average (source: Federal Statistical Office, Wiesbaden).

2010].

Being aware of the before mentioned problems, information about the BF site, consequences of site re-use, and possible re-use alternatives have to be assessed and presented in a transparent manner to enable a stakeholder-based decision process that is accepted by the public.

Considering the issues above complex decision making, stakeholder participation and communication, site investigation and remediation measures are all required at different stages of the revitalization process. Several proposed approaches fulfill the demands of BF revitalization projects in parts like multi-criteria decision making, smart growth concepts, startup plan [e.g. O'Reilly and Brink, 2006, Carlon et al., 2004, Semenzin et al., 2007a, Sorvari and Seppälä, 2010, Mack et al., 2004, Greenberg et al., 2001, Gabriel et al., 2006, Preuß et al., 2006]. In general, decision support systems (DSS) are considered useful tools for informing stakeholders and supporting the decision making process. Decision support systems are interactive computer software systems, which support human decision makers in the management of different tasks. This contrasts with expert systems, that make decisions based on expert knowledge and embedded reasoning mechanisms [e.g. Turban and Watkins, 1986]. An overview on the history of DSS is given in Power [2007]. With respect to BF revitalization, several (spatial) DSS were developed [e.g. Schädler et al., 2011b, Carlon et al., 2007b, Chen et al., 2009, Lesage et al., 2007], but there is still a lack of decision support for integrated, holistic assessment of BF re-use scenarios. Relevant omissions from previously developed DSS include integrated environmental, and economic assessment as well as a sustainability evaluation of re-use options [e.g. Agostini et al., 2007, Agostini and Vega, 2009, Rizzoli et al., 2008, also see Figure 1.3].

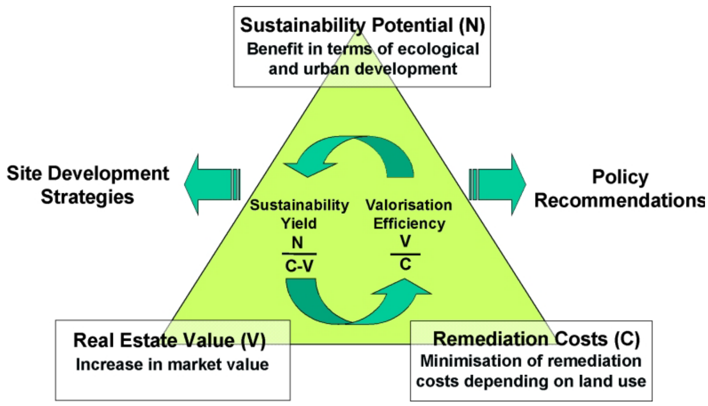


Figure 1.3: Assessment aspects involved with brownfield redevelopment. Fractions inside triangle symbolize trade off of perspectives [modified acc. to SINBRA, 2009].

The motivation of the presented thesis is based on two main objectives, summarized in the following two subsections below.

1.1 Assessment methods for brownfield revitalization

The first objective was to develop methods to gather and process information that allows for the assessment of BF re-use scenarios.

Remediation measures that might be needed to implement a re-use scenario require sufficient knowledge about the magnitude and spatial distribution of subsurface contaminations. Several strategies for the acquisition of contaminant data have been proposed [e.g. Liedl and Teutsch, 1998, O'Reilly and Brink, 2006, Taylor and Ramsey, 2006, Rein et al., 2011]. The methods for estimating contaminant distributions range from experienced-based practitioners best guess, over interpolation and geostatistical modeling [e.g. Bárdossy and Li, 2008, Shlomi and Michalak, 2007, Michalski and Peres, 2005] to analytical [e.g. Ahlfeld and Pinder, 1992, Bayer-Raich et al., 2009a, Liedl et al., 2011] and numerical contaminant transport modeling [D'Affonseca et al., 2008, Wycisk et al., 2009, Miles et al., 2008]. These methods have different demands on the amount and spatial density of physical samples and the information collected on the (hydro-) geological parameters at a site. Especially at early stages of BF assessment, it is a common problem that site data regarding contamination and the affected media (aquifer, unsaturated soil) are scarce. Hence, classical geostatistical models and numerical transport models beyond a conceptual stage are not applicable. Thus, methods are needed to cope with scarce input data about subsurface contamination. In this work a new GIS-based methodology is proposed, which enables to model a groundwater plume from an assumed source zone by amending physical samples with flow field information and auxiliary sampling points in order to enable a segment wise interpolation. The method is called 'Flow Guided Interpolation' (FGI) and is explained in detail in Chapter 3 of this thesis.

The dimensions and efforts for required remediation of a BF depends on a site's surroundings and the actual or planned use of the site. Different land-use types have differing demands regarding the subsurface quality, i.e. the maximum acceptable level of contamination. Ideally these threshold values are specific for each contaminant, compartment and prospected land-use type and its receptors, which are potentially exposed to contaminants via specific pathways. The possible determination of threshold values ranges from site unspecific regulatory values to maximum acceptable concentrations calculated specifically by ecological and/or human health risk-assessment. The determination of remediation target values can be made on basis of e.g. (i) guidance and intervention values ('Prüfwerte / Maßnahmenwerte' in Germany, cf. to [BBodSchV, 1999]), which are land-use specific in parts, or preliminary remediation goals ['PRG', see e.g. ASTM, 2002, Shan and Javandel, 2005], (ii) a site- and use-specific risk assessment that depends on potential exposition of receptors to hazardous substances via relevant pathways [e.g. Strenge and Smith, 2006, McKnight et al., 2010], (iii) estimated mass fluxes in groundwater and contaminant plume characteristics (mass discharge from the site over a control plane and comparison to acceptable mass fluxes or evidence of plume stationarity and absence of threats to potential receptors) [e.g. Leschik et al., 2009, Annable et al., 2005, Goltz et al., 2009], or (iv) negotiation between obliged parties (e.g. strict liability tortfeasors ('Zustandstörer'), and parties obliged to undertake remediation ('Sanierungspflichtige')) and appropriate authorities (in the case of Germany, usually the 'Lower soil protection agency').

To structure and formalize the further evaluation of re-use plans this thesis introduces a scenario–layout concept to assist the decision making process (see Figure 1.4). A scenario defines the composition of a re-use plan including the definition of land-use types and their area ratios, whereas the layout describes the spatial configuration of the land-use types on the site. If a site offers a certain degree of freedom in planning due to its given size there may exist many different layouts of one scenario to choose from. The layouts of the re-use scenario under evaluation have to be translated into a set of spatially explicit, contaminant and site specific threshold values. The need for use-specific remediation measures then can be determined by comparing the distribution of contaminants with these threshold values. In order to carry out this comparison automatically based on digital data, in this thesis the so called 'conflict analysis' is presented.

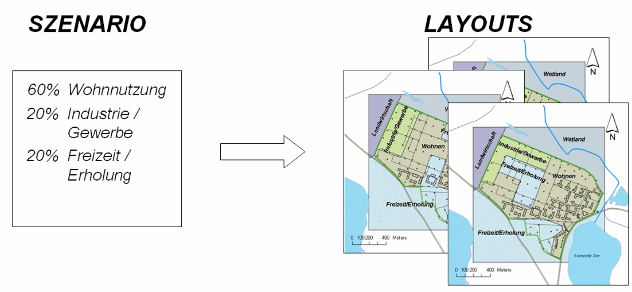


Figure 1.4: Scenario – layout concept for future brownfield use.

The newly developed conflict analysis procedure compares the contaminant distribution by contaminant target value maps specific to the land-use layout yielding exceedance maps for each contaminant and compartment, respectively. The processed data is converted to standard raster grid format (ESRI ASCII grids) in order to ease the spatial processing, where the extent and discretization of the grids is adapted to the site scale. The geoprocessing is automated and can be conducted whether using commercial GIS or with open source GIS (cf. to Sections A.4 and A.5 in the Appendix for references to further information). In addition, conducting a conflict analysis for uniform land-use yields information on where a certain land use could be allocated on the site without causing the need for remedial action. The conflict analysis procedure also delivers information for spatially explicit and land-use specific remediation cost models (cf. to Chapter 2 and Schädler et al. [2009, 2012]).

Remediation costs largely depend on the type, spatial and temporal scale of contamination and also on the selected measures to remove, reduce, or contain the contamination on the site. Different levels of detail with respect to knowledge of contamination at a site demand for different cost estimation models. Empirical models [e.g. Bonnenberg et al., 1992] allow for estimating remediation costs on the basis of contaminated volume, mean unit costs and a set of difficulty factors reflecting type, extent and severity of contamination. Semi-empirical models add the consideration of physico-chemical processes or type of remediation measure to be implemented [e.g. ITVA, 2003, Bayer et al., 2005]. More detailed approaches deliver a listing of cost-relevant positions, services and associated standard reference price needed

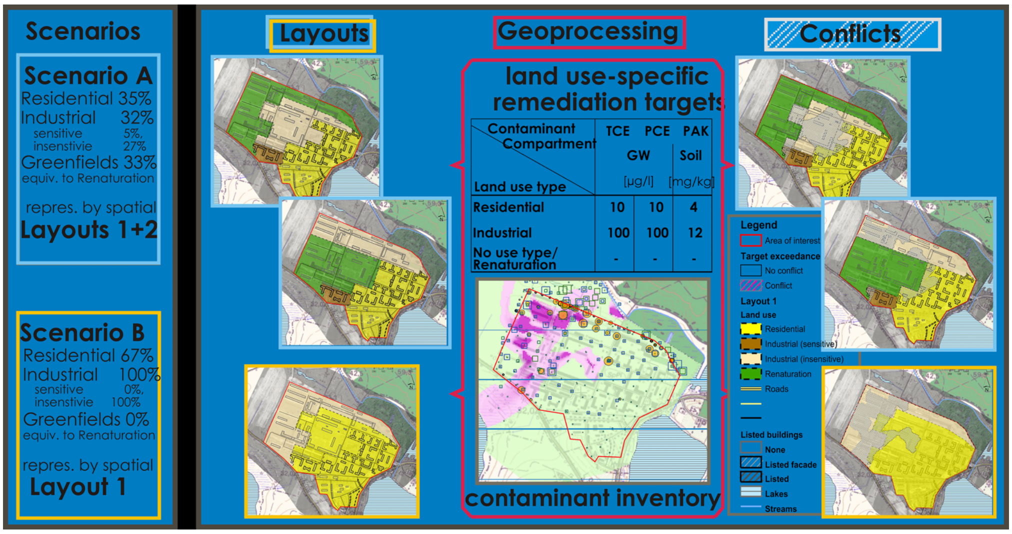


Figure 1.5: Scheme of conflict analysis for identifying remediation needs.

to implement and conduct remediation and clean up measures [e.g. Bracke et al., 2005]. When using conflict analysis as the basis for estimating the price of a remediation plan, cost models with different level of detail and different demands for input data were extended in the context of the presented thesis in order to process spatial input data and deliver land-use specific cost estimates [e.g. Schädler et al., 2010a, 2011b, 2012].

A further important economical aspect is the market oriented valuation of the BF site's re-use scenario. The market value of a BF is usually mitigated by contamination, whether known or suspected, therefore stigmatized by the previous use of the site [Patchin, 1988]. In a site owner's or investor's perspective, clarification on land value of a BF is needed to show risks or on the other hand, raise incentives to invest in the site [Greenberg et al., 2001]. The actual land value of a BF site is controlled by the determination in terms of allowed future use [e.g. Großmann et al., 1996, Sächsiches Landesamt für Umwelt, Landwirtschaft und Geologie, 2001, Finkel et al., 2010]. The value calculation is based on so called reference values that depend on the location and use-types of the site. The site's preparation costs and other possible value reducing factors like previous use, stigma, demand, etc., yielding the remaining land value of the site are subtracted from these reference values. A methodology for a traceable, transparent market value calculation including market value reduction based on expert information was proposed by Bartke and Schwarze [2009a,b].

The implementation of remediation costing and market value assessment methods into an integrated decision support approach is introduced in Chapter 2 and Chapter 4. The integration of these methods into a land-use allocation optimization approach is demonstrated in Chapter 6.

Besides searching for economically attractive and feasible re-use options for BF, the sustainable development of urban and peri-urban areas in the regional context gained stakeholders' and researchers' attention over the last decades [Bettencourt and Kaur, 2011]. While the term sustainability originates from forestry regulations, the Club of Rome and the Brundtland commission extended the term sustainability to include the scope of mankind [Meadows et al., 1972], including societal, ecological and economical aspects of development [e.g. U.N., 1987, Potschin and Haines-Young, 2006]. Applied to the context of BF management and revitalization, sustainability focuses on regional development and is evaluated by site-specific sets of indicators [e.g. Alker and McDonald, 2003, Ulmer et al., 2007, Hartmuth et al., 2008, Müller and Rohr-Zänker, 2009]. Many of the indicator metrics used in those evaluation approaches have a spatial component. This allows for a natural transition into a spatially explicit indicator evaluation system to support land-use decision making. The addition of a explicit evaluation component to the concept proposed by Müller and Rohr-Zänker [2009] is presented in Schädler et al. [2011b] (see also Chapter 5). This spatial concept proposes a new method to expand the sustainability definition into spatially explicit, quantitative evaluation functions. This allows the sustainability indicator evaluation to be applied within the objective function of an optimization algorithm. This way sustainability evaluation yields a score for a future land-use configuration and can be traded off against economical aspects in an integrated decision support framework (see Chapter 6).

1.2 Finding optimal re-use plans using an integrated assessment scheme

The second objective was to embed the methods mentioned in the section above into a BF DSS with the goal of following an integrated assessment approach. The creation of a suitable DSS must integrate approaches and models that stem from different scientific disciplines [e.g. Parker et al., 2002, Rizzoli et al., 2008, Ascough et al., 2008] while simultaneously assuring that stakeholders with different expertise can participate in the assessment process [Kok and Verburg, 2007, Sterk et al., 2011].

The proposed integrated BF assessment scheme can be divided into several steps, where the iterative and participative nature of the decision making takes place at several points in the sequence (see Figure 1.6). The process includes the different assessment methods introduced in the previous section.

At large BF, where re-use scenarios allow for a multitude of mixed-use layout options, establishing optimal re-use plans can be cumbersome, if not impossible, if all relevant assessment criteria have to be considered. The development of a novel model-optimization framework aims to aid the identification of optimal re-use scenarios from an integrated perspective. Within the context of the assessment scheme outlined in Figure 1.6, an existing generic spatial optimization framework [Holzkämper et al., 2006], based on genetic algorithms [Wall, 1996], was adapted and extended to serve the need of BF redevelopment. The newly developed system

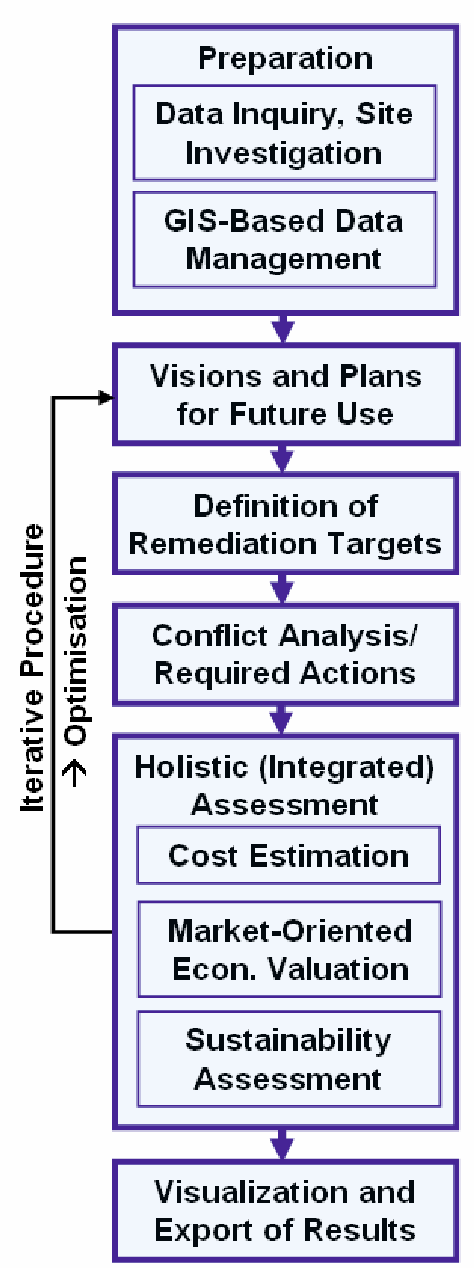


Figure 1.6: Steps of planning and integrated assessment for brownfield reuse projects, after Morio et al. [2011].

- Data acquisition and preparation: GIS-based data management is mandatory for spatial analysis. Demand for site data may change (increase) and be refined during a redevelopment process.
- Generation of land-use scenarios and layouts: Ideas for re-use scenarios need to be developed, ideally in consultation with all involved stakeholders taking into account existing boundary conditions like infrastructure, listed buildings, land-use in the vicinity of the site, planning regulations. Stakeholder may iterate and optimize the scenario-layout generation process on basis of results from previous scenario assessments.
- Use-oriented remediation objectives: Need to be determined for each land-use type that is assessed.
- Conflict analysis: Remediation needs are identified by overlaying land-use maps, related remediation objectives and existing soil and groundwater contamination within a GIS.
- Remediation and site preparation costs are determined by spatial models selected according to the availability and level of detail of input data.
- Sustainability of re-use scenarios: Sustainability metrics must be identified and adapted to the given situation. Scenarios can be compared to each other in terms of sustainability based on these indicator metrics.
- Market oriented valuation: The market value for each scenario and its layouts on the basis of reference land value and of mercantile value reduction for risks and other factors perceived in the market.
- Export/Visualization of results: The results of the integrated assessment should be presented in a clear and easy accessible way including models and underlying assumptions used for assessment.

starts with a re-use scenario as the initial input. Additional input is given by constraints such as the range of allowed deviation from the initial area ratio of land-use types, and the weighing of assessment criteria within the multi-criteria objective function.

For optimizing the re-use scenario towards a goal, which contains multiple criteria, it is possible to decide between different trade-off options. Within the optimization problem, the exploration of the search space allows for the identification of a Pareto front, where solutions (here: re-use layouts) are located on that front, which cannot be dominated by other solutions with respect to the given goals. Such Pareto optimality can be identified by different methods like random sampling, weighting, distance, or constrained trade-off methods [cf. to e.g. Zitzler, 1999]. In contrast to these Pareto-based methods, which can become quite computationally demanding, the weighted sum approach can be utilized. Up to this point, all multi-objective models are based on either Pareto based methods or weighted sum analysis [Cao et al., 2012].

The genetic algorithm approach is based on the idea of biological evolution [for details see e.g. Goldberg, 1989]. By utilizing stochasticity, a set of individuals (solutions) is generated on the basis of an initial map, which is converted to a chromosome representation based on its given planning unit scheme. This set of individuals (population) is evaluated by an objective function, where the better portion of the population is selected to build up a new, improved generation. New offspring individuals are generated on basis of this selection, crossover (pairwise exchange of chromosome parts), and mutation (stochastic change of genes in a chromosome). The evolution propagates over a given number of generations or until a stopping criterion based upon convergence (e.g. a minimum relative change of the individual's fitness over a certain number of generations) is fulfilled.

The weighted sum aggregate fitness score consists of single criterion evaluation functions, which are summed up to a normalized, weighted linear score. The single criteria are:

- Maximization of market value: The most favorable layout is searched on basis of land-use type and location specific market-value evaluation maps.
- Minimization of remediation costs: Land-use specific cost evaluation maps are used to find configurations to minimize remediation expenditures.
- Maximizing the suitability for sustainable development: A set of indicators is evaluated by spatial metrics functions and stakeholder input. The result is an aggregated sustainability score.

The optimization framework and possible trade-off of criteria for finding beneficial re-use scenarios is explained in detail in Chapter 6. This framework is also embedded in a user-friendly BF DSS, the megasite management toolsuite (MMT, for details cf. to Appendix A.4.2).

By optimizing the spatial configuration of multi land-use scenarios and producing several re-use alternatives (layouts) with respect to the possibly contradicting goals of maximizing economic benefit and assuring suitability of a re-use scenario to sustainable development, stakeholder discussion can be fostered and compromises can be made.

1.3 Thesis outline

The remainder of this thesis is organized in Chapters as follows:

Chapter 2 introduces the challenge of supporting decision making for BF revitalization by an integrated assessment that includes economics and sustainability, which are illustrated by means of general assessments at a demonstration site.

In Chapter 3, the above described FGI method to represent groundwater contaminant concentration distribution based on scarce data is introduced. The method particularly intends to support the redevelopment process at early project stages. The applicability of this method and the consequences within the context of a BF redevelopment project is demonstrated in Chapter 4.

Chapter 5 gives a detailed algorithmic formulation of the assessment criteria and their aggregation into an integrated assessment scheme. For a number of re-use scenarios it is illustrated how economic evaluation results can be balanced with a sustainability indicator assessment results.

Chapter 6 presents the development and implementation of a heuristic optimization framework to find near-optimal land-use configurations for BF re-use where trade–off of economical and sustainability factors occurs.

Finally, Chapter 7 summarizes and concludes the work presented and Appendix A gives an overview of project reports that document the implementation of scientific methods into a decision support tool.

Chapter 2

Improving mega-site revitalisation strategies by trading off benefits from future land use and clean-up costs[1]

Abstract Derelict land, where former industrial, military and mining activities have often led to vast contaminations of soil, groundwater and surface waters, is a problem in many urban areas in Europe. Facing competition with Greenfield development, the re-use of these areas is only achievable if management options optimally trade off the conflicting goals of protecting human health and the environment, of microeconomic needs and of regional development. To assist decision-making in finding optimised revitalisation strategies, we propose a GIS- and model-based planning and assessment tool that links land-use planning, risk-assessment, cost and benefit evaluation. The paper describes the key elements of the tool's concept by means of a demonstration project at a former military site in Potsdam near Berlin, Germany.

Key words mega-sites; soil and groundwater contamination; revitalization; remediation; land use planning; cost-efficiency; GIS

2.1 Introduction

In Europe and world-wide, a large number of regions exist where industrial, military and mining activities during the past century have led to vast contaminations of soil, groundwater and surface waters. These so-called mega-sites may severely impact human health and the environment, and hamper the economic revival in corresponding areas [EEA, 2000, EC, 2006]. Mega-site management therefore needs to address the protection of human health and the environment, as well as the economic urban and regional development, targeting both a high sustainability yield and an efficient valorisation. To support decision makers in finding viable revitalisation strategies, there is a demand for tools that help to assess and communicate the

[1]reproduced from: Morio, M., Finkel, M., Schädler, S., Hartmuth, G. and H. Rügner (2008): Improving mega-site revitalisation strategies by trading off benefits from future land use and clean-up costs. Groundwater Quality: Securing Groundwater Quality in Urban and In-dustrial Environments.- IAHS Publ. no. 324, 555-562.

pros and cons of existing plans of site clean-up and future land use, both in terms of market and non-market benefits and costs. In this paper, we describe the concept of the GIS- and model-based planning and assessment tool that is currently being developed within the German research priority programs REFINA [Hauschild et al., 2006] and SAFIRA II [Rügner et al., 2007]. The tool shall support the process of finding optimal revitalisation strategies by trading off minimized clean-up costs and benefits from future land use. The results of a demonstration project at a former military site in Potsdam near Berlin, Germany, are used to illustrate the conceptual approach of the tool.

2.2 The conceptual approach

The overall intention is to support an iterative enhancement of the revitalisation plan for a given site during the planning process. The initial land use plan portrays a scenario on how the site may be used in future. Such a scenario may result, e.g. from considerations of the local authority's planning board or from an investor's development plan. The scenario defines a particular land use allocation for the site. In general, it will be comprised of different land use types, that is, a heterogeneous (non-uniform) use of the site is planned. The quotas of the individual land use types are considered as existing demand for additional areas of the respective use type. The distributions of these quotas form the basic characteristics of a scenario. Since these quotas may be achieved in different ways, we further distinguish between scenario layout, which describe how the land use quotas are specifically arranged in space. Thus, one land use scenario may comprise many different layouts.

In a first step, the monetary benefits and sustainability of the given land use scenario are evaluated. Clean-up and site preparation costs are then estimated for the proposed specific scenario layout. This involves the: (i) specification of the clean-up effort required to solve existing conflicts between the planned land use allocation and present contaminations in soil and groundwater; and (ii) application of an adequate cost model. On the layout level, alternative spatial land-use allocations may be examined and proposed to minimize conflict areas and required clean-up expenses.

Finally, the monetary and non-monetary assessment results for the examined scenario and its layouts are analysed and discussed among the stakeholders. This may result in a revised land use scenario, which will then be evaluated within the next iteration of the planning process.

All steps and sequences of the process described above are supported by corresponding software modules that integrate diverse methods and models (e.g. cost estimation models, sustainability assessment methods, GIS-based data management).

2.3 Site description

The former military site "Kaserne Krampnitz" is located in the outskirts of Potsdam near Berlin, covering an area of about 1.2 km^2. It was built up in 1937 as a motorized cavalry school. From 1945 until 1992 the site was used by the Russian armed forces. The site is partly covered with building ruins (to be deconstructed) as well as listed, historical buildings (see Fig. 2.1). Due to the utilisation as barracks encompassing garages, workshops, storage tanks, dry cleaning facilities, etc. there existed probable cause to assume subsurface contaminations at the site. Various site investigation activities have been carried out [Schädler et al., 2008]. The geological situation at the site is governed by periglacial depositions forming an aquifer mainly consisting of a heterogeneous composition of silty fine to middle grain-sized sands intermixed with moor deposits in the northern part of the area. The flow regime of the partly confined aquifer is controlled by recharge and diverging groundwater flow towards the receiving stream and lakes. Presently known groundwater contamination is dominated by light volatile chlorinated hydrocarbons (CHC, mainly TCE and cisDCE, up to >170 mg/L) (Fig. 2.1) and, to a lesser extent, of BTEX (<1 mg/L). The investigation of the spatial extent of contamination is still ongoing using innovative methods, including tiered refinement of the direct push raster, plant screenings (CHC-uptake via roots) and integral pumping tests (where applicable).

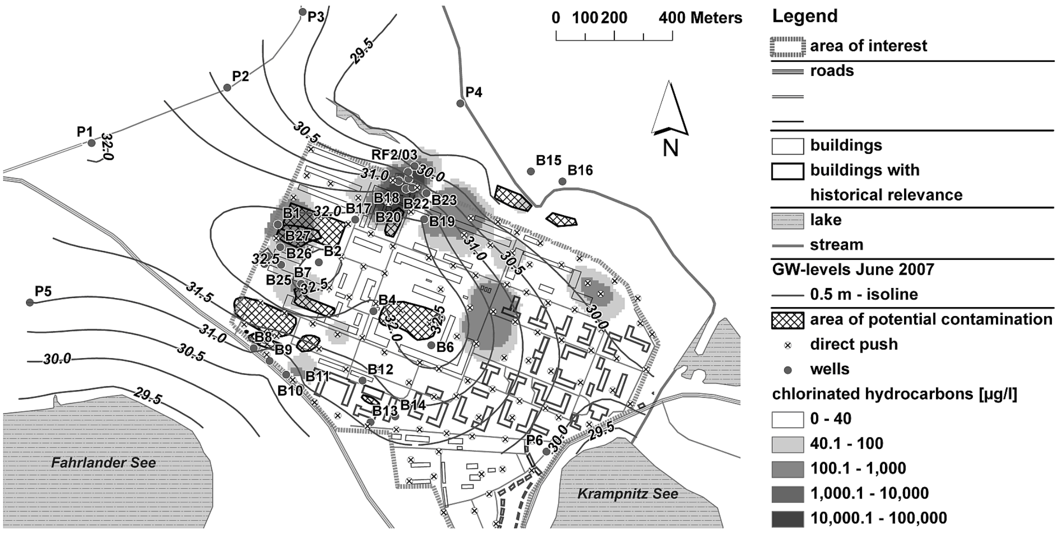


Figure 2.1: Plan view of the former military site "Kaserne Krampnitz" in Potsdam.

2.4 Land use scenario

To demonstrate the methods, a simple and rather hypothetical land use scenario was considered. It includes three different types of land use within the area of interest (see Table 2.1 and Fig. 2.3). In all areas where listed buildings are situated, the land use is fixed to "residential". Agricultural and recreational areas, as well as wetlands (no specific use, but ecological concerns) border the site property.

Table 2.1: Initial (hypothetical) land use scenario for the Krampnitz site.

Land use type	Area (m^2)	Area within the site (m^2)	Quota at site (%)	Restricted area due to historical buildings (m^2)
commercial/ industrial	174595	174595	15.3	–
recreational	1015972	263151	23	˜ 35000
residential	705280	705280	61.7	˜ 355000
Total	1895847	1143026	100	˜ 390000

2.5 Evaluation of monetary benefits and sustainability

The benefits of the development of formerly abandoned land that can be attributed to a particular land use scenario or layout in terms of an increased land value were quantified on the basis of regional average standard land values reflecting the actual development state of the area incl. infrastructure, buildings, facilities, etc. ("Bodenrichtwert").

The following soil values were used: 40 €/m^2 for "residential", 25 €/m^2 for "recreational" and 15 €/m^2 for the "commercial/industrial" use type, respectively. These standard land values, established for non–contaminated land by an advisory committee [WertR, 2002, WertV, 1998], are reduced according to the diminution in value due to the contamination. This includes losses or discounts resulting from the site's bad reputation ("stigma", e.g. Patchin [1991]) or from additional investment and liability risks [Großmann et al., 1996, Sächsiches Landesamt für Umwelt, Landwirtschaft und Geologie, 2001, ITVA, 2007].

The market-oriented economic evaluation of the benefits of site redevelopment is accompanied by a sustainability assessment. Both the clean–up itself and the development of the site will result in a variety of ecological, economic and social changes to the site and in the neighborhood that may influence the stakeholders decision on the selection of the land use plan. There are different assessment approaches available, including different operationalisations of sustainability, different sets and weighting of indicators, different levels of detail and more or less profound involvement of stakeholders [e.g. Hartmuth et al., 2006b,a, Schwarze and Bartke, 2007]. This non–monetary assessment is done at the scenario level. This means that the particular layout of a scenario, as long as it is not fundamentally changed, is assumed to have only a minor influence on the assessment result.

In the proposed evaluation framework, two approaches are considered: (i) the so-called soil-value balance [Umweltbundesamt, 2000] aims at a rather simplified

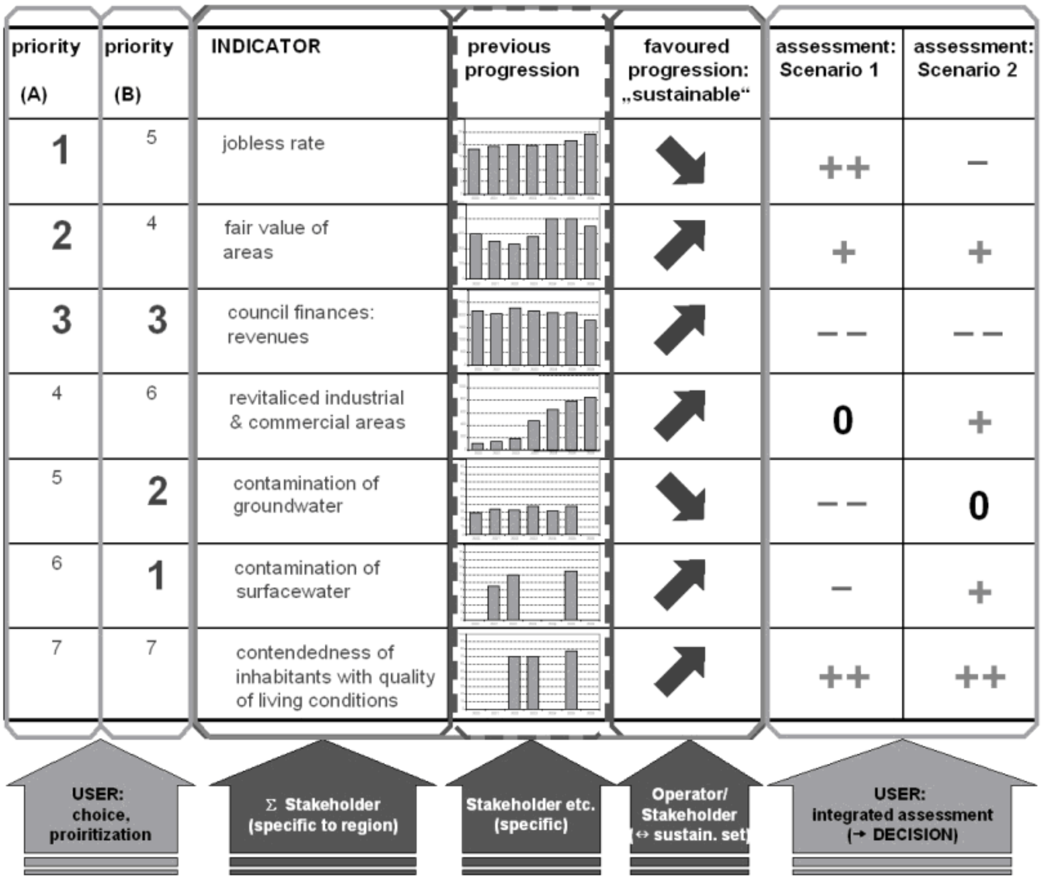


Figure 2.2: Utilization of sustainability indicators for evaluating future land use scenarios.

value system including a monetisation of social or ecological values; and (ii) the approach proposed by Hartmuth et al. [2006b,a] relies on an intensive involvement of stakeholders, not only in the evaluation, but also with respect to the definition and ranking of relevant indicators. Figure 2.2 shows an example of indicators for evaluation of a future land use scenario.

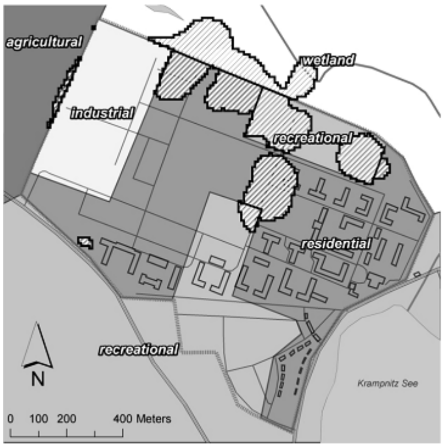
2.6 Evaluation of costs

Conflict analysis The link between land use and required clean-up activities is represented by remediation targets for soil and groundwater. It is assumed that the levels of these targets are a function of the future land use, since exposure scenarios and pathways are specific to the particular land use type. The spatial land use allocation, as described by the scenario layout under consideration, is correspondingly transferred to a map of clean-up targets. Contaminant-specific, as well as use-specific quality targets are given by the responsible environmental agency [LUA, 2006] in terms of concentration threshold values for soil and ground-/surface water.

These threshold values serve as a reference that can be replaced by risk-oriented clean-up targets provided that a site-specific risk assessment [e.g. U.S.EPA, 1990, 1991, ASTM, 2002, Strenge and Smith, 2006] has been conducted.

Table 2.2: Land use and site-specific remedial targets.

Land use type	regulatory or calculated remediation target; TCE (μg/L)	Relevant legal act/ordinance or most sensitive pathway
Industrial	6960	Indoor air inhalation
Residential	100	Indoor air inhalation
Wetlands	20	Quality target
Agricultural	20	according to [LUA, 2006]
Recreational	20	



Land use type		Area (m²)	Exceedance of target (max.) (-)	Conflict area (m²)
wetlands	off site	443477	3632	54349
industrial	on site	174595	1.7	758
agricultural	off site	156477	30.5	3746
recreational	off site	855389	-	0
	on site	263151	8.1	59408
residential	on site	705280	933	77938
total	on site	1143026		138104
	off site	1455343		58095

Figure 2.3: Resulting conflict areas for the initial land use scenario (layout A) and given CHC-contamination.

Intersecting the maps of clean-up targets and contaminant distributions yields contaminantspecific areas of conflict that are then superimposed. In doing so, two maps, one for soil and one for groundwater, describe the extent of unacceptable impairment. Here, for the sake of simplicity, the result of the conflict analysis is only shown for CHC in groundwater (Fig. 2.3).

For the saturated zone, it has to be considered that type and extent of required clean-up activities may not be only a mere matter of the conflict area, but also of the origin of the contamination causing the conflict. The conflict areas in the northern part of the site, for example, are caused by sources located in the area intended for commercial use for which no conflicts were identified (Fig. 2.3). Therefore, source–plume relationships have to be carefully analysed and taken into account when selecting appropriate measures for remediation. Available methods range from rather pragmatic methods, such as particle tracking, to sophisticated approaches, utilising analytical or numerical contaminant propagation models.

Determining clean-up costs Based on the conflict maps and further GIS-managed site information, clean-up costs are estimated by one of several costing approaches currently available. They differ in complexity and input requirements and are selected depending on the level of available knowledge and information [Bonnenberg et al., 1992, Bracke et al., 2005, Schädler et al., 2008]. For the example shown here, remediation costs required to solve the conflicts with respect to groundwater quality were estimated to 3.39 Million €for pump-and-treat. Note that the groundwater clean-up costs for measures solely designed to protect the neighbourhood would amount to about 1.00 Mio €.

2.7 Minimising costs by optimal land use allocation

After having assessed one initial layout ("A") of the land use scenario, further layouts were considered in order to minimize clean-up efforts and costs through optimisation of the land use allocation (using constant overall quotas, as defined by the scenario). The goal is to reduce the extent and magnitude of conflicts. For each of the land use types, a specific region can be specified, where conflicts do not arise (Fig. 4). Clearly, the land use type "industrial", being the least sensitive, has the highest degree of freedom for allocation. An altered land use layout ("B") and the resulting conflict areas are shown in Fig. 5. Due to re-allocation, groundwater remediation costs are now estimated to 2.18 Mio €. That portion of the costs that is related to the specific use of the site has decreased correspondingly, from about 2.39 Mio € to about 1.18 Mio €.

Please note that layout B does not stem from any mathematical optimisation but was chosen from a given set of alternatives to show how layout alterations can reduce clean-up efforts.

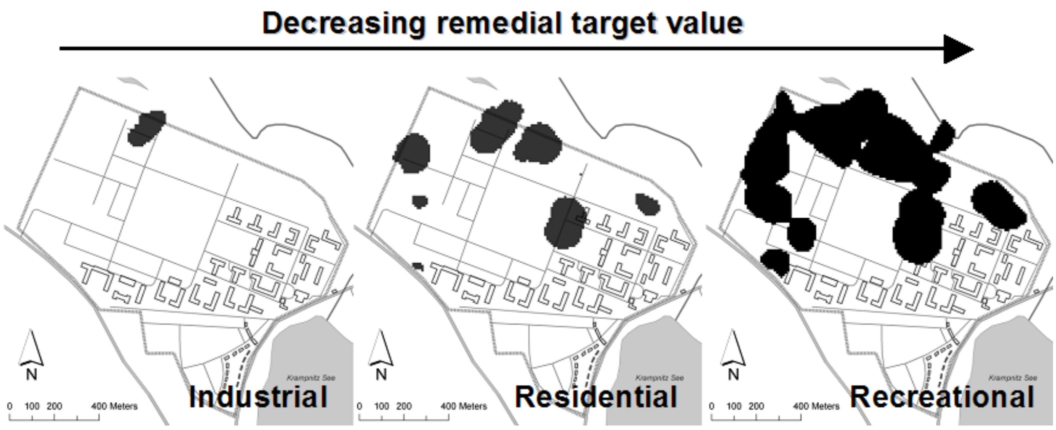
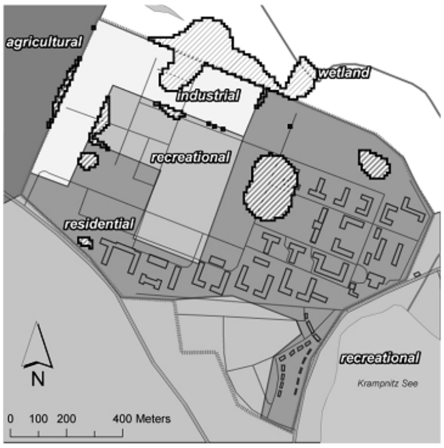


Figure 2.4: Scope for land use allocation without any conflict (non-black area).



Land use type		Area (m²)	Exceedance of target (max.) (-)	Conflict area (m²)
wetlands	off site	443477	3632	53915
industrial	on site	179987	25	14768
agricultural	off site	156477	30.5	3746
recreational	off site	855389	-	-
	on site	278548	6.8	7159
residential	on site	684495	12.7	46628
total	on site	1143030		68555
	off site	1455343		57661

Figure 2.5: Land use allocation layout B and resulting conflicts with the given CHC-distribution.

2.8 Comparison of benefits and costs

Table 2.3 lists the benefits and costs, as evaluated for the exemplary scenario considered here. The initial scenario and its alternative layout have approx. the same land value, since the quotas for the individual land use types differ only slightly. However, the remediation costs for layout "B" are lower due to the differences in layout-specific spatial allocation of use types.

Another scenario that was also analysed labelled "only residential use" (compare Table 2.3 and Fig. 2.4). It would yield a higher land value, but also higher remediation costs. From the mere economical point of view of an investor, this (also hypothetical) scenario may be the most attractive one. However, ranking of options will not be solely driven by clean-up costs and land values, but will also consider the results of non-monetary assessments. The "only residential use" scenario, for instance, may yield a worse result than the initial scenario (e.g. being in contrast to the demands of regional planning or is down-graded in a sustainability assessment).

Table 2.3: Assessment results for different scenarios. *) purely hypothetical results (for the purpose of illustration).

Land Use Scenario/Layout	Land value (€)	Groundwater clean-up costs (€)	Non-monetary Assessment *
Initial Scenario & Layout A	37 408 900	3 390 000	++
Initial Scenario with alternative Layout B	37 270 055	2 180 000	++
Only residential use	45 721 040	2 070 000	o

Please note that, in this paper, we referred to remediation costs for groundwater clean-up only. Note also that the presented concept for estimating costs on the basis of land use specific conflict areas applies in the same way to soil remediation costs [compare Schädler et al., 2008, this issue], and also to site preparation costs (e.g. demolition of ruined buildings and infrastructure, rubble clearance, earthworks, etc.). All these cost types are considered specific to the land use type. In some cases, the additional burden due to the presence of listed historical buildings must also be taken into account.

2.9 Acknowledgments

The authors gratefully acknowledge the support of the German BMBF research priority program REFINA (contract no. 0330757C). Funding for this study also has been provided by the Helmholtz Centre for Environmental Research – UFZ in Leipzig (contract no. 4500029698).

Chapter 3

Flow guided interpolation - a GIS-based method to represent contaminant concentration distributions in groundwater[1]

Abstract This paper introduces a new interpolation method to estimate the spatial distribution of contaminant concentrations in groundwater. The method is intended to identify areas of risks in early investigation stages when groundwater sampling data is typically scarce and available interpolation methods fail to provide reasonable results. As a consequence, the method does not only incorporate available sampling data, but also makes use of information about the groundwater flow field, in order to "guide" the interpolation with e.g. ordinary kriging or inverse distance method. The guidance includes the augmentation of available data by auxiliary point data and the segmentation of the estimated plume area into a series of sectors. The method is evaluated for several settings and different sampling data sets. Each data set reflects a specific level of field investigations at the model site, an abandoned military base in Potsdam near Berlin, Germany. The results reveal that flow guidance improves the representation of contaminant distribution for all cases examined in this study compared to "unguided" interpolation. These findings are underpinned by the results of the method's application to real sampling data. The method especially shows its strength when data of only a few sampling points are available.

Keywords interpolation ; groundwater contamination ; contaminant transport ; chlorinated hydrocarbons ; TCE ; GIS ; particle tracking; ordinary kriging ; numerical groundwater flow modeling

3.1 Introduction

Different approaches exist to estimate the spatial distribution of contaminants dissolved in groundwater. Proposed approaches range from experience-based practitioners' methods, such as best guess delineation of source zones and plumes based

[1]reproduced from: Morio, M., Finkel, M. & E. Martac (2010): Flow guided interpolation – A GIS-based method to represent contaminant concentration distributions in groundwater, Environ. Model. Softw., doi:10.1016/j.envsoft.2010.05.018

on small amounts of sample data and experiences from similar sites and cases, to advanced methods involving geostatistics [e.g. Isaaks and Srivastava, 1989, Deutsch and Journel, 1997, Michalak and Kitanidis, 2004a, 2005], modeling [e.g. Shlomi and Michalak, 2007, Prommer et al., 2002, D'Affonseca et al., 2008] and data assimilation techniques e.g. using Bayesian filtering techniques [e.g. Kalman, 1960, Chen, 2003]. The appropriateness of individual methods is mostly dependent on the type, amount and quality of available data as well as on the particular objectives. Plume delineation focusing on detecting the plume's extent [e.g. Meyer et al., 1994, Storck et al., 1997, McGrath and Pinder, 2003] may call for methods other than the estimation of the concentration distribution [e.g. Boufassa and Armstrong, 1989, MacKay, 1990, Kerry and Oliver, 2007].

Data assimilation techniques such as Particle Filter and Ensemble Kalman Filtering have gained considerable interest in the last decade for utilization of available measurement data to update mathematical model predictions of groundwater flow and plume propagation [e.g. Evensen, 1994, Eigbe et al., 1998, Porter et al., 2000, Chang and Jin, 2005, Chang and Latif, 2009]. Filtering methods seem to be best suited for transient problems of groundwater system state estimation when time series of measurements are to be repeatedly (i.e. sequentially) assimilated into mathematical models [e.g. Liu et al., 2008, Huang et al., 2009, Chang and Latif, 2010].

Geostatistical interpolation methods have been widely applied in the past decades. Mehrjardi et al. [2008] proposed the use of ordinary kriging and cokriging for interpolation of contaminants in groundwater, while Reed et al. [2004] evaluated different interpolation methods to estimate the distribution of perchloroethylene (PCE) in three heterogeneous test cases of different size and complexity for a ground water plume with differing amounts of non-gridded sampling data. They recommend quantile kriging and multigaussian kriging to be most robust and least biased compared to ordinary kriging, intrinsic kriging and inverse distance weighted methods. Journel and Rossi [1989] showed that universal kriging (also called "kriging with trend") yields similar results to ordinary kriging on data sets with trend when the trend component is unknown and kriging is conducted in local neighborhoods for non-stationary data sets.

Cooper and Istok [1988] discusses the requisite of data preparation and analysis, including additivity, stationarity and amount of samples for the estimation using geostatistical interpolation methods. Sufficient data is required, e.g. to make use of an empirical semivariogram [e.g. Deutsch and Journel, 1997, Fuest et al., 1998, Kitanidis and Shen, 1996, Reed et al., 2004, Kistemann et al., 2008]. A practical rule for the minimum amount of samples is given by Journel and Huijbregts [1978]:

$$N(h) > 30\text{-}50 \quad with: \quad |h| < (L/2), \tag{3.1}$$

where $|h|$ denotes the magnitude of separation vector h for N sample pairs and L stands for the longest dimension of the contaminant plume in the direction of h. For a complete list of symbols used in this article, please refer to Table 3.5. Interpolation may utilize concentration measurements either in terms of point observation data from distributed monitoring networks [e.g. Sudicky et al., 1983, Warrick et al., 1998] or in terms of data from so-called control planes or monitoring fences [e.g. Schwarz et al., 1998, King and Barker, 1999, Bockelmann et al., 2001, Basu et al., 2006, Kübert and Finkel, 2006, Bayer-Raich et al., 2009b].

Several suggestions were made to improve interpolation by including additional information in the estimation process, e.g. hydraulic gradient or head data from sampling campaigns [e.g. Burger and Schafmeister, 2000, Shlomi and Michalak, 2007]. Other approaches are based on coupling numerical transport models to interpolation methods [Michalak and Kitanidis, 2004a,b]. Neupauer and Wilson [2003] used a probabilistic numerical flow and transport model to relate concentration measurements to possible upgradient source locations. Rautman and Istok [1996], Istok and Rautman [1996] proposed stochastic geostatistical modeling of contaminant plumes as an approach to derive probabilities of having a contamination at a certain point with respect to a specific concentration threshold and probability cutoff.

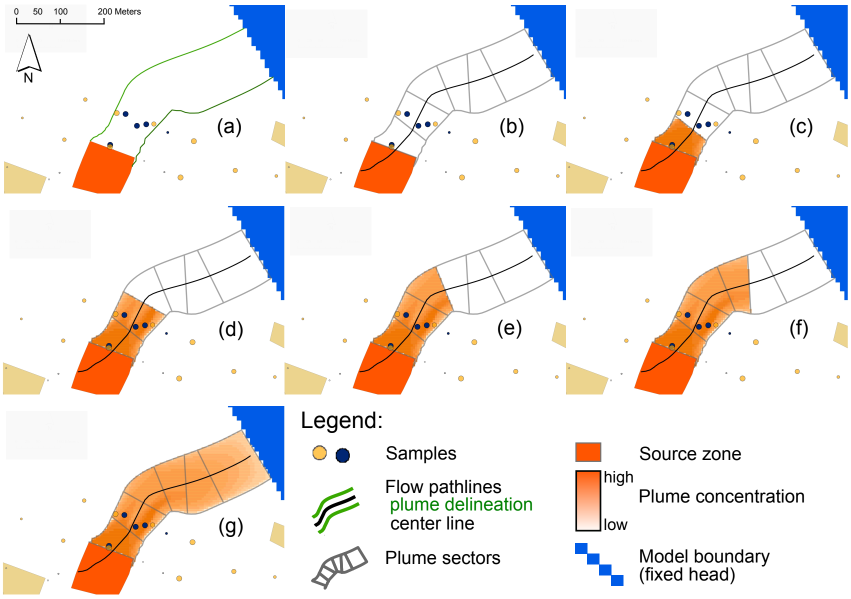


Figure 3.1: Flow guided interpolation: (a) potential source zone with outermost groundwater flow pathlines, (b) segmentation according to curvature of plume's center pathline (here: 6 sectors), (c) interpolation within sector downgradient of the source zone, (d-g) consecutive sector-wise interpolation in downgradient direction. Blue colored circles denote groundwater wells, orange circles stand for direct push samples.

A common problem in practice is that available contaminant concentration measurement data is not sufficient to make sensible use of the abovementioned geostatistical interpolation methods. Numerical transport modeling [e.g. Anderson and Cherry, 1979, Chu et al., 1987], which further requires comprehensive information about aquifer and transport properties, is also inappropriate for this reason [e.g. Batu, 2006]. Limited availability of contaminant data is characteristic of early project stages in tiered decision-making procedures, when information on subsurface contamination only stems from historical data and some initial site investigation. This is particularly true, e.g. when extent and complexity of a site require an early identification and prioritization of focal areas and origins of risks in order to drive further decisions on detailed investigation programmes and remediation measures [compare Triad approach, e.g. in Crumbling et al., 2001, Mack et al., 2004, Critto et al., 2007, O'Reilly and Brink, 2006]. Thus, especially for early site investigation stages, there is a need for enhancement and appropriate processing of sparse amounts of available data in order to produce the premise for a reasonable application of interpolation methods such as kriging.

In this paper we present a flow guided interpolation (FGI) method that has been specifically adapted to the type, scale, and information basis that is typically available in early stages of revitalization projects at contaminated sites. The method proposes to add extra sampling points in a standardized way through coupling of flow data and existing samples plus information about possible source zone extents to enable the application of kriging methods. The purpose of the proposed method is to bridge the gap between elaborate, data intensive approaches and subjective and often non-reproducible methods. The FGI method builds upon a groundwater flow model, assuming that basic information about the groundwater flow regime can be made available at relatively low cost. This model is not supposed to provide a highly sophisticated representation of the flow situation but is supposed to show the major i.e. characteristic features. Guidance by groundwater flow is intended to improve the interpolation especially if contaminant concentration data is scarce. The idea is to incorporate upgradient information in a sequential downgradient interpolation procedure. The relevance of the quantity of available data is addressed through analyzing the FGI method's performance for different knowledge states, i.e. different sample amounts.

The remainder of this paper is organized as follows: the FGI method is described in section 2 by use of pseudo-code algorithms to explain the sequential procedure execution; section 3 gives a description of the model site in which the FGI method was applied; the evaluation of the FGI method for different parameter settings is discussed in section 4; results of the case study are presented in section 5; conclusions are made in section 6.

3.2 Methodology

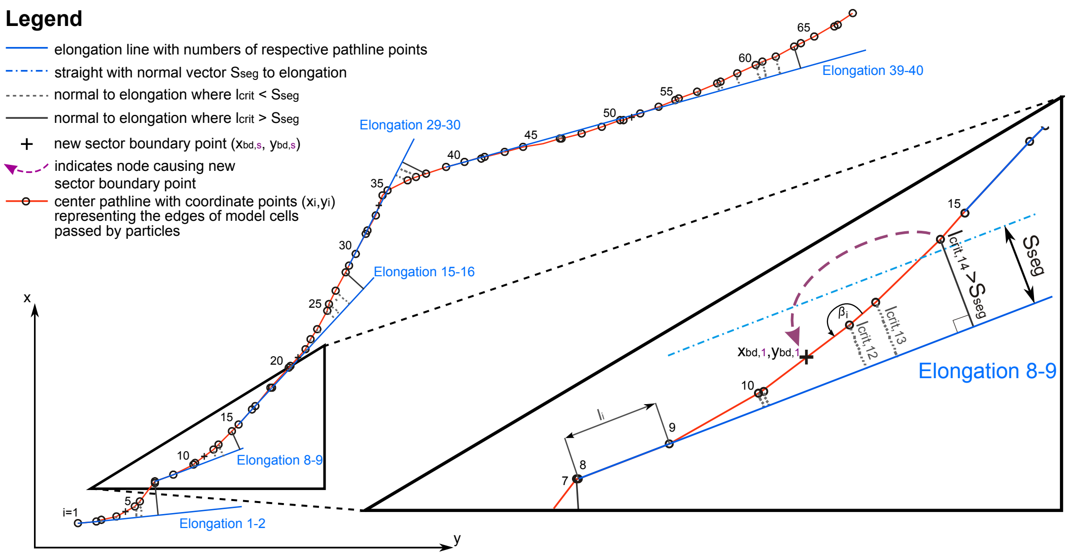
The FGI method is implemented into the geographic information system ArcGIS (ArcMap, Version 9.1 or higher, [ESRI, 2005]) with VBA and ArcObjects [Razavi, 2004, Burke and Arana, 2003]. The method is comprised of a sequence of procedures with major portions that are controlled by VBA modules.

In short, the following steps are performed: (1) delineation of the known or expected source zone of contamination using particles, which are equidistantly distributed along the source zone edges; (2) delineation of the plume fringe by tracing these particles advectively downgradient; (3) segregation of the plume into several sectors according to the plume's tortuosity and curvature; (4) employment of sector-wise flow guided interpolation, utilizing sampling data in the sector, as well as auxiliary sampling point data along the plume fringe and along the boundary to the previously processed sector; (5) merging of the results of all sectors into a single grid by mosaicking.

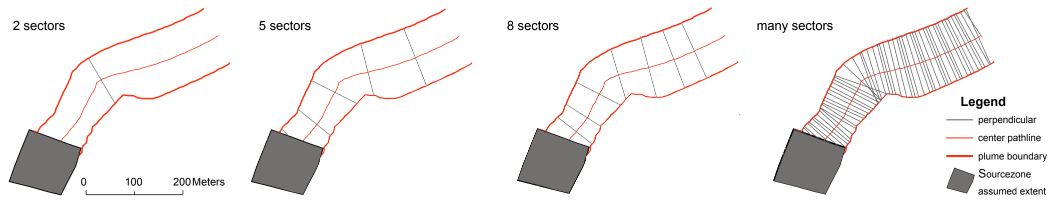
A series of three pseudo-code algorithms describe the process of (i) plume fringe delineation based on the previously defined source zone (algorithm 1 , see also Figure 3.1a), of (ii) segmentation of the derived plume shape dependent on groundwater flow direction (algorithm 2, see also Figure 3.1b) and of (iii) sector-wise interpolation to estimate the spatial concentration distribution within the plume (algorithm 3, see also Figures 3.1c to 3.1g). The procedures are described in more detail below. Please note that multiple source zones and corresponding plumes can be considered. For the sake of clarity we limit the description to one source zone and one plume. The delineation of the plume fringe requires polygon data of the source zone, a numerical groundwater flow model, and a particle tracking module. The flow model is required to calculate the groundwater flow field, which in turn is required to calculate pathlines of groundwater flow by particle tracking. We used MODFLOW 96 [Harbough and McDonald, 1996] and MODPATH 3.0 [Pollock, 1994], respectively, but other models, like a version of ESRI's Groundwater Modeling application [ESRI, 2009], could be used as well after some adaption work (see also the concluding discussion of this section further below). The identification of the source zone is based on desk work examining information on former use of the site, possible locations of contaminant spills, the geological and hydrological situation, and subsurface sampling information. Source zone polygons are then created manually as polygon shape files in GIS, based on the assembly of given data. As shown in algorithm 1, the source zone polygons are converted into a set of equidistantly distributed points, which are then used as water particle starting locations for particle tracking with MODPATH. The pathline data returned by MODPATH is automatically converted to a polyline shape file consisting of polylines for each particle starting point and a corresponding point shape file bearing information on the pathline time steps. The pair of outermost polylines in the shape file represents the plume fringe and is converted to a polygon shape file. The resulting polygon has to be cut in order to account for the expected plume age. Using travel time information from the point shape file, a polygon is created that represents the plume extent corresponding to the given time after spill.

Please note that this purely advective approach may underestimate the real plume extent. However, assuming that macroscale heterogeneity is sufficiently described in the flow model used, the neglected effect of hydrodynamic dispersion is believed to be minor.

The segmentation of the plume into distinct sectors is based solely on the curvature of the plume's center pathline and one further input parameter, the so-called segmentation criterion, S_{seg}. The segmentation of the center pathline is illustrated in Figure 3.2a and is comprised of diverse steps as described by algorithm 2. These steps are processed mostly automatically by the VBA code. The center pathline is



(a) Principles of segmentation process. Righthand-side triangle shows an enlarged section of the pathline on the left-hand side of the figure. β_i denotes the angle between two adjacent pathline elements.



(b) Results of plume segmentation for different values of S_{seg} (from left to right 50 m, 2.5 m, 0.5 m, and 0.05 m)

Figure 3.2: Illustration of the plume segmentation process dependent on the curvature of the plume's center pathline

provided as a result of algorithm 1 in terms of a polyline and its corresponding point shape file. S_{seg} serves as a criterion for the maximum deflection of the center pathline that causes the creation of a new sector. Sector boundary points are determined along the center pathline. The deflection of a center pathline point i is quantified as normal distance $l_{crit,i}$ of this point to an 'elongation line' representing the center pathline's initial direction (cf. Figure 3.2b). A new boundary point will be created if $l_{crit,i} > S_{seg}$ midway between point i and the initial point from where the elongation line starts (cf. purple arrow in Figure 3.2b). This process of segmentation is repeated in downgradient direction to determine all sector boundaries until the tip of the plume is reached. Lines perpendicularly oriented to the center pathline are created on the newly derived boundary points. These lines are then used to clip the plume polygon into distinct sectors. The number of sectors resulting from plume segmentation increases as the S_{seg} value is lowered and as the plume shape becomes

Algorithm 1 FGI-WORK FLOW: PLUME DELINEATION INVOKING AN ARCGIS-MODPATH INTERFACE

Require: Source zone polygon data {GIS (multiple sources at a site possible)}
Require: Numerical flow model {here: MODFLOW 96}
Require: Advective transport i.e. particle tracking module {here: MODPATH 3.0}
Read model extent and discretization {ArcGIS-MODPATH interface, works automatically, if not noted otherwise.}
Convert source polygon to points (equidistantly distributed, here: point distance Δl = 10 m)
Create MODPATH particle starting locations
Run MODPATH, output: pathline file
Import MODPATH pathlines in GIS , **Convert** to:
○ ESRI raster grid representing cells passed by particles
○ Polyline shape file {pathlines}
○ Point shape file with attribute: cumulative travel times
for all source zone(s) **do**
  Select outermost pathlines and **Convert** {Manually}:
  ○ Polyline to polygon shape file representing plume
  ○ Polyline to point shape file with points on model cell edges
  Select center pathline's polyline and **Convert** {Manually}:
  ○ Polyline to point shape file with points on model cell edges
  With point shape files: **Select** points that equals spill age {Attribute: cumulative travel times}
  Extract selected points and convert to polyline
  Split polygon by polyline {Result: Polygon with plume extent}
end for

more winding (cf. Figure 3.2b). The sector polygons are then converted into points which are subsequently used to create auxiliary sampling points (ASPs) at the upgradient sector boundary, and at the lateral boundaries along the plume fringe. The plume segmentation provides additional geometrical variables, which serve as input for the subsequent interpolation procedure, namely the total plume length L_{tot}, and for each sector s the mean width W_s, and anisotropy angle α_s.

The sector-wise flow guided interpolation itself is described in algorithm 3. Sectors are distinguished by index s. The interpolation starts in the sector located directly downgradient of the source zone ($s = 1$). The processing of the first sector is different compared to the subsequent ones because there is no upgradient neighboring sector except for the source zone. The source zone boundary is populated with ASPs, the location of which coincide with the particle starting locations. To each of these ASPs a concentration value needs to be assigned that represents the source zone conditions. In this study we assign a unique value, the mean of available concentration measurements in proximity of the source zone, to all points. If detailed information is available, spatially varying concentration values may be used. Sample values at ASPs along the lateral boundary of the sector (plume fringes) are set to some lower threshold concentration C_{tc} (e.g the detection limit of the contaminant of concern). All ASPs and the real samples available in the sector in process are added to the sample list to be used for interpolation. If no real sample is available, real samples (but not the ASPs) of the neighboring sector downgradient are added to the sample list. If the neighboring downgradient sector also does not contain real sample points, the next downgradient sector is considered, and real samples of this

Algorithm 2 FGI-WORK FLOW: PLUME SEGMENTATION BASED ON FLOW DIRECTION

Require: Centerline point and polyline shape file {output from algorithm 1 with n no. of points on center pathline}
Read Gauss Krüger coordinates of vertex points
Calculate descriptive variables to describe center pathline: lengths of line elements l_i and angles β_i of l_i, the directions of lines between adjacent nodes $\overline{(x_i, y_i)(x_{i+1}, y_{i+1})}$ against horizontal
s=1 {sector number}
for $i = 1 \rightarrow n$ **do**
    $n_{step} = 0$ {additional increment variable}
    while $l_{crit,i+n_{step}} < S_{seg} \wedge i + n_{step} < n$ **do**
        $l_{crit,i+n_{step}} = |(y_{i+1} - y_i) \cdot (x_i - x_{i+n_{step}}) - (x_{i+1} - x_i) \cdot (y_i - y_{i+n_{step}})| / l_i$ {Calculate normal distance of plume center pathline node $i + n_{step}$ to elongation line (cf. Figure 3.2a)}
        $n_{step} = n_{step} + 1$
    end while
    $i = i + n_{step}$
    if $i < n$ **then**
        {Determine sector boundary coordinate on the middle between two existing points.}
        $x_{bd,s} = (x_{i+1-\lfloor n_{step} \cdot 0.5+0.5 \rfloor} + x_{i-\lfloor n_{step} \cdot 0.5+0.5 \rfloor})/2$
        $y_{bd,s} = (y_{i+1-\lfloor n_{step} \cdot 0.5+0.5 \rfloor} + y_{i-\lfloor n_{step} \cdot 0.5+0.5 \rfloor})/2$
    end if
    $s = s + 1$ {Increment number of sector}
end for
Calculate azimuth of straigt line defined by adjacent sector boundary coordinates $(\overline{x_{bd,s} y_{bd,s}, x_{bd,s+1}, y_{bd,s+1}})$ {Yields anisotropy angle α_s for each sector}
Calculate cumulative length L_{tot} of point to point distances l_i
Create new boundary points table with $x_{bd,s}$ $y_{bd,s}$ α_s
Create polyline shape file with lines perpendicular to center pathline through each of its vertices {Done by VBA script}
Select a subset of lines that intersect sector boundary points on center pathline by new sector boundary points from new boundary points table {Done by SQL type of GIS query function}
Clip plume polygon with subset of lines to create sectors
Calculate mean Width W_s for each sector.
Create equidistantly distributed points along sector boundaries (here: point distance Δl = 10 m).

sector are then added to the sample list of the sector in process. Note that the additivity assumption of sample data is fulfilled since effective porosity and thickness of the aquifer are assumed to be constant for this study [compare Cooper and Istok, 1988]. Note further that sample data outside the plume fringe are not considered for interpolation. If there is evidence for a contamination outside the delineated plume fringe belonging to the given source zone we suggest to consider a revision of the flow model or of the source zone extent.

Ordinary kriging is then conducted with a sector-specific values of anisotropy ratio RA_s (derived from the ratio L_{tot}/W_s) and angle α_s, which is provided by algorithm 2. The respective parameters for the interpolation procedure in each sector are noted in Table 3.1. Please note that a trend within the sample data, i.e. a component or tendency of the data to change their values according to their spatial position, is not considered here. Due to the small amount of sample data available within the individual sectors, it does not seem practicable to estimate a reliable trend compo-

Algorithm 3 FGI-WORK FLOW: ESTIMATING CONTAMINANT DISTRIBUTION

Require: C_{source}, C_{tc} {Source and plume fringe concentration}, $x_{bd,s}, y_{bd,s}, \alpha_s, W_s, L_{tot}$, plume sector polygons and according boundary points {Result of algorithm 2}
for $s = 1 \rightarrow s_{tot}$ **do**
  Assign concentration values to auxiliary sampling points on upper sector boundary
  if $s = 1$ **then**
    $C_{ub,s} = C_{source}$ {Use source concentration values in 1st sector}
  else
    $C_{ub,s} = C_{lb,s-1}$ {Use results from previous sector}
  end if
  Extract $C_{ub,s}$, add to XYZ-file of sector s {Using ArcGIS Toolbox Sample_SpatialAnalyst}
  Assign C_{tc} to lateral plume boundary as ASP in sector s (add to XYZ-file of sector s)
  if Samples in sector s $\exists$ **then**
    Select samples within sector (add to XYZ-file of sector s)
  else
    Select samples from next sector containing samples from (add to XYZ-file of sector s)
  end if
  Calculate $RA_s = L_{tot}/W_s$ {anisotropy ratio}
  α_s anisotropy angle, calculated in algorithm 2
  Perform Ordinary Kriging on XYZ-file of sector s using RA_s and α_s
end for
Mosaic sectors' concentration rasters to one seamless raster for entire plume.

nent and to model a corresponding variogram. The grid of estimated concentration values has the same resolution as the flow model grid. The grid extent is clipped to the sector in process and sampled at the downstream boundary points to generate the ASPs required for interpolation in the next sector. The interpolation of the 2nd and any further sector follows the same procedure. The grids calculated for the single sectors are finally mosaicked, i.e. sector-specific results are merged to a single raster grid, to produce the grid of concentration values for the entire plume.

To ease the application of the FGI method, it is recommended to process and manage all available site data in the GIS. The FGI method can also be implemented in GIS packages other than ArcGIS. Open source GI-Systems and packages include i.e. GRASS-GIS, QuantumGIS, the geodata abstraction library GDAL (http://www.gdal.org) or R with the rgdal-package [GRASS Development Team, 2009, Quantum GIS Development Team, 2009, R Development Core Team, 2009]. The pseudo-code algorithms presented above may serve as a guideline for such an implementation process. The FGI method presented in this paper may also be adapted for using other codes to simulate groundwater flow and advective transport (particle tracking).

3.3 Model site: Investigation data and flow model

The model site is an abandoned military base covering 120 hectares on the outskirts of Potsdam near Berlin, Germany. The site was turned into a brownfield in the early 1990s. It was used by German and Russian armed forces until 1945 and 1991, respectively. Gas stations and a dry cleaning facility represent the major sources of

Table 3.1: Available sampling data and sector-specific interpolation parameters in plume sectors for different cases of segmentation and investigation levels.

Sectors[a] (-)	Sector no. s (-)	No. of samples[b] Wells,DP1,DP2/Tree–core	Mean sector flow direction[c] α_s (°, $E = 0°$, CCW)	Anisotropy ratio RA_s(-)	Total plume length L_{tot}(m)	Mean sector width in sector s W_s(m)
2	1	4, +3, +1 / 13	41.0	4.4	400	90
	2	0, +0, +0 / 9	25.0	3.4		115
5	1	1, +1, +0 / 4	47.0	4.4	400	91
	2	3, +2, +1 / 9	60.5	4.4		90
	3	0, +0, +0 / 2	31.8	4.0		100
	4	0, +0, +0 / 3	17.8	3.2		125
	5	0, +0, +0 / 4	26.5	3.0		135
8	1	1, +1, +0 / 4	48.6	4	400	91
	2	0, +0, +0 / 0	51.1	5.5		90
	3	3, +2, +1 / 9	63.4	4.2		94
	4	0, +0, +0 / 1	47.2	3.8		105
	5	0, +0, +0 / 1	14.2	3.8		106
	6	0, +0, +0 / 3	17.4	3.1		127
	7	0, +0, +0 / 2	22.8	3.2		125
	8	0, +0, +0 /2	27.1	3.2		105

[a]This columns indicates the amount of sectors, into which the plume is segmented.

[b]This column denotes the amount of samples that are available in the particular sector s after investigation campaign "Wells" and the amount of samples that became additionally available after campaigns "DP1" and "DP2". The numbers given for investigation phase "Tree-core" stands for on own and are not to be added to the samples of the other investigation campaigns.

[c]i.e. anisotropy angle

subsurface contamination. Since 1992, the site has been revisited and investigated several times by various groups of consultants and researchers. Four major investigation campaigns have resulted in an increasing net of monitoring wells, from a rather scarce net of observation points in 1996 to a quite dense net after a comprehensive direct push campaign and sampling of tree-cores in 2007.

The presently known groundwater contamination is dominated by volatile chlorinated hydrocarbons (CHC, mainly trichloroethylene (TCE) and cis-dichloroethylene, up to more than 170 mg/l). Contaminants originate from diverse source zones, as shown in Figure 3.3. Contaminated groundwater flows from the site towards two lakes, nature reserves and other potential receptors (Figure 3.3).

A two-dimensional finite difference flow model was used to simulate groundwater flow in the unconfined aquifer consisting of fine sand to silty deposits. The model domain is represented by a cell-grid with an extent of 2500 × 4000 m using a discretization of square cells of 10 × 10 m. A fixed head boundary condition is defined along gaining streams and lakes. No-flow boundary cells are set where model boundaries coincide with groundwater flow lines (see Figure 3.3). Hydraulic conductivity values of the calibrated model range from $K = 6.23 \cdot 10^{-8}$m/s to $K = 1.32 \cdot 10^{-3}$m/s (geometric mean $K_{geom} = 1.34 \cdot 10^{-5}$m/s), aquifer thickness from 3.6 to 20 m. The model calibration is based on hydraulic heads measured at 27 groundwater monitoring wells and 20 temporary direct push wells [Rein et al., 2008b]. The groundwater level varies approx. between 2 and 6 m below ground surface.

In correspondence to this stepwise site investigation since 1996, four different knowledge states (investigation stages), representing different levels of extent and density of concentration data, can be distinguished [Schädler et al., 2008]. For TCE, which is used here as a model compound, the first level of information is comprised of concentration measurements at 17 groundwater wells. This level is hereafter denoted as ”Wells”. Two direct-push campaigns provided further data (three additional points in campaign #1 and another one in campaign # 2) and result in investigation levels ”DP1” and ”DP2”. Finally, an intensive sampling of tree-cores [Holm, 2007, 2009, Rein et al., 2008a] in the area of interest strongly improved the measurement network (level ”Tree-core”). Tree-core sampling utilizes contaminant accumulation in plants providing semiquantitative information about shallow tetrachloroethene and trichloroethene contaminations in soils and groundwater [e.g. Schumacher et al., 2004, Larsen et al., 2008].

In this study we focus on one contaminant plume in the northern part of the site. Since little information about the vertical contaminant distribution was available, only a two-dimensional analysis was performed.

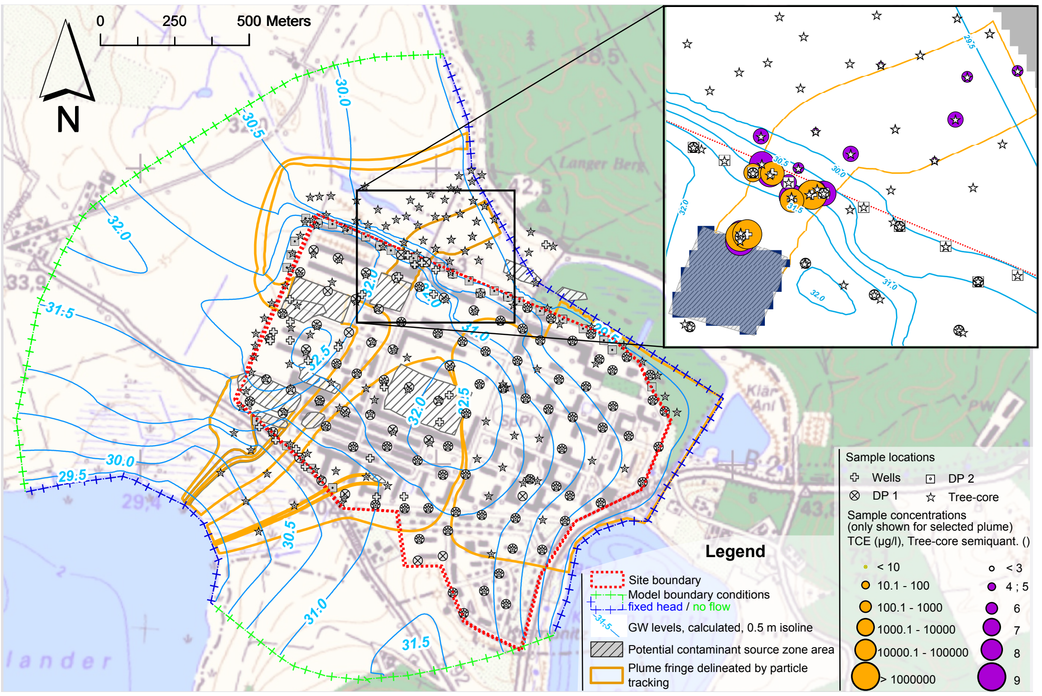


Figure 3.3: Field site with model boundaries, area of interest and zoomed-in study area. Colored circles illustrate magnitude of sampled TCE concentrations (orange) and semiquantitative tree-core sample values (purple).

3.4 Method evaluation

3.4.1 Purpose

In order to examine the appropriateness and performance of the proposed FGI method, it was applied to a synthetic close-to-reality test case. Through the creation of a data grid of reference values of TCE concentration, we could evaluate the performance of the method for different values of segmentation criterion S_{seg} and different investigation stages, simply by comparing the estimated concentration distribution with the assumed 'true' distribution, as given in the form of the reference data grid.

3.4.2 Evaluation test case

The continuous reference values of TCE concentration in the area of interest (see Figure 3.4 and Table 3.2) were generated by implementing a transport model using MT3DMS [Zheng and Wang, 1999]. Data input regarding the heterogeneous flow field was taken from the MODFLOW results (see previous section). Transport parameters were set based on field data (e.g. from tracer tests and soil column analyses). The total organic carbon content f_{oc} varies between 0.02 to 1.17%. The effective porosity n_e ranges from 0.10 to 0.34. The distribution coefficient K_d for TCE was set as the product of 'measured' f_{oc} values and literature values of the sorption constant K_{oc} [e.g. Mehran et al., 1987, Schwarzenbach et al., 2003], assuming that pure forward modeling serves the purpose of generating a reasonable close-to-reality contaminant concentration data field. In accordance with observations made in the field, a steady-state plume and a constantly emitting source zone were assumed. The constant concentration boundary condition equals the saturation concentration of TCE in groundwater ($C_{source} = 1.2 \cdot 10^6 \mu g/l$). Longitudinal and lateral dispersivity were set to 1 m and 0.01 m, respectively. In-situ degradation of TCE was modeled as 1st order process using a degradation rate constant of $0.002\,d^{-1}$, in accordance with literature [Gorder et al., 1996, 1997]. The generated plume is shown in Figure 3.4. It should be pointed out that the transport model is used here only to produce the reference data for the method's evaluation. It is, however, not needed for the application of the FGI method itself.

The generated plume (i.e. the modeled concentration data grid) was then sampled at the sample locations given by the different investigation campaigns. For each of the four campaigns one set of synthetic concentration point measurements was produced (see Table 3.2).

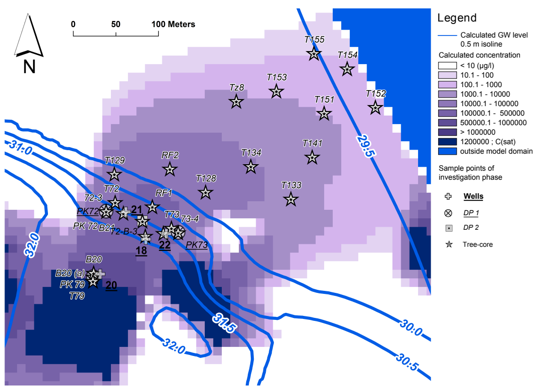


Figure 3.4: Modeled TCE concentration distribution in groundwater in area of interest. C(sat) denotes saturation concentration.

Table 3.2: Sample types and reference concentrations, for X,Y-coordinate, refer to Table 3.3.

Type	Name	Samples reference (μg/l)
Well	B 18	313666
Well	B 20	946668
Well	B 21	181586
Well	B 22	1848830
DP1	PK72	141450
DP1	PK73	135161
DP1	PK79	976230
DP2	72-B-3	248389
Tree-core	T72	125708
Tree-core	T73	135161
Tree-core	T79	1200000
Tree-core	T128	38730
Tree-core	T129	36260
Tree-core	T133	2473
Tree-core	T134	11709
Tree-core	T141	2397
Tree-core	T151	860
Tree-core	T152	218
Tree-core	T153	847
Tree-core	T154	193
Tree-core	T155	86
Tree-core	Tz8	1733

3.4.3 Evaluation method

The quality of the FGI method was quantified by comparing the estimated concentration values of all grid elements with the respective values in the reference data grid. We utilized the normalized root mean square error (NRMSE) to obtain an overall measure of quality (equation 3.3). The root mean square error (RMSE) is determined by:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{j}(c_i^{ref} - c_i^{est})^2}{j}}, \tag{3.2}$$

where j is the number of grid node elements considered within the plume, x_i^{ref} and x_i^{est} denotes the concentration values of the reference distribution and of the estimated distribution, respectively. The NRMSE is further calculated by:

$$NRMSE = \frac{RMSE}{\max c^{est} - \min c^{est}} \tag{3.3}$$

with $\max c^{est}$ and $\min c^{est}$ being the maximum and minimum values of estimated concentrations in all grid elements covering the plume area.

3.4.4 FGI performance

The FGI method was applied to the test case with different sets of sampling data and different values of segmentation criterion S_{seg}. The latter was varied between S_{seg} = 50 and S_{seg} = 0.5. The resulting segmented plumes consist of 2 to 8 sectors, accordingly (compare Figure 3.2b). The number of samples that are located in the individual sectors and the parameters used for sector wise interpolation are listed in Table 3.1. When using a plume divided into only two sectors, for example, the second sector contains no real samples for the investigation levels "Wells", "DP1", and "DP2", whereas the fourth investigation level, "Tree-core", provides 9 sample points. Similar conditions apply to the cases with 5 and 8 sectors, respectively, where sectors located further downgradient also do not contain sample information for the first three investigation levels. Note also that the density of available data may fluctuate from sector to sector depending on the distribution of given sample points (e.g. sequence of sectors 1-2-3-4 in the case of 8 sectors). The interpolation was performed with the commercial computer program Surfer 8 (Golden Software) using ordinary (point) kriging without modeling a variogram nor incorporating slope or trend. The resulting estimation grids were converted to ESRI ASCII grids with the free software GridConvert (www.geospatialdesigns.com) for further processing within GIS. The comparison of the estimations to the reference distribution was calculated using Matlab©(R2009a, The MathWorks, Natick, Massachusetts).

Figure 3.5 shows the matrix of evaluation results obtained with the FGI method depending on the number of sectors (matrix rows) at different investigation levels (matrix columns). For the purpose of comparison, the last row displays the results obtained with 'un-guided' ordinary kriging (OK). A visual inspection of the results suggests that the FGI method provides reasonable concentration distributions for all cases. Missing sampling points in the farther downgradient sections result in slightly overestimated concentrations in these sectors. This might be explained by the propagation of estimates from upgradient sectors. Further analysis reveals that FGI particularly outperforms OK in the case of sparse sampling data. Quantitative assessment also supports these findings (see Figure 3.6). While OK (standard interpolation) exhibits a distinct dependency on available sampling information, the FGI method shows a rather consistent performance. Guiding the interpolation by flow information obviously compensates for missing data in downgradient plume regions. Figure 3.6 also indicates a shift in the ranking of the results obtained with the three different degrees of segmentation. Although the NRMSE decreases with increasing number (density) of available sampling points for all degrees of segmentation, more data (levels "DP2" and "Tree-core") seems to favor a finer segmentation while a coarser segmentation apparently performs better when little data is available (levels "Wells" and "DP1"). For the purpose of comparison, interpolation was also done by the inverse distance weighted method (IDW) using squared distances and the same anisotropy angle and ratio as was used for OK (see Table 3.1). Although IDW does not perform as well as OK, again flow guidance clearly improves the quality of the results as can be seen from the NRMSE values given in Figure 3.6.

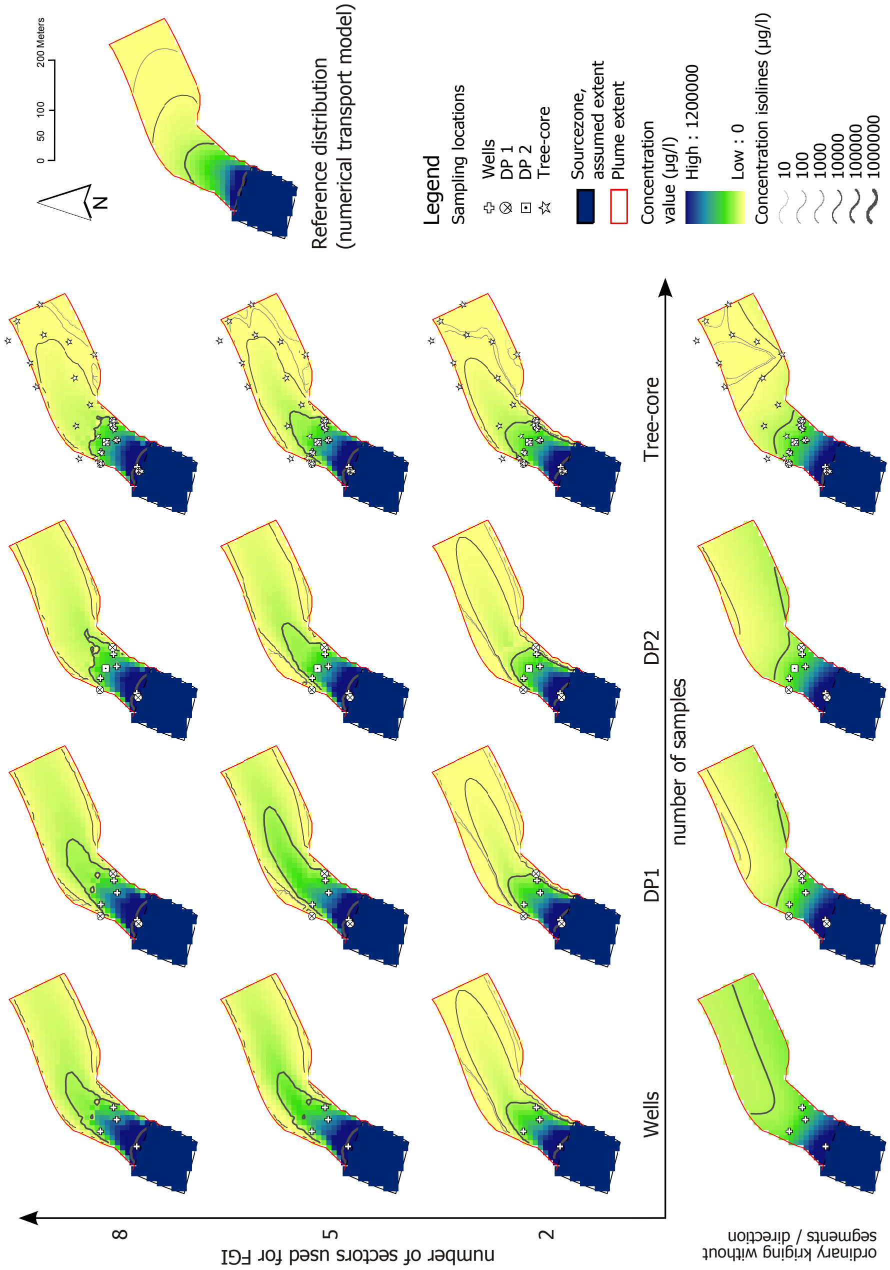


Figure 3.5: Results of the FGI method at different investigation levels in comparison to ordinary kriging (OK) and the reference distribution. Number of samples at different investigation levels increases in the following order: “Wells”, “DP 1”, “DP 2”, and “Tree-core”.

3.5 Method application

Based on the results of the evaluation described in the previous section, the FGI method was applied to the real sampling data sets available for the area of interest. Segmentation settings that performed best in the evaluation were chosen for

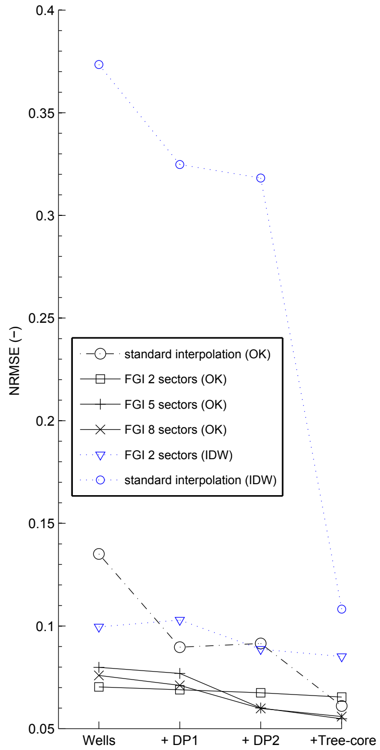


Figure 3.6: Normalized root mean square error NRMSE for concentration estimates as a function of increased knowledge status (cf. Fig. 3.5). Comparison of results from FGI conducted with ordinary kriging (OK) and the inverse distance weighted method (IDW), and from 'un-guided' interpolation with OK and IDW.

each of the four investigation levels (comp. Figure 3.6): 2, 5, and 8 sectors were respectively used for levels "Wells", "DP1", and both "DP2" and "Tree-core". The application results are depicted in Figure 3.7. Once again, FGI results are compared with the results from OK. Please note that the application at the "Tree-core" level had to take into consideration that tree-core sampling provides only semiquantitative values. Results from tree-core sampling were provided on a scale from 1 (below detection limit) to 9 (high concentration in groundwater close to solubility) representing peak areas determined by gas chromatography. To get a complete and consistent sample list for the "Tree-core" level, we converted the groundwater concentration values measured at the sampling points of the first three investigation stages to the semiquantitative tree-core scale (Table 3.3) using an approximative log-scaled conversion scheme (Table 3.4). Comparison of converted values with tree-core results at pairs of sampling points located close to each other (T79 vs. PK79: 9 vs. 8; T72 vs. B21: 7 vs. 7; T73 vs. PK73: 6 vs. 5) shows a good agreement and confirms the adequacy of this approximation for this particular case.

The ASP values along the downgradient edge of the source zone were set to $C_{source} = 1.2 10^5 \mu g l^{-1}$ representing the mean measured TCE concentrations in wells

Table 3.3: Sample locations and concentrations used for interpolation procedures at field application

Type	Name	X	Y	Samples field (μg/l)	Tree -core (-)
		GK coordinates			
Well	B 18	3366921	5814676	77440	7
Well	B 20	3366868	5814635	119703	8
Well	B 21	3366898	5814708	72962	7
Well	B 22	3366945	5814682	174181	8
DP1	PK72	3366874	5814708	6089	6
DP1	PK73	3366959	5814684	820	5
DP1	PK79	3366859	5814632	121605	8
DP2	72-B-3	3366917	5814697	8229	6
Tree-core	T72	3366885	5814719	–	7
Tree-core	T73	3366951	5814689	–	6
Tree-core	T79	3366859	5814627	–	9
Tree-core	T128	3366991	5814731	–	6
Tree-core	T129	3366884	5814752	–	6
Tree-core	T133	3367091	5814723	–	4
Tree-core	T134	3367044	5814761	–	3
Tree-core	T141	3367116	5814772	–	6
Tree-core	T151	3367130	5814823	–	5
Tree-core	T152	3367190	5814830	–	5
Tree-core	T153	3367074	5814849	–	3
Tree-core	T154	3367157	5814875	–	3
Tree-core	T155	3367118	5814893	–	3
Tree-core	Tz8	3367027	5814837	–	4

B20 and PK79, located in close proximity to the source zone. For level “Tree-core” the source zone concentration was accordingly set to $C_{source} = 9$ (compare Tables 3.4 and 3.3). The threshold concentration values C_{tc} assigned to the ASP on the lateral sector boundaries were set to zero at all investigation stages.

Naturally, no absolute quantitative assessment of the results could be carried out since true values at unsampled locations are unknown. Still, visual inspection reveals evident differences between the results obtained with the FGI method and OK . The FGI method yielded plausible results at all investigation levels. Results at low investigation levels appear to be confirmed by results at higher levels. The series of estimated concentration distributions exhibits a successive refinement (see Figure 3.7, from left to right). In contrast, OK results were found to be rather arbitrary and strongly dependent on available data. This disparity between the methods’ results is particularly apparent when comparing the plumes’ shape at level “DP2” with the shape at level “Tree-core”. It should be mentioned that the FGI conducted for level “Tree-core” was performed in the same way as for the groundwater concentration values of investigation levels “Wells”, “DP 1” and “DP 2”. Thus, the inputs for “Tree-core” are scaled using integer intervals but the estimated results on the grid consist of floating-point numbers.

Table 3.4: Conversion scheme for tree core sample analogues at well and DP locations

Tree-core (-)	Hypothetical analog concentration for groundwater (µg/l)
1	unverifiable
2	< detection limit (< 0.1)
3	< 10
4	10 – 99
5	100 – 999
6	1000 – 9999
7	10000 – 99999
8	100000 – 999999
9	> 1000000

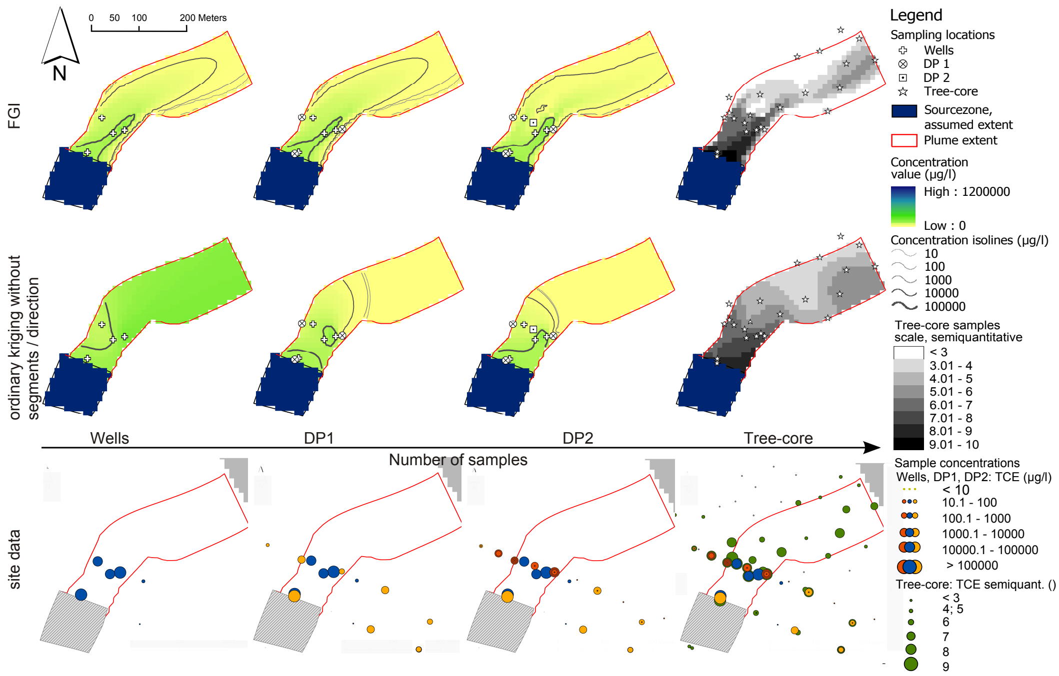


Figure 3.7: Results of segmented interpolations using field data within plume

3.6 Summary and conclusions

In this paper we introduced and tested a new method, flow guided interpolation (FGI), for generating continuous concentration data in the area of contaminant plumes in groundwater. In comparison to pure interpolation by ordinary kriging, FGI offers clear advancement in the use of modeled data on flow direction and the respective shape of the contaminant plume: (i) the sampling point list used for interpolation is complemented by auxiliary sampling points along the plume fringe and (ii) the plume area is segmented into a series of plume sectors, depending on the plume's curvature. The interpolation is therefore termed "flow guided". The new method also features a sequential sector-wise interpolation in downgradient direction. Results generated in one sector are used for subsequent interpolation of the next sector, i.e. information is virtually propagated downgradient. In this way, the FGI method counteracts the decline in available measurement data with increasing distance to the source zone, as is typically observed in practice.

The FGI method has been implemented in ArcGIS using VBA code to automize major steps of the method's procedures. Based on the detailed descriptions and illustrations given in this paper, these procedures may easily be transferred to other geographical information systems that allow for expanding and customizing functionalities.

The evaluation of the method using varying segmentation settings and sample data sets of different size showed the robustness of the method. Estimated concentration distributions agree well with the reference distribution, independent of the setting and the data set which have been chosen. Results from the method's application to a model site confirm its practicability. The advantage of the FGI-method over "unguided" ordinary kriging was shown to be especially large when available sampling data is scarce. Although a rigorous analysis of the FGI method's performance by means of numerical experiments remains to be completed, the results presented in this paper obviously demonstrate that the method meets the demands of a realistic representation of contaminant plumes in groundwater at early investigation stages.

3.7 Acknowledgments

The authors gratefully acknowledge the support of the German BMBF research priority program REFINA (contract no. 0330757C). Funding for this study also has been provided by the Helmholtz Centre for Environmental Research - UFZ in Leipzig (contract no. 4500029698). The authors would also like to thank Margaret Hass for language editing of the manuscript.

3.8 List of symbols

Table 3.5: List of symbols, their definitions and units

α_s	anisotropy direction angle for sector *s*	(°, E = 0°, CCW)
β_i	angle between adjacent plume center pathline elements	(°, E = 0°, CCW)
c_i^{est}	estimated concentration value on grid node *j*	(μgl^{-1})
c_i^{ref}	reference concentration value on grid node *j*	(μgl^{-1})
$C_{lb,s}$	concentration at downgradient boundary of sector *s*	(μgl^{-1})
C_{source}	source concentration	(μgl^{-1})
C_{tc}	threshold concentration at lateral plume fringe	(μgl^{-1})
$C_{ub,s}$	concentration at upgradient boundary of sector *s*	(μgl^{-1})
h	separation vector of sample pair	(m)
i	generic increment variable	
j	number of grid node elements in estimated raster grids	
L	longest dimension of contaminant plume in direction of separation vector *h*	(m)
$l_{crit,i}$	normal distance of plume center pathline node to elongation line	(m)
l_i	length of center pathline element between to nodes	(m)
L_{tot}	total plume length in direction of groundwater flow	(m)
n_{step}	generic increment variable	
n	total number of points on plume's center pathline	
N	number of sample pairs	
RA_s	anisotropy ratio in sector *s*	
s	sector number	
S_{seg}	segmentation criterion	(m)
W_s	mean width of sector *s* (m)	
x	point x–cordinate	(m Gauss-Krüger)
y	point y–cordinate	(m Gauss-Krüger)
$x_{bd,s}$	sector boundary point x–cordinate	(m Gauss-Krüger)
$y_{bd,s}$	sector boundary point y–cordinates	(m Gauss-Krüger)

Chapter 4

A screening level method to derive contaminant distributions in groundwater for early stage assessments of brownfields[1]

Abstract The complexity and scale of groundwater contamination at mega-sites requires an early identification and prioritization of focal areas and risks in order to drive further decisions concerning detailed investigation programmes and remediation measures. There is a need for the enhancement and appropriate processing of sparse amounts of groundwater contamination data, especially during the early investigation stages of mega-sites. We present a flow guided interpolation method (FGI) that has been adapted to the type, scale and information basis that are typically available at the early stages of revitalization projects at contaminated sites. Comparison of remediation cost estimations against investigation expenses show how uncertainty about required remediation measures and associated costs change during tiered brownfield revitalization projects.

Keywords particle tracking; interpolation; mega-site management; groundwater contamination; GIS; remediation costs; FGI

4.1 Introduction

Proposed methods to estimate the spatial distribution of contaminants dissolved in groundwater range from experience-based practitioners' methods to advanced model-based methods [e.g. Michalak and Kitanidis, 2004a, Miles et al., 2008]. The appropriateness of individual methods is dependent on the amount and quality of available data as well as on the particular objectives. Plume delineation focusing on determining the extent of the plume [McGrath and Pinder, 2003] may call for methods other than the estimation of the concentration distribution using geostatistical interpolation methods [e.g. Boufassa and Armstrong, 1989, MacKay, 1990,

[1]reproduced from: M. Morio, M. Finkel (2011): GQ10: Groundwater Quality Management in a Rapidly Changing World (Proc. 7th International Groundwater Quality Conference held in Zürich, Switzerland, 13-18 June 2010). IAHS Publ 342, 189-193, 2011.

Deutsch and Journel, 1997, Kerry and Oliver, 2007]. A common problem in practice is that available contaminant concentration measurement data is not sufficient to make sensible use of geostatistical methods. Limited availability of contaminant data is characteristic of early project stages when the only available information on subsurface contamination stems from historical data and some initial site investigations. In this paper we demonstrate the aptness of a flow guided interpolation (FGI) method developed by Morio et al. [2010], which is specifically designed to cope with limited contaminant data. In particular we show the implications of FGI results obtained at a field site for different investigation stages for the assessment of future land use scenarios regarding groundwater contamination.

4.2 Methods

4.2.1 Flow guided interpolation

The FGI method builds upon a steady-state groundwater flow and advective transport model (here: MODFLOW96 and MODPATH), assuming that basic information about the heterogeneity of the groundwater flow regime can be made available at relatively low cost. Guidance by groundwater flow is intended to improve the interpolation, especially if contaminant concentration data is scarce. The method proposes to add extra sampling points in a standardized way through coupling of flow data and existing samples plus information about possible source zone extents to enable the application of kriging methods. Interpolation is done sector-wise from source zone in downgradient direction and incorporates information from upgradient areas generated before (Fig. 4.1 (A)). A detailed explanation of the method and its underlying assumption is given in Morio et al. [2010].

We apply a simple model for the estimation of investigation costs. It considers unit costs for sampling well installation and for sample analytics. Unit cost factors for the demonstration site are listed in Table 1.

Remediation costs are calculated as a function of the planned land use. Individual land use types (e.g. housing, trade, recreation) are translated into contaminant-specific subsurface quality targets, which in turn are translated to raster maps representing the spatially distributed remediation target values. These maps are compared with the contaminant distribution in groundwater, estimated using the FGI. A GIS-based conflict analysis yields exceedence maps for each of the contaminants being considered. These maps, together with further site specific information, serve as an input to the remediation cost estimation model. Cost estimates are based on the volume of unacceptably high contaminated groundwater (following Bonnenberg et al. [1992]; see also Schädler et al. [2008]). See Morio et al. [2008] for a detailed description of the conflict analysis method.

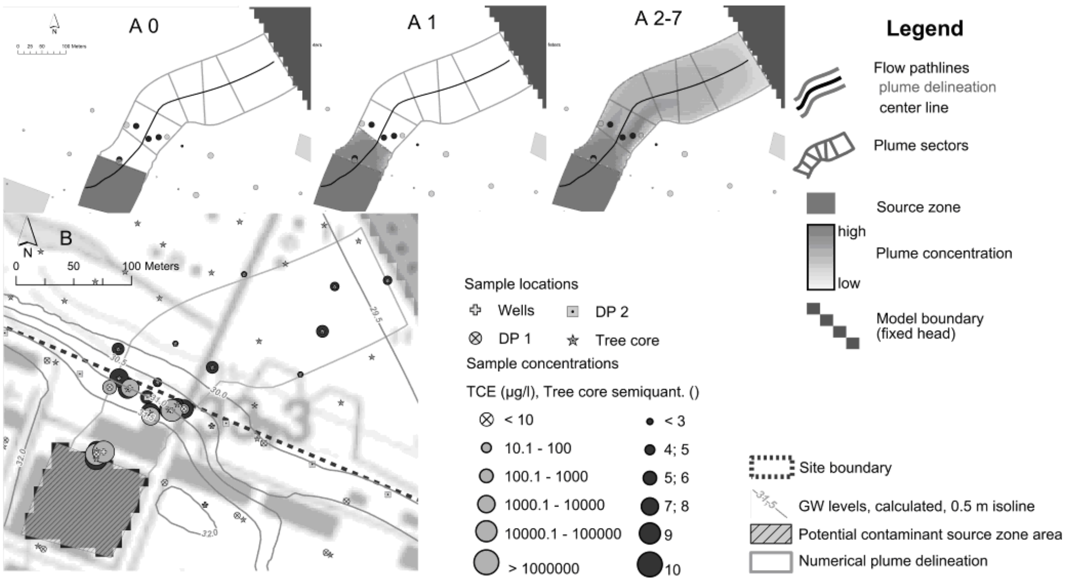


Figure 4.1: FGI Method (A0-7) and demonstration site showing field data (B).

4.3 Application, results and discussion

The model site is an abandoned military base covering 120 ha on the outskirts of Potsdam near Berlin, Germany. The site was turned into a brownfield in the early 1990s. Gas stations and a dry cleaning facility represent the major sources of subsurface contamination which, as far as known, is dominated by light chlorinated hydrocarbons. A detailed site description and information about conducted subsurface investigation are available in Morio et al. [2008], Rein et al. [2008a], and Schädler et al. [2008]. In this study we focus on a TCE plume that has been investigated in several campaigns, denoted as “Wells”, “DP1”, “DP2” and “Treecore” (Table 4.1). Conflicts were identified for two land use scenarios. Scenario (A) assumes a uniform residential land use with a constant TCE target value of 20 μg/L. Scenario (B) assumes a residential area within the premises of the site and a renaturation area outside the site in the north, where no relevant exposure is expected.

Table 4.1: Investigation cost estimation. *) Cost for analysis of samples: 100 €/sample; **) DP stands for Direct Push.

Investigation phase	Sample points (–)	Type	Installation costs/point (€)	Samples analysed (–)*)	Total costs (€)
Wells	4	GW-well	2500	4	10400
DP1	3	DP-well**)	600	7	2500
DP2	1	DP-well	600	8	1400
Treecore	22	Plants	–	30	3000
Total	30	–	–	49	17300

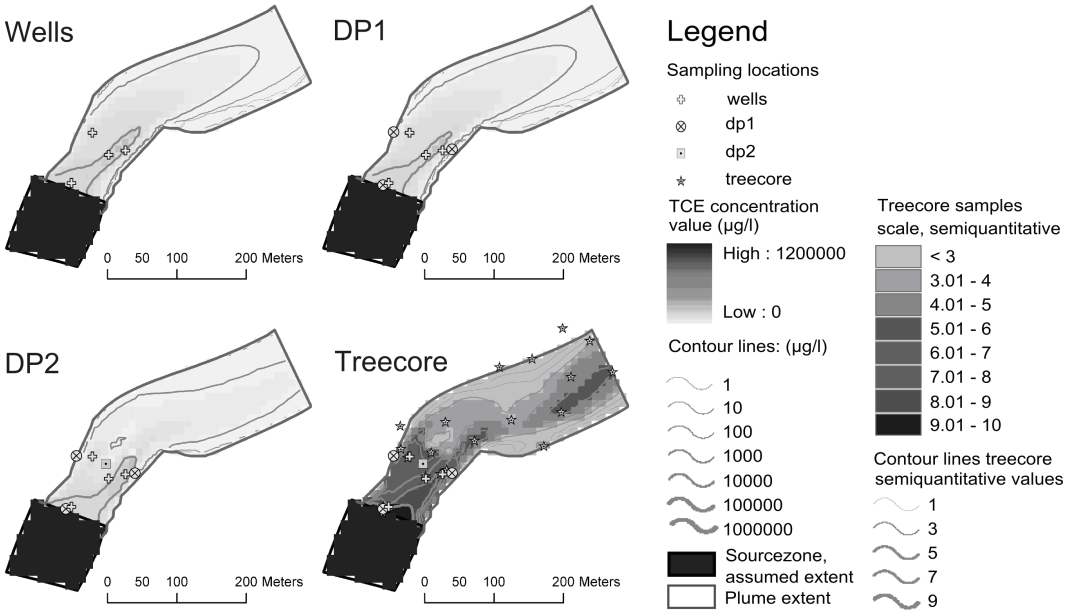


Figure 4.2: FGI Results of segmented interpolations (FGI) using field data within plume.

The results of the FGI application are depicted in Fig. 4.2. Estimated contaminant distributions were used to calculate remediation costs based on conflicts of existing contamination with remediation targets (Fig. 4.3). To show the effect of the interpolation method on the cost estimates, results obtained for concentration distributions derived with ordinary kriging (OK, no anisotropy, no trend) are shown for comparison. Differences between FGI and OK do strongly depend on the particular land use scenario. For Scenario (B) cost estimates vary only slightly as costs are driven only by contamination within the site premises, where estimates of both OK and FGI are similar, both being dominantly influenced by source zone data. For Scenario (A) differences are considerably larger and do vary in magnitude depending on the investigation phase. Using FGI, similar estimates of remediation costs for the phases “Wells”, “DP1” and “DP2” indicate that new data do not essentially change the interpretation, as all investigations are focused on the area close to the source zone (Fig. 4.2). “Treecore” data of the plume section further downstream considerably changes cost estimates.

4.4 Acknowledgements

The authors gratefully acknowledge the support of the German BMBF research priority program REFINA (contract no. 0330757C). Funding for this study also has been provided by the Helmholtz Centre for Environmental Research - UFZ in Leipzig contract no. 4500029698). Thanks go also to Kirsten Oswald for language

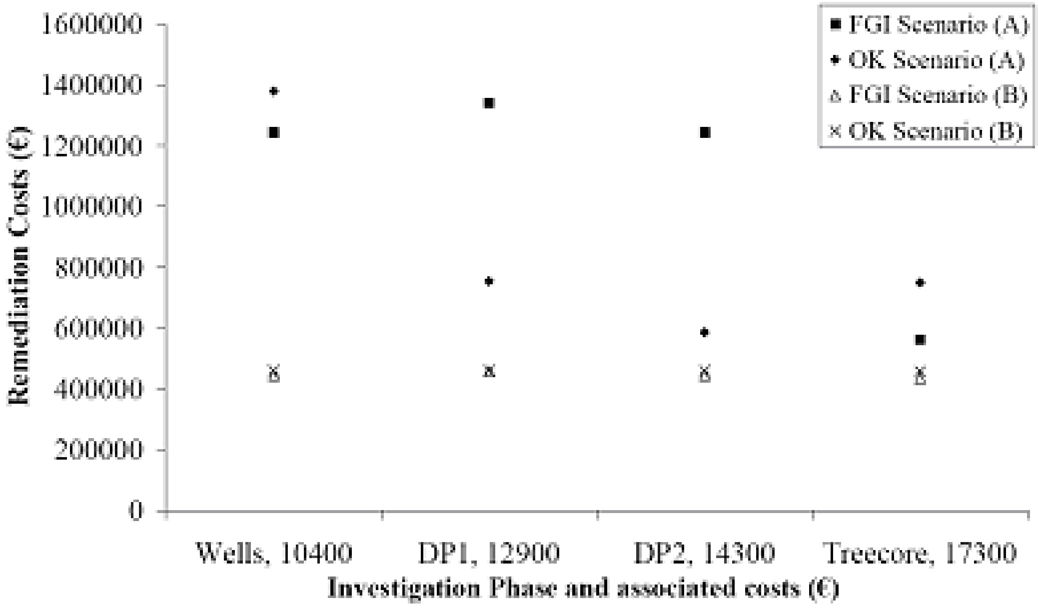


Figure 4.3: Investigation phase vs remediation cost estimation.

editing of the manuscript.

Chapter 5

Designing sustainable and economically attractive brownfield revitalization options using an integrated assessment model[1]

Abstract We describe the development of an integrated assessment model which evaluates redevelopment options of large contaminated brownfields and we present the application of the model in a case study. Aiming to support efficient and sustainable revitalization and communication between stakeholders, the presented assessment model integrates three pinnacles of brownfield revitalization: (i) subsurface remediation and site preparation costs, (ii) market-oriented economic appraisal, and (iii) the expected contribution of planned future land use to sustainable community and regional development. For the assessment, focus is set on the early stage of the brownfield redevelopment process, which is characterized by limited data availability and by flexibility in land use planning and development scope. At this stage, revealing the consequences of adjustments and alterations in planning options can foster efficiency in communication between the involved parties and thereby facilitates the brownfield revitalization process.

Results from the case study application indicate that the integrated assessment provides help in the identification of land use options beneficial in both a sustainable and an economical sense. For the study site it is shown on one hand that brownfield redevelopment is not automatically in line with sustainable regional development, and on the other hand it is demonstrated that additional contributions to sustainability are not intrinsically tied to increased costs.

Keywords brownfield; integrated assessment; sustainability; remediation cost; decision making; contaminated land appraisal

[1]reproduced from: Schädler, S., Morio, M., Bartke, S., Rohr-Zänker, R. and M. Finkel (2011). Designing sustainable and economically attractive brownfield revitalization options using an integrated assessment model. Journal of Environmental Management 92(3),827 – 837, DOI:10.1016/j.jenvman.2010.10.026.

5.1 Introduction

5.1.1 Brownfield revitalization

Different definitions in both Europe and the US similarly describe brownfield sites as abandoned or underused properties, for which intervention is required to ensure beneficial reuse because of the real or suspected presence of hazardous substances, pollutants or contaminants [CABERNET, 2005, U.S.EPA, 2002]. The health and economic threats of Brownfields as well as the challenges and potential of their reuse are recognized world-wide and international literature describes concerns related to brownfields e.g. in Africa [e.g. Haylamicheal and Dalvie, 2009, Kaufman et al., 2005], Asia [e.g. Cao and Guan, 2007, Zhang and Wong, 2007], Australia [e.g. Apostolidis and Hutton, 2006, Toms et al., 2008], and Canada [e.g. C.De, 2001, NRTEE, 2003]. Estimated costs for restoration of large brownfield sites in the US range from $100 billion [U.S.EPA, 2003] to over $650 billion [NRTEE, 2003] and for the European Union amount to almost EUR100 billion [EEA, 2000].

When brownfields are especially large in terms of area, prominence, relevance, seriousness, regional significance, complexity of contamination and of stakeholder networks, they are typically referred to as megasites in more recent literature [Agostini et al., 2007, Bardos, 2004]. The revitalization process of such sites may be complicated e.g. by extensive investigation efforts, intricate negotiation among stakeholders with potentially differing interests, large uncertainties, and time-consuming and costly cleanup that may outrun any market interest by far [Bardos, 2004, NRTEE, 2003]. The consequence of this is that many of the most complex brownfields to date remain undeveloped.

On the other hand, successful brownfield revitalization can benefit from the typically prominent location of the sites and of already existing infrastructure and it can drastically enhance sustainable regional development [Bardos et al., 2000] by contributing to a reduction of land consumption and urban sprawl [Nuissl and Schroeter-Schlaack, 2009]. Large sites additionally provide developers with a wide scope of planning for the design of future land use options, i.e. the use types considered and their allocation on the site. Only if this freedom is exploited in order to optimally trade-off between the partly conflicting goals of maximizing land value (i.e. realization of valuable land use types), minimizing remediation costs (i.e. by optimal definition and allocation of land use types with respect to exposure to contaminants), and at the same time contributing to a sustainable urban and regional development, revitalization of large brownfields can be successful [De Sousa, 2006].

5.1.2 Necessity for appropriate decision support systems

The concept of spatial decision support systems (sDSS) evolved from the need to make decisions based on quantitative and qualitative spatial data in geographic information systems (GIS) [Densham and Goodchild, 1989]. Interest in sDSS research has been continuously increasing [Malczewski, 2006] and so has their use for comparative analysis of environmental management alternatives [Ascough et al., 2008], when the high uncertainty associated with forecasting consequences to future actions [Walker et al., 2003] could otherwise result in inaction or improper action like excessive data collection [Reichert and Borsuk, 2005, Smit and Smit, 2003, Wang and McTernan, 2002].

A wide variety of methods to date deal with one or a number of aspects of brownfield revitalization such as risk assessment [e.g. Carlon et al., 2008, Semenzin et al., 2007b, Strenge and Chamberlain, 1995], policy analysis [e.g. Linkov et al., 2006], optimization of remediation [e.g. Ahlfeld et al., 1995, Burger et al., 2007, Wang and McTernan, 2002], remediation cost assessment [e.g. Kaufman et al., 2005], general success factors for brownfield redevelopment [e.g. Lange and McNeil, 2004, Nijkamp et al., 2002], infrastructure redevelopment [Attoh-Okine and Gibbons, 2001], urban planning and site prioritization under budget constraints [e.g. Alvarez-Guerra et al., 2009, Stevens et al., 2007] and mediation of negotiation [Sounderpandian et al., 2005].

Despite the variety of models, several authors have recently described additional need for DSS for contaminated land reuse, which integrate the manifold relevant topics into one system and manage the complicated balance between complexity of information and transparency of results [e.g. Agostini and Vega, 2009, Agostini et al., 2007, Bardos et al., 2001, Tam and Byer, 2002], and that provide guidance to stakeholders while analyzing the huge number of factors that influence optimal future land use on large contaminated sites [Carlon et al., 2007a]. In particular further development of DSS that integrate an assessment of sustainability has been claimed [Hassan, 2004]. Although several definitions of sustainability criteria are described in literature, as well as models to assess the sustainability of land use options [e.g. Wedding and Crawford-Brown, 2007, Zavadskas and Antucheviciene, 2006], most DSS today still do not integrate such assessments. This is explained by the topic's abstract notion [Esty et al., 2005], its multidimensionality [Doick et al., 2009, Jakeman et al., 2008], and a perceived lack of transparency and objectivity.

5.1.3 Objectives

The objective of this work was to provide an integrated assessment model, which is based on the use of screening level data and serves as a spatial decision and communication support system for the comparative evaluation of alternative brownfield redevelopment options. The following key factors (modified from Tam and Byer [2002]) were considered in this sDSS:

1. Examine alternative clean up goals.

2. Examine alternative site use options.

3. Examine the social, economic, and ecological sustainability of land use alternatives.

4. Estimate all of the economic implications, including clean-up costs, liability, and site use benefits.

5. Examine uncertainties.

6. Be computationally feasible and accessible to stakeholders.

7. Generate results that are understandable to stakeholders (not only to experts in the respective fields).

By encouraging stakeholders to communicate their different expectations towards brownfield redevelopment, the model is meant to promote concerted, constructive and site-specific compromises, thereby fostering the optimal exploitation of the sites' physical planning scope which enables successful revitalization. The focus of this paper is the description of the framework of methods that underlie the integrated assessment, as well as the discussion of results from their application to a case study site.

5.2 Description of Methods

5.2.1 Data Requirements

The proposed integrated assessment requires a set of general site-specific data and subsurface conditions including aquifer geometry, properties and contamination (Table 5.1). In addition to this, the redevelopment options of the site need to be specified in terms of land use maps (i.e., the spatial allocation of defined land use types on the site). Redevelopment options that shall be assessed may stem from proposals made by the local authority's planning board or from the investor's plans, but can also be the result of stakeholder discussions and/or iterative re-planning guided by the results of an assessment model as is presented herein. The description of the redevelopment options is complemented by a set of parameters that characterize the particular land use types being considered.

The parameter set is composed of reference values for the price of clean land in order to reflect the land use-specific potential revenues from revitalising the site, and compliance criteria for contaminant concentration in soil and groundwater. These compliance criteria define levels of environmental quality, which need to be achieved in order to permit the planned future use of the site. Levels may be defined using human health risk assessment methods [e.g. Marsland and Carey, 1999, Strenge and Chamberlain, 1995, U.S.EPA, 1991] or based on regulatory remediation goals [Rügner et al., 2006], and they should always be established in cooperation with local authorities in order to achieve the commensurate and reasonable levels required by law [Begley, 1996]. For the sustainability assessment and market value appraisal further information needs to be gathered about the (non-)existence of several key features, attributes and attractions of the site (assuming the redevelopment option under consideration has been implemented) and the surrounding region.

Table 5.1: Required input data for the integrated assessment model.

		Spatial data	Non-spatial data
Site-specific	Location and extent of site	x	
	Digital Elevation Model	x	
	Depth and thickness of contamination in soil and groundwater	x	
	Aquifer top and bottom	x	
	Hydraulic conductivity	x	
	Distribution of contaminant(s)	x	
	Contaminant properties		x
	Unit cost data for remediation		x
	General conditions of the site (social, economic, ecological)	x	x
Option-specific	Reference values for price of clean land		x
	Compliance criteria for contaminant concentration		x
	Planned allocation land use options	x	
	Buildings to be deconstructed		x
	Information on site features, attributes, and attractions		x

5.2.2 Conflict Analysis

The conflict analysis is comprised of a set of GIS-based procedures which identify those regions on the site that will require remediation given the information on the distribution of contaminants, as well as on the map of compliance criteria attributed to each specific redevelopment option. The resulting raster maps of exceedance factors for each contaminant of concern indicate areas and magnitudes of conflicts and serve as an input for the estimation of soil and groundwater remediation costs.

In addition, conflicts can be assessed under the assumption that the entire site is uniformly used. This enables planners to identify land use type allocations which are free of conflicts and thus do not require remediation. These supplementary conflict maps provide insight into the opportunities offered when future land use is optimally allocated and give valuable support for an iterative re-planning of land use options.

5.2.3 Estimation of Costs for Site Preparation

The cost estimation model covers (i) groundwater remediation costs and (ii) soil remediation costs, which from the real estate appraisers' point of view are among the most influential cost factors to affect investors' decisions on the redevelopment of brownfield sites [e.g. Dotzour, 2002, Healy and Healy, 1992], as well as (iii) costs related to the deconstruction of buildings. Costs of other and more specific site preparation activities that may be required (e.g., demolition of subsurface infrastructure, asbestos disposal, etc.) are not considered due to the simplicity of this model.

5.2.3.1 Groundwater Remediation Costs

Costs for groundwater remediation are estimated using two models: (i) a model to calculate costs of remedial activities on site that are necessary to resolve conflicts between planned land use and the contamination situation, and (ii) a model to estimate costs of additional measures in order to avoid unacceptable risks to neighbours. Such measures may be necessary if the contaminant flux across site boundaries is expected even after revitalization has taken place, e.g. because contamination on site is partly or entirely left in place due to insensitive land use and associated compliance criteria. In this case costs for plume containment along the concerned site boundary are considered.

Model I estimates the land use related costs for groundwater clean-up, C_{GW} [EUR], based on the volume of contaminated groundwater and the respective magnitude of exceedance factors as calculated previously in the conflict analysis. Based on this, costs are calculated with an empirical method following Bonnenberg et al. [1992] who designed and validated the method for a quick and convenient evaluation of a large number of sites without explicit differentiation between remediation techniques. The method only requires little detail in input data for the estimation of groundwater remediation costs: spatial information about top and bottom of the contamination (yielding the contaminated volume V [m^3]) as well as about the type and level of contamination. For a map of exceedance factors that contains n conflicting cells, groundwater clean-up costs C_{GW} [EUR] are summed up as follows:

$$C_{GW} = \sum_{i=1}^{n} C_{u,GW} V_i f_{D,i} f_{K,i} f_{L,i} n_{eff} \tag{5.1}$$

where $C_{u,GW}$ [EUR/ m^3] are standard unit costs of contaminated groundwater clean-up, n_{eff} is the effective porosity of the contaminated aquifer volume [%], and f_D [-], f_K [-] and f_L [-] are spatially variant factors considering the severity of the contamination in terms of depth (shallow, medium, deep), contaminant group and degree of contamination (low, medium, high and non-aqueous phase), respectively.

Additional costs for plume containment along the site boundaries are calculated using model II in terms of a screening level estimation based on the contaminant flux across site boundaries. A permeable reactive barrier (PRB) filled with zero-valent iron is taken as a reference plume containment technology for chlorinated hydrocarbons (see case study below). Investment costs C_I [EUR] for containment of each contaminant plume are estimated following the cost functions introduced by Bürger et al. [2003] and are based on an approximate calculation of required PRB dimensions.

$$C_I = \underbrace{w S_{het,1} m_{Aq} T}_{V_B} (C_{RM} f + C_E (1 - f)) + C_S \tag{5.2}$$

The required PRB volume V_B [m^3] is represented by the width w [m] of the contaminant plume, corrected for the safety factor $S_{het,1}$ [-] that accounts for flow direction variability [Benner et al., 2001, Elder et al., 2002], the aquifer thickness m_{aq} [m], and the thickness of the reactive barrier T [m]. The latter is defined by $T = K_f n_{eff} I S_{het,2} t_c$, where multiplication of the hydraulic conductivity K_f [m s^{-1}], the hydraulic gradient I [-], and the effective porosity n_{eff} [-] yields the groundwater flow velocity in the barrier. The safety factor $S_{het,2}$ [-] accounts for variations in this flow velocity due to aquifer heterogeneities [Benner et al., 2001, Elder et al., 2002], and t_c [s] is the necessary contact time $t_c = \log(c_0/c_{target})\lambda$ between the contaminant and the reactive material, which depends on the actual concentration c_0 [μgl^{-1}], the compliance value i.e. accepted maximum concentration c_{target} [μgl$^-1$], as well as on the contaminant's degradation rate constant λ [s$^-1$]. CE [EUR m^{-3}] and CRM [EUR m^{-3}] represent unit costs per volume of earthworks and reactive material (here: zero-valent iron), respectively. Where the barrier thickness T equals values smaller than the technically achievable thickness T_{min}, the dimensionless factor $f = T_{min}/T$ corrects the actual physical thickness of the barrier and the amount of reactive material. Otherwise f equals 1. C_S [EUR] represents site mobilization costs.

In order to account for deactivation of zero-valent iron during PRB operation, these investment costs are applied again as reactivation costs after regular periods during the required total operation time and discounted to present value costs [see e.g. Lemser and Tillmann, 1997].

It should be noted that literature values are available for many of the above mentioned parameters as shown in the supplementary data. These can be used for a screening-level assessment if site-specific data is not available.

5.2.3.2 Soil remediation costs

The model for estimating soil remediation costs C_s follows the framework KONUS commissioned by the German Federal Environmental Agency [Umweltbundesamt, 1995]. Cost estimates are calculated based on contaminated soil volume V_{cont} [m^3] and technology-specific unit costs $C_{U,k}$ [EUR]:

$$C_s = V_{cont} \min C_{U,k}, \quad k \in i : A(M_i) \geq th_A \times A(M_j) \forall i, j \in 1, \ldots, n_M \tag{5.3}$$

with

$$A(M_i) = \sum_{l=1}^{n_c} (a_c a_A a_D a_{Kf})_l$$

For each of the n_M remediation methods M considered (here $n_M = 12$), the method's technical appropriateness $A(M_i)$ for the prevailing mixture of a number of n_c contaminants is determined by specific suitability values a_c, a_A, a_D and a_{Kf}, which depend on the contaminants present, size of the contaminated area, depth of the contamination and on the aquifer's hydraulic conductivity, respectively. Only those remediation methods are considered which show a sum of suitability values that is above a certain threshold fraction th_A of the best of all methods. Among those, the least costly method is chosen for the cost estimation. Similar to the approach described by Kaufman et al. [2005], the model considers 11 typical contaminant groups which are described by specific properties concerning mobility and oral and respiratory toxicity.

5.2.3.3 Building deconstruction costs

The calculation model for building deconstruction costs *BDC* [EUR] is adapted from Umweltbundesamt [1995]. The cost calculation is based on gross cubic space V [m^3] of the buildings and a set of refining factors:

$$BDC = \sum_{i=1}^{n} (f_u f_W f_S f_H C_u V)_i \tag{5.4}$$

where f_U [-], f_W [-], f_S, [-] and f_H [-] represent empirical cost-driving factors for the kind of use, the wall thickness, slab thickness and the height of each of a total number of n buildings, respectively. C_u [EUR m^{-3}] is the unit cost which again depends on the type of building, as well as on gross cubic space categories for each building.

5.2.4 Market value estimation and mercantile value reduction (MVR)

Although it is theoretically possible to derive the value of brownfield sites in a comparative purchase price analysis of (previously) contaminated sites which have been sold, the necessary market data of comparable transactions is often not available in practice. Therefore, the market value of a contaminated property is traditionally estimated using a residual value approach, in which expected costs for site preparation are subtracted from the value of a comparable uncontaminated site [Adair et al., 2001, Rinaldi, 1991]. However, due to perceived remaining risks, revitalized brownfields are usually prized considerably below this value, as has been described in literature within the last three decades [cf. Bell, 1999, Jackson, 2001, Mundy, 1992, Patchin, 1988, Syms and Weber, 2003]. In order to correctly account for these value reductions, our model uses two steps to assess the site's market value. In a first step a so-called theoretical land value $V_{L,theor}$ of cleared land is estimated in a residual value approach by subtracting site preparation costs from the reference value of a comparable but clean real estate. The latter is obtained using reference land values per square meter of distinguished land use types [e.g. GSD, 2010]. Costs for soil and groundwater remediation and deconstruction of buildings are subtracted from the $V_{L,theor}$ in order to obtain the preliminary land value $V_{L,pre}$.

In a second step, a mercantile value reduction (MVR) is applied (equation 5.5). MVR is a scoring method proposed by Bartke and Schwarze [2009b] with the scope of reducing the contradictions frequently found between existing risks and those perceived by marketers [Patchin, 1991, Mundy, 1992]. The concept is based on an international real estate literature survey and a poll of German appraisal experts and it represents a market value markdown (here: a reduction of $V_{L,pre}$) caused by perceived uncertainties regarding rehabilitation, risk of future liability claims, investment risks, utilization risks, as well as stigma and marketability risks. The method quantifies a risk rebate based on (i) local site characteristics, (ii) the information level of the site's redevelopment costs, and (iii) the ability to pass on the monetary risk to others.

Following the concept of Bartke and Schwarze [2009b], a set of local site characteristics (e.g. "Poor demarcation of (suspected) contamination", "Great media attention for contamination risk") are key determinants of the value reduction of a brownfield site as derived from a literature analysis [e.g. Jackson, 2002, Kleiber et al., 2007]. These key characteristics are specified during a site evaluation by the stakeholders' input U. The average value diminution level m_i [-], as well as the respective weights $w_{S,i}$ [-] of each key local characteristic are median values from the aforementioned expert poll, and thus represent extensive empirical knowledge from previous revitalization projects. Evaluation of the sum of local characteristics results in a relative value reduction FL between 5% and 30%, which is subsequently adjusted for the factors "time" F_T and "risk" F_R.

$$MVR = V_{L,pre} \underbrace{\sum_{i=1}^{15} (m_i(U) w_{S_i})}_{F_L} \times \underbrace{\sum_{T_i=1}^{2} (w_{T_i} - 1)}_{F_T} \times F_R \qquad (5.5)$$

The informational factor "time" F_T , which is determined by the weights w_{T_1} and w_{T_2}, reflects the fact that MVR drops over time (i) before site rehabilitation due to increasing availability of detailed information about remediation costs from site investigation (Table 5.2), and (ii) after site rehabilitation as remaining stigma of the previously contaminated site diminishes over time. Finally, the "risk" factor F_R corrects for the fact that, depending on the market situation, potential risks could be passed on from the sellers to the buyers of a site, thus decreasing the value reduction. The MVR risk factor F_R takes values between zero (for acute shortage and great demand in a booming market) and one (big oversupply of similar properties), and will equal 0.5 in a balanced market.

The site's market value is obtained by subtracting MVR from the preliminary land value only where $V_{L,pre}$ is positive. Otherwise both MVR and the market value are set to zero.

5.2.5 Sustainability assessment

The sustainability assessment method evaluates the compatibility of land use types and specific future planning options with the goal of sustainable urban development in terms of the principles of the Agenda 21 [ICLEI, 1994, United Nations, 1992] and the three fundamental dimensions of ecological, social and economic sustainability.

Table 5.2: Empirical uncertainty in remediation costs as a function of investigation/information levels [Kerth and van de Griendt, 2000], and the resulting "time" factors for estimation of MVR as evaluated by Bartke and Schwarze [2009b].

Information level	No study	Historical investigation	Phase 1 investigation	Phase 2 investigation	Phase 3 investigation	Remediation Plan	Remediation completed
Lower limit	10%	20%	50%	70%	80%	85%	100%
Upper limit	280%	260%	200%	160%	140%	130%	100%
Resulting factor "time"	1.45	1.4	1.25	1.15	1.1	1.08	1

Within this general framework the focus was set on the main areas of local governments' planning policies [see e.g. pilot projects of sustainable urban development in Germany: Deutsche Umwelthilfe e.V., 2004, Fuhrich, 2004, ICLEI, 2004, Teichert, 2000], which are reflected by five first level goals (i) sustainable land management, (ii) preservation of nature and landscape, (iii) preservation of resources and reduction of emissions by intelligent mobility management, (iv) high quality residential environment, and (v) strengthening of municipal economy. These goals are represented by a set of indicators, as is common practice in international sustainability evaluations [Esty et al., 2005, Hansen, 2009, Shmelev and Rodríguez-Labajos, 2009], especially on larger scales with comparably limited data density, where a convenient comparison of results and promotion of further detailed stakeholder discussion is achievable only by simplification. The assessment method, namely the anticipation of effects of different types of land use on a specific site and its vicinity, made it necessary to develop new indicators since most of the commonly applied indicators of sustainable urban development (a) are used for ex post comparisons but not for predictive assessments [Singh et al., 2009] and (b) are not focused on specific characteristics of a brownfield site's allocation.

The resulting 22 indicators (Table 5.3) are related to forms of settlement and land use and describe qualitative and quantitative features of a site and its vicinity. The existence or absence of these features is used to express whether and how a specific land use option will either foster or contradict the goals of sustainable urban development. For each spatial planning unit and attributed land use type, it is evaluated whether the descriptive statements of the individual indicators k are applicable or not. This evaluation is done based on spatial data created according to regional maps, aerial photographs data from (historical) site investigations and stakeholder knowledge. The resulting Boolean (TRUE/FALSE) answers translate into integer values (Table 5.3) which are multiplied with the individual weight for each indicator k to obtain a positive or negative actual score p_k^+ and p_k^-. The degree of suitability

Table 5.3: Sustainability first and second level goals, and representative indicators used for assessment. Evaluation by "TRUE/FALSE" statements translates into integer value pairs (TRUE: first value, FALSE: second value). "n": no relevance with respect to the given land use type (i.e. "0/0").

	Weighting (%)	I. Residential	II. Local Services	III. Recreational	IV. Trade/ Industries	V. Emitting industries	VI. large-space business centres	VII. Monofunctional facilities w/ large open spaces
1. SUSTAINABLE LAND MANAGEMENT								
1.1: Realization of short distances by complementing land uses								
1.1.1 Residential Areas in the surrounding area	10	n	-1	1/0	1/0	n	n	n
1.1.2 Green spaces in the surrounding area	10	1/0	n	n	n	n	n	n
1.1.3 Local supplies within walking distance	10	1/0	n	n	n	n	n	n
1.1.4 Neighbouring uses are strongly emitting	20	-1/0	n	-1/0	n	n	n	-1/0
1.2: Prevention from additional soil sealing								
1.2.1 Site contains <40% sealed soil	10	n	n	-1	-1/0	-1/0	-1/0	-1
1.3: Support for urban inner development								
1.3.1 Site location within urban area	40	-1	-1	n	-1	n	n	n
2. PRESERVATION OF NATURE AND LANDSCAPE								
2.1: Preservation of sites important for urban ecology								
2.1.1 Site is part of a local habitat	40	-1/0	-1/0	n	-1/0	-1/0	-1/0	-1/0
2.1.2 High value tree or plant populations	20	n	n	n	n	-1/0	-1/0	n
2.2: Conservation of natural reserves								
2.2.1 Direct vicinity to nature reserve	40	-1/0	n	n	n	-1/0	-1/0	n
3. RESOURCE-CONSERVING & EMISSION-REDUCING MOBILITY MANAGEMENT								
3.1: Preventing overburdening of local road system								
3.1.1 Low capacity of access roads	30	n	n	n	-1/0	-1/0	-1/0	-1/0
3.2: Reduction of individual car use								
3.2.1 Good access to public transport	40	-1	-1	1/0	-1	n	-1	-1
3.3: Protection of residents from transport emissions								
3.3.1 Access to clearway	20	n	n	n	n		-1	n
3.4: Support for non-motorized mobility								
3.4.1 Good accessibility for bikers	10	-1	-1	-1	-1	1/0	1/0	1/0
4. HIGH QUALITY RESIDENTIAL ENVIRONMENT								
4.1: Good local supplies								
4.1.1 Local amenities in walking distance	10	-1	n	n	1/0	n	n	n
4.1.2 Primary school in walking distance	10	-1	n	n	n	n	n	n
4.2: Preservation and development of local recreational space								
4.2.1 Great impact on recreational areas	20	-1/0	-1/0	n	-1/0	-1/0	-1/0	-1/0
4.3: Preservation and upscaling of historic cityscape								
4.3.1 Historically relevant buildings	10	1/0	n	-1/0	1/0	-1/0	-1/0	1/0
4.3.2 Great influence on cityscape	10	n	n	1/0	n	-1/0	-1/0	n
4.4: Minimizing land use conflicts								
4.4.1 Neighbouring uses sensitive to immissions	40	n	n	n	n	-1/0	-1/0	n
5. STRENGTHENING OF LOCAL ECONOMY								
5.1: Small burden for local budget by investment/follow-up costs related to local infrastructure								
5.1.1 Good supply and disposal infrastructure	20	-1	-1	n	-1		-1	-1
5.2: Small burden for local budget related to site remediation								
5.2.1 Site strongly contaminated	30	-1/0	-1/0	-1/0	n	n	n	-1/0
5.3: Enhancement of local attractiveness by innovative businesses								
5.3.1 Site suitable for innovative industries	30	n	n	n	1/0	n	n	n
5.4: Preservation of business location								
5.4.1 adjacent enterprises w/ precarious sense of security	20	-1/0	n	n	n	n	n	n
maximum positive score: P+,max = f(weights)		160	120	80	170	50	90	90
maximum negative score: P-,max = f(weights)		-300	-210	-80	-210	-260	-300	-210

E is then calculated according to

$$E = \left(\frac{\sum_{k=1}^{22} p_k^+}{P_{max}^+} \times 100 \right) - \left(\frac{\sum_{k=1}^{22} p_k^-}{P_{min}^-} \times 100 \right) \tag{5.6}$$

where P_{max}^+ (P_{min}^-) represent the positive (negative) boundary for each land use type which is obtained by calculating the sum over each indicator's maximum (minimum) possible score (Table 5.3).

Case-study-specific default weights were applied for each indicator. These weights represent the state of scientific discussion about the relative importance of each respective goal and indicator for sustainable urban development in this specific context of the case study site. This setup may be changed by the evaluating experts to improve the representation of specific local conditions.

To evaluate specific redevelopment alternatives that consist of a number of n_P different planning units, equation 5.6 is evaluated separately for each planning unit i. The results for each planning unit are then weighted by the fraction of the area of the planning unit $A_{P,i}$ and the total site area A_S, and summed up into one resulting value E_{tot} for the entire site as shown in equation 5.7.

$$E_{tot} = \sum_{i=1}^{n_P} E_i \frac{A_{P,i}}{A_S} \tag{5.7}$$

This evaluation allows for a convenient and direct comparison of different site redevelopment options with respect to their contribution to sustainable development. Further details on the methodology are given in Müller and Rohr-Zänker [2009].

5.3 Case study

5.3.1 Description of model site

The model site is a former military site situated on the outskirts of the city of Potsdam near Berlin, Germany (see Figure 5.1). The site with an area of approximately 113 ha was used by German and Russian armed forces until 1945 and 1991, respectively. The operation of gas stations and a dry cleaning facility has led to vast contamination dominated by chlorinated solvents, which affect an aquifer with a thickness of 5 m. The depth of the water table is 2 m to 6 m below ground surface. Contaminated groundwater flows from the site towards two lakes, nature reserves, local recreation areas and other potential receptors. The surrounding areas contain businesses and industry as well as residential areas.

The site contains both listed historical buildings and economically worthless buildings constructed after 1945. Since 1992, the site has been investigated several times by various groups of consultants and researchers. More detailed site and data descriptions are given in Morio et al. [2008] and Rein et al. [2011].

The input data used for this case study is based on information from a detailed expert report about a site inspection in 1996 and on data from two groundwater

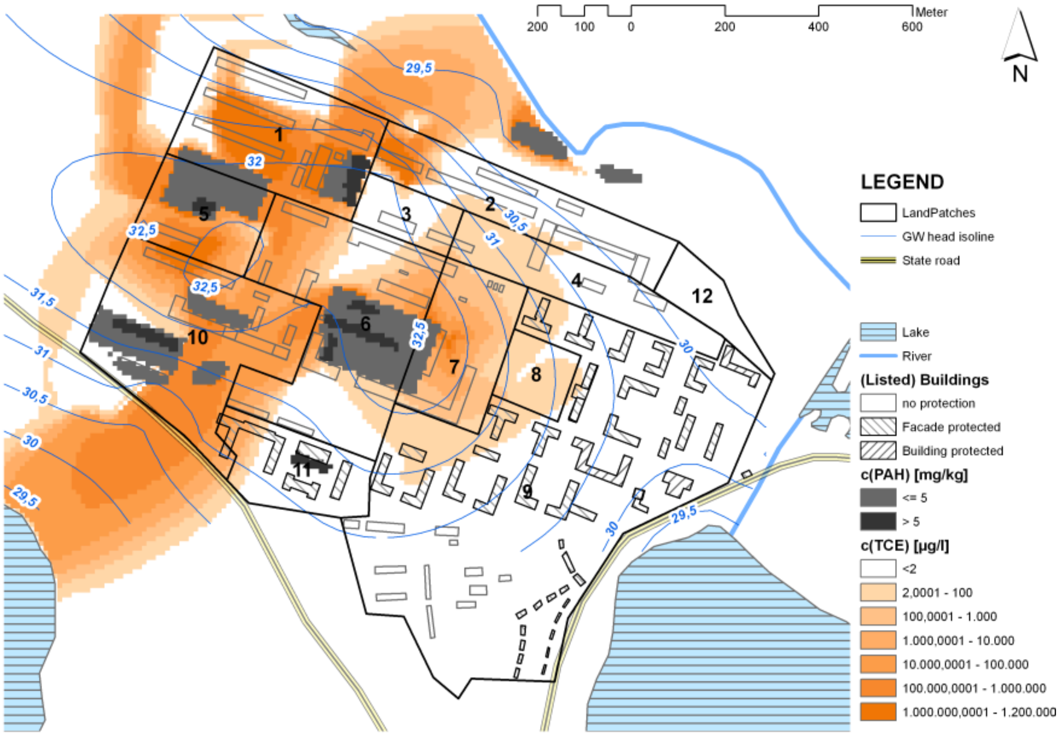


Figure 5.1: Case study site data: Information about groundwater regime and subsurface contamination, existing buildings, state roads, and water bodies, as a basis for subdivision into 12 planning units ("land patches").

investigation campaigns, conducted in 2000 and 2001 (with 24 sampled wells), and in 2007 (direct push investigation with 123 measurement points). According to this data, the contamination at the site is dominated by three priority contaminants/contaminant groups, i.e., TCE and PCE in the groundwater and PAHs in the soil. Please note that information about soil contamination is uncertain and limited to the delineation of potentially contaminated areas.

In order to conceive a set of basic redevelopment options, the site was subdivided into 12 planning units (i.e. land patches, compare Figure 5.1). In this study the definition of planning unit boundaries is based on spatial features of the site such as distribution of contamination, existing buildings (some of which are partially or entirely listed as protected monuments), proximity to state roads, environmentally protected areas in close vicinity to the site, infrastructure and neighbouring recreational areas.

5.3.2 Characterization of land use types and definition of redevelopment options

For the definition of redevelopment options, the following exemplary land use types were considered: "housing area" (HA), "trade/industries" (TI), "recreational" (RE), "no use" (NU), and "high tech industry" (HT) as a special type of "trade and industry". Sensitivities with respect to tolerable exposure to contaminants are reflected by specific remediation standards assigned to each land use type. Corresponding concentration threshold values are shown in Table 5.4. Absence of target values for the "no use" type indicates that no conflicts will be considered in relevant areas as no risk is anticipated due to restricted access.

For evaluating sustainability, the land use types considered here were further characterized as follows: (1) neither land use types "Trade/Industry" nor "High Tech Industry" are strongly emitting, (2) the close surrounding area is not populated (corresponds to today's situation but may not remain true in future), and (3) "Housing area" includes local supplies, but not the building of an additional school (compare sustainability indicator 4.1.2).

Table 5.4: Considered land use types and their properties

		TI, HT	**HA**	**RE**	**NU**
Compliance criteria:	TCE [μg/l]	100	10	60	n.a.
	PCE [μg/l]	100	10	60	n.a.
	PAH [mg/kg]	10	2	4	n.a.
Reference Land Value RLV [EUR/m^2]		40	95	10	0
Site preparation [% RLV]		75	80	50	0

Based on these land use types a total of 10 different redevelopment options were defined as shown in Figure 5.2. Option A is based on stakeholder discussions; options A' to H are additionally drafted for comparison in order to exemplify possible benefits and drawbacks of alternative redevelopment plans. Each option comprises one or more land use type in different fractions, which are assigned to the 12 planning units.

As a simplification, costs for the deconstruction of buildings are assumed to be constant through all land use options, i.e., all buildings except for the listed ones are deconstructed. Further specification requires additional methods for appraisal of buildings as well as spatially explicit deconstruction cost estimation, both of which require detailed data beyond the screening level sought here.

The planning horizon for discounting was set to 50 years, with a relevant PRB reactivation period of 10 years and an annual discount rate of 5 %. All further assumptions as well as literature values that were taken as input data for the assessment model are listed in the Supplementary Information.

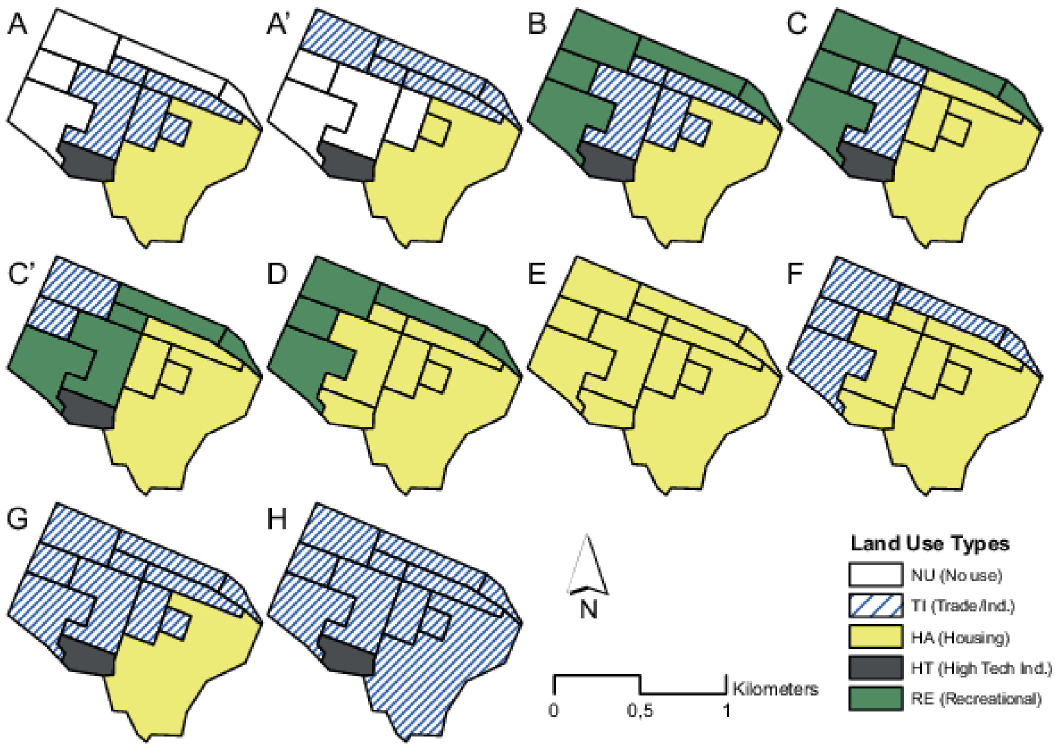


Figure 5.2: Definition of land use options A–H by allocating distinct land use types on the 12 planning units.

5.4 Results and Discussion

5.4.1 Evaluation of redevelopment options

We first evaluated redevelopment option A, which is the result of stakeholder discussions. The intention of option A was to avoid costly remediation on the site by restricting access to the most severely contaminated areas in the western part of the site: "no use" (NU) is assigned to the respective land patches and the contamination is left in place. Therefore, in these areas, costs will be incurred for measures to sufficiently reduce the risk to neighbours affected by the chlorinated solvent plumes emitted from the site. In the Eastern part of the site, valuable residential areas are allocated on mainly uncontaminated land with a high number of listed buildings and good access to two state roads (patch 9). A trade and industry area conveniently separates the residential area from the highly contaminated western parts of the site and ensures a good sustainability rating as will be discussed below. Conflicts between land use and existing contamination in groundwater are completely avoided in this option, and only a small volume of soil in patch 6 shows contamination above the limit concentration for use type "TI". Only the costs for the deconstruction of derelict buildings lead to a significant decrease of the theoretical land value, and after a mercantile value reduction of about 0.6 million EUR, the remaining market value is positive. The combination of complementary land use, good accessibility, and the non-relevance of those parts of the site that remain unused, leads to an overall slightly positive sustainability rating (compare Table 1.5).

Option A' results from searching for a redevelopment option with fractions of land use types that are similar to the ones in option A. A re-allocation of land use was sought that minimizes conflicts between existing contamination and land use-specific subsurface quality requirements. The consequences are decreased costs for both soil remediation and plume containment. Hence, the market value increases to 2.9 million EUR. However, at the same time the sustainability rating of option A' is significantly lower than in option A (A' ranking 9th out of ten as compared to A ranking 2nd). This is due to the anticipated increase in motorized transport resulting from the fact that in option A' trade and industry have been re-allocated onto land use patches that are not easily accessible by public or non-motorized transport (sustainability indicators 3.2.1 and 3.4.1).

The use pattern in option B is similar to option A with the only difference being the "no use" planning units from option A replaced by recreational areas. The underlying idea is to better support the principle of reusing land and to minimize land consumption, and to consider "no use" areas only where extreme remediation costs make an economically feasible land use impossible. One consequence is that in this option the compliance criteria ensure a total remaining TCE flux below the limit flux, so that no additional cost for the reduction of risks to neighbours is added. However, to enable the sensitive land use in the strongly contaminated north-western part of the site, cleanup of the vast soil contamination is now required which makes the costs for remediation exceed the preliminary land value in option B: the resulting market value would be negative and in practice it is set to zero: The sustainability rating in option B equals that of option A: the only change in land use, i.e., the change from no use to recreational use, does not affect the rating, as the recreational use is rated neutrally.

Options C, C', D and E represent the goal to raise market value by a stepwise increase of the spatial fraction of residential use (being the most valuable among the defined land use types here, see Table 5.4). Starting with the placement of additional housing in low contaminated areas, its fraction was increased from 48% (options C and C') to 67% (option D) and eventually to 100% (option E). Despite a considerable increase in the theoretical land value VL,theor (9.8 million EUR for options C and C', 11.5 million EUR for option E, and 16.7 million EUR for option F), resulting market values are much lower compared to the value of options A and A'. This is due to a disproportionately high increase in remediation costs that diminish the market value strongly (as was shown before for option B).

Remediation costs of options D and E differ only marginally (estimates for both options are approx. 10.6 million EUR). The replacement of recreation by housing areas and associated changes in compliance criteria (Table 5.4) only very slightly alter the conflicts that need to be resolved by remediation. This is due to the fact that levels of existing contamination are well above the remedial targets throughout the site. Therefore, option E, having the highest of all possible land values VL,theor,

Table 5.5: Results of the integrated analysis of redevelopment options.

Land Use Option	**A**	**A'**	**B**	**C**	**C'**	**D**	**E**	**F**	**G**	**H**
Land Use Type [ha]										
Housing Area (HA)	40	42	40	54	54	76	114	76	40	0
Trade/Industry (TI)	31	28	31	17	15	0	0	38	69	109
High Tech Industry (HT)	5	5	5	5	5	0	0	0	5	5
Recreational (RE)	0	0	38	38	40	38	0	0	0	0
"no use" (NU)	38	39	0	0	0	0	0	0	0	0
Economic Evaluation [Mio EUR]										
$V_{L,theor}$	8.7	8.7	8.9	9.8	9.8	11.5	16.7	14.1	11.4	8.8
BDC	4.1	4.1	4.1	4.1	4.1	4.1	4.1	4.1	4.1	4.1
GW[a] remediation costs	0	0	0.8	0.8	0.8	0.9	0.9	0.9	0.7	0.7
Soil remediation costs	0.9	0.6	7.2	7.8	8.2	10.6	10.6	5.2	1.8	1.8
Costs for reducing risks to neighbours	0.5	0.4	0	0	0	0	0	0	0	0
Preliminary land value	3.1	3.6	-3.2	-2.9	-3.3	-4.2	1	3.9	4.7	2.1
MVR	0.6	0.6	0	0	0	0	0.2	0.7	0.9	0.4
Market value[b]	**2.6**	**2.9**	**(-3.2)**	**(-2.9)**	**(-3.3)**	**(-4.2)**	**0.8**	**3.2**	**3.9**	**1.7**
Sustainability Evaluation [%]										
Housing Area	17	17	17	4	4	4	-13	7	11	-
Trade/Industry	8	-35	8	8	8	-	-	2	8	-4
High Tech Industry	30	30	30	30	30	-	-	30	30	30
Recreational	-	-	0	0	0	0	-	-	-	-
Sustainability Rating E_{tot}	**9.4**	**-7.1**	**9.4**	**5.3**	**5.3**	**2.7**	**-13**	**6.6**	**10.1**	**-2.3**
Sustainability Ranking	2	9	2	5	5	7	10	4	1	8

[a]GW: groundwater
[b]negative market values are shown in bracktets – in practice they would be set to zero

results in a distinctly higher market value than option D. A clear drawback, however, is a strongly negative sustainability rating (ranked 10th and thus worst of all options considered), which can be attributed to the location of the site on the outskirts of the city Potsdam: a homogeneous i.e. pure residential use is not rated sustainable because distances to existing public facilities in the city of Potsdam and its surroundings are too large (compare indicators 1.1.3, 1.3.1, 3.2.1, 3.4.1, and 5.1.1). Contrary to this, redevelopment options involving a mixture of residential areas, recreational areas and trade and industry that inherently form a sustainable unit (i.e. a well functioning quarter) are rated more sustainable. The poor rating for option E thus reflects the fact that this option lacks the positive aspects of mixing complementary land use types.

Design of the mixed use options F and G reflects the findings of the previously discussed options: The mixing of trade/industry and residential areas in different ratios yield very good results with respect to market value as well as sustainability rating. Bad effects identified before are most widely avoided, as well as required soil remediation, which is reduced to a minimum by smart land use allocations on the patches.

Considering the slight improvement in assessment results that was achieved by increasing the fraction of trade/industry from option F to option G, consequently a pure trade and industry option H was investigated. However, because remediation costs cannot be further reduced when compared to option G, and as the sustainability rating is distinctly worse due to the uniform use, this is not a favourable option.

5.4.2 Discussion

The integrated assessment of revitalization options enables stakeholders to identify and explain strengths and weaknesses in particular options and to systematically improve land use planning on brownfields by comparing alternative options. The quick comparison at screening level enables assessment of consequences to adjustments of land use allocation plans or land use characteristics such as clean-up goals or reference land values. In this way, the model helps to identify potentially valuable revitalization options on the basis of one common data set, and supports discussions on possible adjustments in order to achieve optimal redevelopment solutions.

In the evaluation presented herein, site redevelopment options F and G can be seen as the result of a learning process that was encouraged by the integrated assessment model, where positive aspects learned during the evaluation of previous options, like a mix of complementary uses [e.g. Evans and Foord, 2007], were applied in an iterative improvement.

The sustainability assessment results of this case study show two major aspects of sustainable brownfield revitalization: While they underline the statement by Eisen [1999] that it is wrong to suspect all brownfield redevelopment to be inherently sustainable, more importantly it is shown that sustainable land use options are not necessarily economically unfavourable. Figure 5.3 compares the sustainability rating of the redevelopment options with their market value after remediation with no correlation seen between results of the economic and sustainability assessment for the options considered here. Hence, the preconception that sustainability is intrinsically costly, which would result in a negative correlation between the two results, cannot be supported by this data. For the subset of economically qualified options having a positive market value (A, E, G, H), even a positive correlation between market value and sustainability can be observed. The best options among the given set of 10 candidates are most valuable in terms of both money and sustainability. The results of the evaluation would thus promote that these options, A, F, and G are worthy of further refinement and a more detailed investigation.

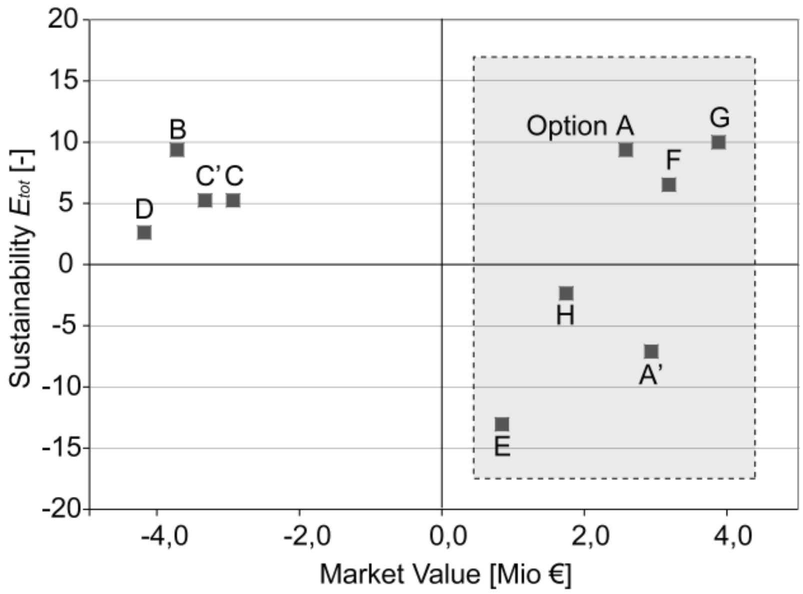


Figure 5.3: Model site's sustainability factor $E_t ot$ versus market value of analysed land use options.

5.5 Conclusions

The intention in developing an integrated assessment model for brownfield revitalization options was to obtain a screening level sDSS which reveals the economic and social consequences of alternative redevelopment plans on large contaminated sites. The aim was to foster communication among stakeholders particularly in early phases of a redevelopment project. Due to the integration of remediation cost estimation, mercantile value reduction, and evaluation of sustainability with respect to regional development, the model proves helpful especially for contaminated sites in urban areas.

The integrated assessment model consequently employs only simplified methods that require relatively little input data. Obviously, refining these methods and implementing the assessment of further aspects of the revitalization process could extend the applicability of the sDSS to later project stages when accumulated data and information allow for the use of more sophisticated methods. Further model development may include, among other issues, a sustainability evaluation with a site-specific (local) definition of sustainability by stakeholder involvement [e.g. Curtis et al., 2005, Hartmuth et al., 2008] addressing additional issues such as sustainable remediation and green building [e.g. Wedding and Crawford-Brown, 2007], and differentiation between technological remediation scenarios.

5.6 Acknowledgements

The authors gratefully acknowledge the support of the German BMBF research priority program REFINA (contract no. 0330757C) and of the Helmholtz Centre for Environmental Research – UFZ in Leipzig (contract no. 4500029698).

Chapter 6

A multi-criteria genetic algorithm framework for the identification of holistically optimum brownfield redevelopment options[1]

Abstract The re-use of underused or abandoned contaminated land, so-called brownfields, is increasingly seen as an important means for the reduction of land consumption and natural resources. Seeking sustainable re-use solutions, many existing decision support systems are not appropriate as they do focus mainly on economic aspects, neglecting sustainability issues. To fill this gap, we present a framework for spatially explicit integrated planning and assessment of brownfield redevelopment options. A multi-criteria genetic algorithm allows to determine optimal land-use configurations with respect to one or more assessment criteria and given constraints on the composition of land-use classes. Assessment criteria include sustainability indicators and economic aspects (minimization of remediation costs and maximization of land value). The context-specific sustainability evaluation framework is based on criteria for sustainable urban development in Germany. A set of 23 indicators is automatically evaluated as part of the objective function of optimization. The framework is applied to a case study at a former military site near Potsdam, Germany. Emphasis is given on the trade-off between economic goals and the need for sustainable development in the regional context of the brownfield site. The results show that the quantitative integration of sustainability may considerably improve the basis of decision-making. Another amendment is the separated optimization of economic criteria, which revealed that reuse options with similar economic outcomes may considerably differ in terms of the environmental state that will be achieved.

Keywords optimization, genetic algorithms, GIS, remediation, costs, market value, sustainability, land-use allocation

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[1]submitted for publication to Environmental Modelling & Software, Authors: M. Morio, S. Schädler, and M. Finkel

6.1 Introduction

6.1.1 The brownfields issue

The scarcity of land for food production, energy crops, living or other uses is becoming a major problem in our world [Lambin and Meyfroidt, 2011, Böhner, 2006]. One important aspect in efficiently using available land resources is the reduction of unnecessary land consumption. An essential means in this context is the promotion of inner-development of urban areas instead of sprawling development to greenfields. A major challenge is the (re-)use of derelict and devastated land, i.e. brownfield sites [U.S.EPA, 2002, CABERNET, 2005, Lee et al., 2004]. Especially if these sites are considerably large and contaminated they may represent an economic as well as human and ecological health risk [e.g. Agostini et al., 2007, De Sousa, 2003, Apostolidis and Hutton, 2006, Cao and Guan, 2007, Kaufman et al., 2005].

6.1.2 Integrated assessment and decision support

Redeveloping brownfields means dealing with potentially conflicting objectives. Soil and water acts call for appropriate and reliably dimensioned risk mitigation measures, whereas economic goals include the minimization of related efforts and costs. The maximization of financial benefits that will be derived from re-using the site, in turn, may lead to re-use visions that contradict societal interests such as sustainable development aiming at optimizing the wellbeing of concerned local parties. For a long time, the search for economically feasible options has shaped the decisions on how to redevelop a brownfield. Over the last years the issues of sustainable development caught more and more stakeholders' and researchers' attention. Adequate decisions can be made only if advantages and disadvantages of any particular re-use option are carefully weighed up against each other, taking into account the often divergent stakeholders' choices and objectives [Linkov et al., 2006]. To amend this process, decision support systems (DSS) are required, which provide an integrated evaluation of possible options of future use that is based on a formally clear and, if possible, quantitative multi-criteria assessment scheme [e.g. Parker et al., 2002, Carlon et al., 2007a, Kok and Verburg, 2007, Schädler et al., 2011b]. The use of a DSS may generate an added value especially by making the routes to decisions transparent [Pollard et al., 2004]. Manifold criteria and characteristics might be relevant for assessment of a brownfield site, depending on its size and former use, its surroundings, and the existence of possible receptors that might be affected. Quantification of these criteria is typically done in different terms, as monetary costs or benefits, in physical units, as risk levels or as rather abstract indices such as e.g. 'social acceptance' or 'sustainability index'. A critical review of existing brownfield classification systems and of the criteria these systems do consider, is presented in Dasgupta and Tam [2009]. A multitude of indicators have been proposed to measure the sustainability of any redevelopment in relation to its site-specific context [e.g. Hartmuth et al., 2008, Pediaditi et al., 2010, Singh et al., 2009, Wedding and Crawford-Brown, 2007, Zavadskas and Antucheviciene, 2006].

However, most of the DSS available today do not integrate the assessment of sustainability for want of transparency and objectivity.

6.1.3 Spatial optimization approaches

A multitude of GIS-based approaches have been proposed for facilitating decisions related to land-use suitability analysis i.e. to the identification of the most appropriate spatial pattern of future land uses according to the specific requirements and preferences. Approaches are usually based on combinations of map overlay modeling, multicriteria evaluation using landscape metrics, and some optimization method or artificial intelligence technique [Malczewski, 2004].

Attempts in finding metrics to describe the structure of landscapes quantitatively have especially been made in the field of landscape ecology [e.g. Forman, 1995, Gustafson, 1998, Turner, 1990, Reynolds and Wu, 1999, Uuemaa et al., 2007]. An overview on different metrics was presented recently by Antrop et al. [2009]. Guidance on the selection of metrics, their proper use and interpretation is given in e.g. Botequilha Leitão and Ahern [2002], Li et al. [2005], Cushman et al. [2008], Uuemaa et al. [2005]. A distinction is generally made between spatially non-explicit metrics to characterize features associated with the presence and amount of different patches within a landscape mosaic, i.e. its ‘composition’, and spatially explicit metrics to quantify the landscape’s ‘configuration’ referring to the physical distribution or spatial character of patches within it [McGarigal and Marks, 1995].

Among the optimization methods used are linear solvers [e.g. Romanos and Hatmaker, 1980, Wright et al., 1983, Aerts et al., 2003a], tabu search [Qi et al., 2008], simulated annealing [Aerts and Heuvelink, 2002, Aerts et al., 2003b, Duczmal and Assuncao, 2004, Duh and Brown, 2007, Sante-Riveira et al., 2008a], genetic algorithms (GA) [e.g. Matthews et al., 2006, Aerts et al., 2005, Holzkämper and Seppelt, 2007b, Xiaoli et al., 2009, Tong et al., 2009] and evolutionary algorithms [e.g. Bennett et al., 2004, Xiao et al., 2007, Xiao, 2008].

The various fields of application include: forestry [Bos, 1993, Adams et al., 1996, Mendoza, 1997, Strange et al., 2001, Kangas et al., 2001, Venema et al., 2005, Gaucherel et al., 2006, Mathey et al., 2008], habitat search and reserve planning [McDonnell et al., 2002, Fischer and Church, 2005, Holzkämper et al., 2006, Holzkämper and Seppelt, 2007a], marine biodiversity and ecosystem planning [Possingham et al., 2000, Stewart and Possingham, 2005, Crossmann et al., 2007], and rural or urban planning [Openshaw, 1983, Matthews et al., 1999, 2000, Carsjens and van der Knaap, 2002, Forman et al., 2002, Caro et al., 2004, Ligmann-Zielinska et al., 2005, 2008, Sante-Riveira et al., 2008b, Meyer and Grabaum, 2008, Xiaoli et al., 2009].

6.1.4 Objectives

In this paper, we present a novel simulation-optimization framework for the identification of optimum brownfield redevelopment options from a holistic perspective.

The framework combines an integrated spatial assessment model and a heuristic optimization algorithm for land-use allocation [Holzkämper, 2006]. With this framework we wish to answer the request for an improved DSS for contaminated land re-use as has been expressed in the recent past [e.g. Agostini et al., 2007, Agostini and Vega, 2009]. The work presented here develops the previous achievements of Schädler et al. [2011b,a, 2012] further, who provided a consistently quantitative integrated assessment scheme for use within spatial optimization.

The proposed framework allows for spatial analysis and optimization of land-use scenarios (i.e. landscape configurations) with given constraints in size and shape, trading off the minimization of economic costs (i.e. the maximization of benefits) against the maximization of the suitability with respect to sustainable redevelopment. An existing genetic algorithm optimization framework was selected and extended for this approach [Holzkämper and Seppelt, 2007b]. The emphasis is given to the formulation of objective functions and trade-off of different evaluation criteria rather than to optimization methodology itself.

The remainder of this paper is organized as follows: the assessment methods, the optimization algorithm and associated spatial evaluation functions that are used in the novel framework are described in Chapter 2. Chapter 3 illustrates the case study, the result of which are presented and discussed in Chapter 4.

6.2 Methods

6.2.1 Integrated assessment of mixed re-use options

The approach presented in this manuscript is especially designed for sites, which, because of their size, have a certain degree of freedom with respect to both composition and configuration of redevelopment plans. We, therefore, assume the redevelopment to be targeted at a mixed use of the site, allocating different land-use classes to multiple planning units. How many and which particular land-use classes shall be considered for allocation can be freely defined in accordance to existing demands and suggestions of the stakeholders involved in the planning project. Nevertheless, each land-use class needs to be characterized by (i) compliance criteria with respect to subsurface contamination i.e. contamination target concentrations for the contaminants of concern (CoC) in soil and groundwater (clean-up goals), (ii) a reference land value, and (iii) the attribution to one of the use types defined for the assessment of sustainable development (Table 6.1).

6.2.2 Problem representation

The representation of the evaluation problem follows Holzkämper et al. [2006], and is based on raster grids with land-use classes allocated to specific, predefined planning units (hereafter also denoted as patches). An adaption was made to the notation of the model grid and its associated attributes to make it suitable within the scope of this manuscript.

Table 6.1: Classification of land-use types s for sustainability potential assessment after Müller and Rohr-Zänker [2009].

No.	Sustainability land-use type
1	Residential: all types of residential buildings and green spaces directly adjacent
2	Local Services: retail sales, elementary schools, welfare stations, community health centers
3	Recreational: public parks, places, sports- and playgrounds
4	Trade/Industries: commercial services, handicrafts business, gastronomy, hotels, administration, cultural, social, or sports facilities (indoor)
5	Emitting industries: emitting production facilities, logistics centers
6	Large-space business centers: large administration facilities, spas, sports facilities, amusement parks
7	Monofunctional facilities with large open spaces: large public or private facilities for education (e.g. university campus), hospitals with surrounding green spaces, sports hotels and similar uses
8	no use type assigned

The model's problem representation is based on a discrete grid $G = \{(i,j)|i_{min} < i < i_{max}, j_{min} < j < j_{max}; i_{min}, i, i_{max}, j_{min}, j, j_{max} \in \mathbb{N}\}$. The grid resolution d [m] has to be adapted to both the scale of the planning units and to the spatial resolution of given site information (e.g. level of detail for underground contamination).

Each grid cell can have n attributes, which are derived from several (input) raster maps such as the land-use class $l : G \rightarrow L = \{100, 200, \ldots, a * 100\}$, with a being the number of defined classes, uniform land-use specific underground remediation costs $c_l : G \rightarrow C_l = \{0, \ldots, \mathbb{R}_0^+\}$, market values $v_l : G \rightarrow V_l = \{0, \ldots, \mathbb{R}_0^+\}$, and sustainability potential type $s : G \rightarrow S = \{1, \ldots, 8\}$ (land-use types considered in sustainability assessment, see Table 6.1). The configuration as well as the composition of land-use classes l are subject to change in the optimization algorithm (GA). All other attributes are considered as static/constant variables.

The land-use grid G is converted into a patch topology according to the given planning units. Land use within a planning unit is (by definition) uniform. Membership of a raster cell to one of the given planning units is identified by an unique patch identifier id. m denotes the number of modifiable planning units $u : G \rightarrow id = 1, 2, 3, \ldots; u(i,j) = id = 1, 2, 3, \ldots, m$, with its inversion function providing a set of connected cells of same class of l in G, denoted as $u^*(id) = \{(i,j)|l(i,j) = \text{const., connecting set}\} \subset G$.

For the next paragraphs, each specific spatially explicit land-use configuration will be referred to as a land-use map M, with the properties and attributes of M being defined in the corresponding grid G.

6.2.3 Economic Assessment

6.2.3.1 Identifying the need for remediation: conflict analysis

By utilizing a set of GIS-based procedures, those regions on the site that will require remediation are identified given the information on the distribution of contaminants, and on the map of clean-up goals attributed to the specific redevelopment option M. The resulting raster maps of exceedance factors for each CoC indicate areas and magnitudes of conflicts between existing and required environmental conditions. Exceedance maps $X_{coc,t,l}$ for each contaminant (index coc), media type (index t, here: soil and groundwater), and land-use class l are generated, which serve as an input for the calculation of remediation cost maps.

6.2.3.2 Remediation and site preparation costs

Costs for remediation of subsurface contamination are estimated using empirical models following Bonnenberg et al. [1992]. We focus on costs of remedial activities on the site that are necessary to resolve the abovementioned conflicts in soil and groundwater. Costs of any further measures, for example to avoid unacceptable risks to neighbors (e.g. for the case when contaminant flux across the site boundary is expected even after revitalization has taken place), are not taken into account. Costs for deconstruction of devastated buildings were not considered either, since they are assumed to be constant for the case of a site re-use within the scope of our approach. A detailed description of the cost models can be found in Morio et al. [2008], Morio and Finkel [2010], Schädler et al. [2010b, 2011b].

The land-use related costs for groundwater clean-up, $C_{l,GW}$[EUR] are estimated based on the volume of contaminated groundwater and the respective magnitude of exceedance factors for each of the CoC, as calculated in the preceding conflict analysis. The costs for any particular grid cell (i,j) of the model domain can be estimated for each land-use class l by:

$$c_{l,GW,i,j} = \begin{cases} \max_{coc}(C_{u,GW} V_{GW,i,j}\, n_{e,i,j}\, f_{D,i,j}\, f_{C,coc,i,j}\, f_{L,coc,i,j}) & \text{if } x_{coc,GW,l,i,j} > 1 \\ 0 & \text{otherwise} \end{cases} \quad (6.1)$$

where $C_{u,GW}$[EUR m^{-3}] denote standard unit costs, $V_{GW,i,j}$[m^3] is the volume of contaminated groundwater, $n_{e,i,j}[-]$ is the effective porosity. $f_{D,i,j}$ [-], $f_{C,i,j}$ [-], and $f_{L,i,j}$ [-] are difficulty factors that reflect the severity of the contamination in terms of depth (shallow, medium, or deep), contaminant group and degree of contamination (low, medium, high, and non-aqueous phase; derived from exceedance factor $x_{coc,GW,l,i,j}$), respectively.

The soil-remediation costs $c_{l,Soil}$[EUR] are computed similarly:

$$c_{l,Soil,i,j} = \begin{cases} \max_{coc}(C_{u,Soil} V_{Soil,coc,i,j}\, \rho_{i,j} f_{D,i,j}\, f_{C,i,j}\, f_{L,i,j}) & \text{if } x_{coc,Soil,l,i,j} > 1 \\ 0 & \text{otherwise} \end{cases} \tag{6.2}$$

Here, $C_{u,Soil}$[EUR m^{-3}] denote the standard unit costs, $V_{Soil,coc,i,j}$[m^3] is the contaminated soil volume in accordance to the land-use class specific depth below grade that is to be remediated, $f_{D,i,j}$ [-], $f_{C,i,j}$ [-], and $f_{L,i,j}$ [-] are difficulty factors, and $\rho_{i,j}$[kg m^{-3}], is the soil's bulk density.

Finally the remediation costs for soil and groundwater are summed up for each land-use class l to a total cost value:

$$c_{l,i,j} = c_{l,Soil,i,j} + c_{l,GW,i,j} \tag{6.3}$$

The costs for a specific land-use configuration represented by a map M are obtained by:

$$C_{tot}(M) = \sum_{i,j}^{i_{max},j_{max}} c_{l,i,j}(M) \tag{6.4}$$

where l at $i,j = l(M)$.

6.2.3.3 Site market value

The fact that the values of identical but differently situated sites may strongly vary from one another depending on their locations, is considered with the help of location quality factors, which were specified for each planning unit and land-use class, resulting in a location-quality correction factor matrix $q_l : G \to Q = \{0.75, \ldots, 1.04\}$ [see Schädler et al., 2012, for more details].

Starting from the reference value $V_{l,ref}$ [EUR/m^2] of a comparable, but clean real estate, which can usually be obtained from regional committees of valuation experts, the market value assessment takes into account the specific quality of the location, a cost factor for site preparation with respect to the actual state of development of the site (SPC [%]), and the so-called mercantile value reduction (MVR [%]).

The MVR is calculated according to Bartke and Schwarze [2009a,b]. It represents a market value markdown, which comprises perceived uncertainties regarding rehabilitation, risk of future liabilities, investment risks, utilization risk, stigma effects, and marketability risk, which may play a considerable role in the prizing of brownfields [see e.g. Patchin, 1991, Syms, 1999, Mundy and Kilpatrick, 2003, Jackson and Pitts, 2005]. The MVR method quantifies a risk rebate on the basis of local site characteristics, information level on redevelopment costs for the site, and the ability to pass the monetary risk to others. Together with the SPC [%], it forms a diminution factor D [cmp. Schädler et al., 2011b].

The location-quality corrected market value v_l [EUR/m^2] is then obtained by multiplying the land-use specific D_l [%] with $V_{l,ref}$ multiplied with the location-quality factor:

$$v_{l,i,j} = \begin{cases} (V_{l,ref}\, q_{l,i,j}) D_l & \text{if } > 0 \\ 0 & \text{otherwise} \end{cases} \tag{6.5}$$

with $q_{l,i,j}$ [-] being the land-use class specific location quality correction factor at position i, j of matrix Q.

The market value V_{tot} [EUR] for the specific land-use map M is calculated by:

$$V_{tot}(M) = \sum_{i,j}^{i_{max}, j_{max}} v_{l,i,j}(M) d^2 \tag{6.6}$$

where l at $i, j = l(M)$, with d^2 [m^2] representing the grid cell area.

Finally, taking the remediation costs into account, the overall remaining value for a map is:

$$R(M) = V_{tot}(M) - C_{tot}(M) \tag{6.7}$$

6.2.4 Sustainability Assessment

The assessment of consequences for a brownfield's re-use with regard to sustainable development is based on an indicator scheme proposed by Müller and Rohr-Zänker [2009] to evaluate the suitability of future land use options regarding their compatibility with sustainable urban and regional development according to, e.g. ICLEI (International council for local environmental initiatives, see e.g. in Jeb [1996]) and AGENDA 21 [United Nations, 1992]. The indicator scheme consists of the evaluation of five sustainability goals, which are divided into sub-goals that form 23 particular sustainability indicators.

Based on the work of Schädler et al. [2011b], these indicators were implemented into a raster based spatial assessment scheme (Table 6.2). The indicators describe features of the site and its vicinity. The existence or absence of these features is used to express whether and how a specific land-use option will either foster or contradict the goals of sustainable urban development. For the evaluation of each of the indicators, certain spatial queries are made on the actual land-use configuration (see below). Most of the indicators are relevant only for certain land-use types, as defined in Table 6.1. The column 'Affected type s' (Table 6.2) lists the land-use types s to which the particular indicator is relevant, whereas the 'Evaluation use-type' column indicates land-use types and infrastructural or environmental features that affect the evaluation of the indicator. When indicators are assessed with respect to features, which are not attributed to a particular land-use type, evaluation rasters are utilized for evaluation (as named in column 'Evaluation type'). These features can be e.g. public transportation stations, whose positions are represented by an evaluation raster ‘pubtrans’, nature reserve areas are indicated by a raster grid ‘reserves’, et cetera. Some indicators are answered globally, in terms of a stakeholder or expert predication. For each spatial planning unit and attributed land-use type, it is evaluated whether the descriptive statements of the individual indicators are applicable or not. The resulting Boolean answers translate into integer values (see columns "True" and "False" in Table 6.2). Depending on the given answer and the land-use type, the result for an indicator can be +1 or -1, illustrating the use-type’s compatibility or incompatibility with sustainable development, respectively. The result is zero when the answer for the given land-use type is of no relevance for sustainable development. These values are multiplied with the individual indicator’s weighting to obtain a positive or negative actual score. Indicator’s weightings were used as defined in Müller and Rohr-Zänker [2009], and sum up to 100 % for each of the five sustainability goals.

Table 6.2: Sustainability indicators of the optimization algorithm's evaluation function. Indicator numbers in 2nd column acc. to Schädler et al. [2011b]. Vector positions of values in columns 'True' and 'False' stand for land-use type according to Table 6.1. Default values only valid for the presented case study.

No. x	Indic. no.	Indicator description	Evaluation function	Affected use-type s	Evaluation use-type s/grid	Weight w_x[%]	True	False	dThresh [m]	aThresh [m^2]	Default
	1.	*Goal: Economical land management*									
1	1.1.1	Residential areas in the surrounding area	Distance	2,3,4	1	10	0,1,1,1,0,0,0,0	0,-1,0,0,0,0,0,0	500	50000	
2	1.1.2	Green spaces in the surrounding area	Distance	1	3	10	1,0,0,0,0,0,0,0	0,0,0,0,0,0,0,0	500	0	
3	1.1.3	Local supplies within walking distance	Distance	1	4	10	1,0,0,0,0,0,0,0	0,0,0,0,0,0,0,0	500	0	
4	1.1.4	Neighboring uses are strongly emitting	Neighbor	1,3,7	5	20	-1,0,-1,0,0,0,-1,0	0,0,0,0,0,0,0,0	-	0	
5	1.2	Site contains <40% sealed soil	Distance	3,4,5,6,7	soilSealing40	10	0,0,+1,-1,-1,-1,+1,0	0,0,-1,0,0,0,-1,0	-	-	True
6	1.3	Site location within urban area	Neighbor	1,2,4	1,2	40	1,1,0,1,0,0,0,0	-1,-1,0,-1,0,0,0,0	-	50000	False
	2.	*Goal: Preservation of nature and the landscape*									
7	2.1.1	Site is part of a local habitat	Distance	1,2,4,5,6,7	biotopes	40	-1,-1,1,-1,-1,-1,-1,0	0,0,0,0,0,0,0,0	<cell	0	False
8	2.1.2	High value tree or plant populations	Distance	5,6	highGradeTrees	20	0,0,0,0,-1,-1,0,0	0,0,0,0,0,0,0,0	<cell	0	False
9	2.2	Direct vicinity to nature reserve	Neighbor	1,5,6	reserves	40	-1,0,0,0,-1,-1,0,0	0,0,0,0,0,0,0,0	-	0	True
	3.	*Goal: Mobility management that saves resource and reduces emissions*									
10	3.1	Low capacity of access roads	Global	4,5,6,7	–	30	0,0,0,-1,-1,-1,-1,0	0,0,0,0,0,0,0,0	-	0	False
11	3.2	Good access to public transport	Distance	1,2,4,6,7	pubtrans	40	1,1,0,1,0,1,1,0	-1,-1,0,-1,0,-1,-1,0	500	0	
12	3.3	Access to clearway	Global	5,6	–	20	0,0,0,0,1,1,0,0	0,0,0,0,-1,-1,0,0	-	0	True
13	3.4	Good accessibility for bicyclists	Global	1,2,3,4,5,6,7	–	10	1,1,1,1,1,1,1,0	-1,-1,-1,-1,0,0,0,0	-	0	True
	4.	*Goal: High quality of environment for housing and living*									
14	4.1.1	Local amenities in walking distance	Distance	1,4	2	10	1,0,0,1,0,0,0,0	-1,0,0,0,0,0,0,0	500	0	
15	4.1.2	Primary school in walking distance	Distance	1	elmtrySchool	10	1,0,0,0,0,0,0,0	-1,0,0,0,0,0,0,0	500	0	True
16	4.2	Great impact on recreational areas	Global	1,2,4,5,6,7	–	20	-1,-1,0,-1,-1,-1,-1,0	0,0,0,0,0,0,0,0	-	0	True
17	4.3.1	Historically relevant buildings	Distance	1,3,4,5,6,7	listedBuildings	10	1,0,-1,1,-1,-1,1,0	0,0,0,0,0,0,0,0	<cell	0	True
18	4.3.2	Great influence on cityscape	Distance	3	affCityscape	10	0,0,1,0,0,0,0,0	0,0,0,0,0,0,0,0	<cell	0	False
19	4.4	Neighboring uses sensitive to immissions	Neighbor	5,6	1,3	40	0,0,0,0,-1,-1,0,0	0,0,0,0,0,0,0,0	-	0	
	5.	*Goal: Strengthening of the local economy*									
20	5.1	Good supply and disposal infrastructure	Global	1,2,4,5,6,7	–	20	1,1,0,1,1,1,1,0	-1,-1,0,-1,-1,-1,-1,0	-	0	True
21	5.2	Site strongly contaminated	Distance	1,2,3,7	ROCO_lutype	30	-1,-1,-1,0,0,0,-1,0	0,0,0,0,0,0,0,0	<cell	0	True
22	5.3	Site suitable for innovative industries	Global	4	–	30	0,0,0,1,0,0,0,0	0,0,0,0,0,0,0,0	-	-	True
23	5.4	Adjacent enterprises with precarious sense of security	Global	1	–	20	-1,0,0,0,0,0,0,0	0,0,0,0,0,0,0,0	-	0	False

The patch wise evaluation scheme presented by Schädler et al. [2011b] was extended by grid-based evaluations for the indicators. Each indicator is evaluated by one of the following three indicator evaluation functions:

1. Distance (affected type – evaluation use type) < threshold. The distance to a relevant land-use type or another feature (grid cell of an evaluation raster) is assessed. Positive or negative evaluation depends on whether the distance is below or above a given threshold distance (cmp. column 'dThresh' in Table 6.2). In some cases, an additional check is made with respect to the total area of the 'evaluation use-type' that is found within the threshold distance. Indicators are evaluated as 'True' only if this area surmounts the given threshold (column 'aThresh' in Table 6.2). See Algorithm 4 for functioning of this type of evaluation (see annex).

2. Neighbor == evaluation type. This patch based evaluation checks for favored or unwanted neighborhood relations, e.g. if an emitting industry patch touches a housing patch. The inspection is made cell wise. If the check of one cell with relevant affected use-type gets answered with 'True', the respective indicator result (+1, -1, or zero) will be assigned to all cells in the corresponding planning unit.

3. Global. This evaluation is independent of the actual land-use map configuration. Indicators have to be "answered" for the entire site (i.e. global) by stakeholders and/or experts (compare column 'Default' in Table 6.2). All grid cells of the actual map attributed with affected land-use type get assigned the positive or negative indicator results accordingly.

For each indicator x, one of the three indicator evaluation functions is applied (cf. Table 6.2), returning land-use type specific indicator value matrices $E_{x,s} = (e_{x,s,i,j})$. These values are multiplied by the respective indicator weighting w_x. The positive (negative) values $e_{x,s,i,j}$ of each land-use type are summed up over all 23 indicators, and divided by the land-use type specific maximum possible positive (negative) score $P^+_{max,s}$, $(P^-_{max,s})$ [-] (cf. Table 6.3) times the number of cells of the respective land-use type s. The sustainability result E_s for the land-use type s is calculated by:

$$E_s = \frac{\sum_{x=1}^{23} \sum_{i,j}^{i_{max},j_{max}} \left(e^+_{x,s,i,j} w_x \right)}{P^+_{max,s} A_s d^{-2}} 100 - \frac{\sum_{x=1}^{23} \sum_{i,j}^{i_{max},j_{max}} \left(e^-_{x,s,i,j} w_x \right)}{P^-_{max,s} A_s d^{-2}} 100 \tag{6.8}$$

where the fraction of the land-use type area and cell area (A_s/d^2) stands for the land-use type's number of cells.

Consequently, the suitability of sustainable development E_{tot} [-100,...,+100] for a map M is derived by:

$$E_{tot}(M) = \sum_s \left(E_s \frac{A_s}{A_{tot}} \right) \tag{6.9}$$

land-use type s	1	2	3	4	5	6	7	8
$P^{+}_{max,s}$	160	120	80	170	50	90	90	0
$P^{-}_{max,s}$	-300	-210	-80	-210	-260	-300	-210	0

Table 6.3: Maximum positive and negative score of indicator results for respective sustainability evaluation use-type s (cf. Table 6.1).

with A_s/A_{tot} representing the land-use type area ratio.

6.2.5 Evaluation of shape and compactness of land use pattern

For the work presented in this paper, we tested several metrics described in McGarigal and Marks [1995], like shape index, mean and largest scale index, fractal dimension, cohesion, contagion, total edge, number of patches, patch richness, and proximity index. Preliminary testing with a varying number of 2 to 7 different land-use classes and different grids ranging from 20 x 20 to 400 x 250 cells revealed the total edge metric to be the most effective one in terms of finding a good compromise between a satisfying result and calculation time.

Land-use class-specific total edge values T_l equal the sum of the lengths [m] of all edge segments of connected planning units of same land-use class l [cf. to McGarigal and Marks, 1995]. Here, the total edge T is calculated as sum of T_l values for all effectively considered land-use classes of a particular map M:

$$T(M) = \sum_{l} T_l \tag{6.10}$$

The fact that using a simple total edge count metric for each land-use class delivers satisfying results is due to the representation of the problem in a land-use map consisting of patches that are predefined in terms of m planning units. Thus, the shape of the land-use patches is already pinned down by the shape of the planning units as the resulting land-use patches coincide with one planning unit or a composite of neighboring planning units.

6.2.6 Optimization Algorithm

The optimization procedure used for the approach presented in this paper builds upon an existing generic optimization framework for land-use pattern optimization which was adapted and extended here for the purpose of finding economically, as well as socially, favorable brownfield land-use configurations. The heuristic optimization framework LupoLIB [Holzkämper, 2006] utilizes the genetic algorithm library GAlib [Wall, 1996].

The optimization framework is formulated as a C++-code, where all parameters and inputs, like settings for the genetic algorithm, weightings and constraints for evaluation functions and objectives, as well as gridded data (initial land-use map, planning units, and evaluation maps) are read from ASCII files.

An initial land use input map M_{init} serves as a basis to generate the initial population. It represents one random land-use configuration respecting the defined planning units $u^*(id)$ according to the given ID-map. Other members of the initial population are stochastically generated by changing the assigned land-use classes in a patch wise manner with a given probability p_{init}. The areal ratios of the considered land-use classes, i.e. the composition of M_{init}, will serve as the reference in the subsequent optimization. Specified areas or land-use classes of the initial map can be excluded from optimization by not assigning patches on the ID-map or excluding the land-use class from change during the optimization. For instance, if a certain land-use class allocation is set fix to specific patches, or if the respective area is not within the site boundary.

The initial population consists of *popSize* individuals, each represented by a genome consisting of a vector of m genes, where each gene represents a land-use patch with land-use class l. An individual (i.e. one specific land-use configuration), therefore, comprises different land-use classes and is defined by its vector of planning units $g : (l_h)_{h=1,...,m}$ with $l_h \in L_g$, where $L_g = \{100, 200, \dots, a * 100\} \in L$.

Genetic operators are used to obtain different individuals within one generation and a reasonable evolution with proceeding generations, i.e. an increasing fitness. The optimization algorithm uses one-point crossover [cf. to Wall, 1996] with a probability of p_{cross}. Mutation is conducted with a probability of p_{mut}. Parents for the next generation are selected by roulette-wheel selection [Goldberg, 1989], where the size of the wheel section is proportional to the fitness value of every individual. The individuals with the lowest fitness values are removed from the population. Here, a steady state GA with overlapping populations is applied, where a specified proportion p_{repl} of the population is replaced in each generation by new offsprings. The optimization routine follows the process described in Algorithm 5 (see annex).

6.2.7 Formulation of objective function

Based on the assessment methods introduced above (Equations 6.4, 6.6, 6.9, and 6.10), four functions F_1 to F_4 are defined that evaluate the fitness of a given individual or genome g, i.e. a particular land-use option that is represented by the map $M(g)$ with respect to individual aspects of the assessment. These aspects are: (i) remediation costs, (ii) market value of land, (iii) sustainability, and (iv) shape and compactness of areas allocated to each land-use class. All functions are formulated such that the range of function values is between zero and unity and will be subject to maximization within the optimization.

The function F_1 for evaluating remediation costs of any specific land-use option represented as map M(g) is

$$F_1 = \frac{1 - C_{tot}(M(g))}{C_{tot,max}} \tag{6.11}$$

where

$$C_{tot,max} = \sum_{i,j} \max_{l} (c_{l,i,j}), \tag{6.12}$$

represents the maximum of remediation costs and is used to normalize the function. The market value is described by:

$$F_2 = \frac{V_{tot}(M(g))}{V_{tot,max}} \tag{6.13}$$

where

$$V_{tot,max} = \sum_{i,j} \max_{l} (v_{l,i,j}) \tag{6.14}$$

Please note that only effectively allocatable (defined in M_{init}) land-use classes l are considered for calculating the evaluation functions.

The evaluation function for the degree of suitability with respect to sustainable development is formulated as:

$$F_3 = \frac{E_{tot}(M(g)) + 100}{200} \tag{6.15}$$

The patch compactness of land-use map $M(g)$ is computed by:

$$F_4 = 1 - \frac{T(M(g))}{T_{max}} \tag{6.16}$$

with

$$T_{max} = \sum_{l} \frac{T_l}{4 d p_l k_l} \tag{6.17}$$

T_{max} is an approximation for the upper limit of possible T of the total edges of all land-use classes l present in $M(g)$, where p_l denotes the number of patches present in $M(g)$, k_l is the number of land-use classes present in the initial map M_{init}, and d stands for the cell size of the land use map's raster grid. T_{max} is dependent on the discretization of G, on the number of grid cells to be allocated in M, the respective shape of the total allocatable area, and on the number and size of patches.

Having defined its elements F_1 to F_4, the mathematical formulation of the objective function (OF) is

$$\max J(M(g)) = \sum_{i=1}^{4} F_i w_i \tag{6.18}$$

such that

$$\sum_{i=1}^{4} w_i = 1 \tag{6.19}$$

and

$$c_1 + 1 \geq \frac{A_l(M(g))}{A_l(M_{init})} \geq \begin{cases} 1 - c_1, & \text{if } c_1 \leq 1 \\ 0, & \text{if } c_1 > 1 \end{cases}, \quad \forall\, l \in L_g \tag{6.20}$$

where $J(M)$ represents the fitness score (of the map representation) of genome g, which is subject to maximization. The particular aim of an optimization is determined by the setting of the weightings w_i. If brownfield redevelopment shall be optimized with respect to only one single aspect, the value of the corresponding weighting factor is set to unity while the other weightings become zero. Other settings of the weightings can be used to formulate multi-objective optimization goals.

A class-area constraint c_1 [-] is set regarding the composition of the land-use options (Eq. 6.20). The areal fraction of individual land-use classes, where A_l is the total area of the respective land-use l, must not deviate from the respective fraction in the initial land-use map M_{init} by more than a given factor c_1. Otherwise, the individual's objective score will be set to zero.

6.3 Case study

6.3.1 Site description

The model site is a former military base situated in the vicinity of Potsdam near Berlin, Germany. It was used by German and Russian armed forces until 1945 and 1991, respectively.

The site covers an area of about 113 hectares. Operation of a dry cleaning facility, gas stations and other activities led to considerable contamination of the subsurface. Groundwater is mainly affected by volatile chlorinated hydrocarbons, i.e. tetrachloroethylene (PCE) and trichloroethylene (TCE). For soil, several areas were identified that are suspected of being contaminated by polycyclic aromatic hydrocarbons (PAH). Details about the site investigations and the model study, which have been undertaken to delineate the contamination, are presented in Rein et al. [2010] and Morio et al. [2008, 2010].

6.3.2 Basic land-use scenario and initial land-use configuration

The presented study considers a sub-set of three land-use classes consisting of: 'residential', 'commercial', and 'recreational' use. A basic land-use composition was defined such that the total area fraction of all three use types is approximately the same (tolerance $\pm 3\%$). Hence, for the arbitrarily allocated land-use configuration that serves as starting point for all OR, the land-use classes are assigned to the planning units (Figure 6.2) and converted to raster grids in a way that residential use holds 35.2% (34.4%), commercial use 33.2% (34.1%), and recreational use 31.6% (31.5%) of the area, depending on the grid discretization used (values for $d = 10$m raster grid and, in brackets, for $d = 50$m raster grid discretization, not depicted in Fig. 6.2).

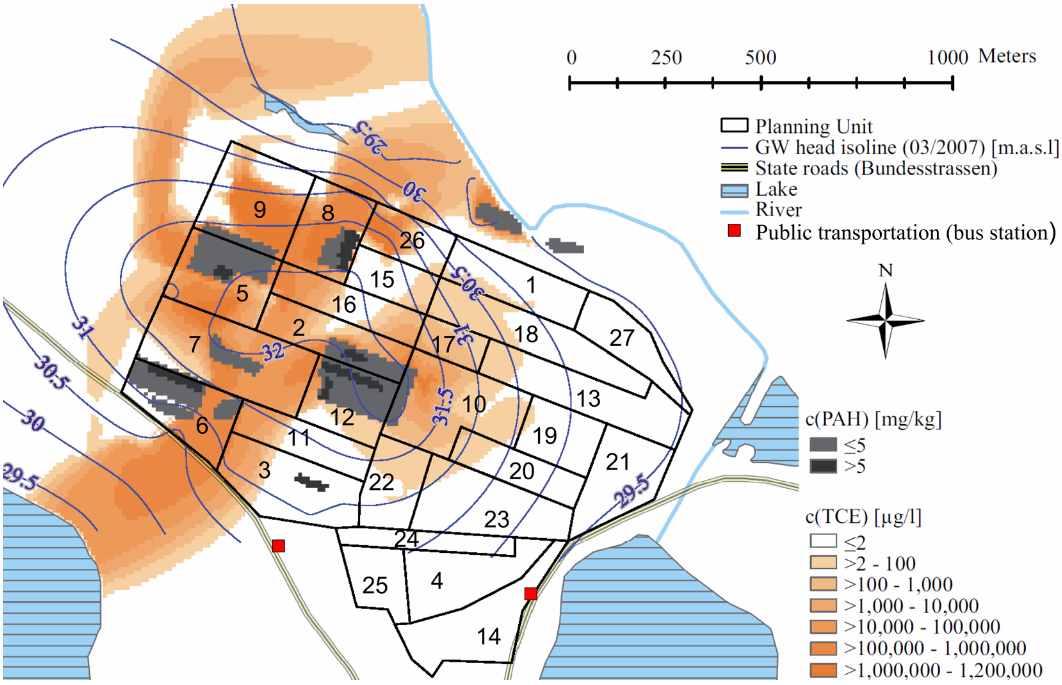

Figure 6.1: Demonstration site subdivided into planning units (black solid line polygons), the groundwater table, and the suspected contamination in groundwater (TCE) and soil (PAH). [m.a.s.l.: meters above sea level]. Figure adapted from Schädler et al. [2012].

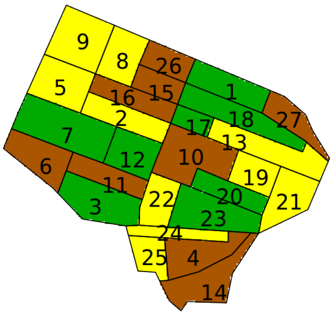

Figure 6.2: Initial map with residential (yellow), recreational (green), and commercial (brown) land-use classes. Each class has an area fraction of about 1/3 of the site's area.

6.3.3 Economic valuation data

The cost maps and land value maps for the evaluation of the individuals according to Equations 6.4 and 6.6 can be calculated in advance of the OR because cost and land value data of any particular evaluation grid cell are exclusively a function of the cell's attributes (type of future use, existing contamination in soil and groundwater, location quality) and are independent of neighboring relations (i.e. for the valuation of the cell under consideration, it does not matter what the situation is in its neighborhood). The costs for soil and groundwater remediation were calculated for each land-use class based on clean-up goals listed in Table 6.4, yielding raster grids of costs per area (Figure 6.3). Raster grids of land value were calculated accordingly (see Figure 6.4) using the reference land-values and respective factors given in Table 6.4.

Table 6.4: Characteristic attributes for the three land-use classes considered in the case study (following Schädler et al. [2012]).

	Land-use option class		
	Residential	Commercial	Recreational
Clean up goals for:			
- TCE in GW [μg/l]	10	100	60
- PCE in GW [μg/l]	10	100	60
- PAH in soil [mg/kg]	2	10	4
Relevant soil depth below grade [m]	0.35	0.10	0.10
Reference land value $V_{l,ref}$ [EUR/m^2]	95	40	10
Diminution factor D [%]	80	75	50
Location quality factor $q_{l,i,j}$ [-]	0.87…1.04	0.82…0.99	0.75…0.95
Related land-use type acc. to Table 6.1 (sustainability assessment)	1	4	3

The cost maps illustrate an overlay of the revealed conflicts between present contamination and clean-up goals of the proposed land-use. Close inspection of Figure 6.3 reveals that (i) in the uncontaminated south and northeastern parts of the site, no costs will be incurred and that (ii) the highest remediation costs can be expected where soil contamination coincides with groundwater contamination.

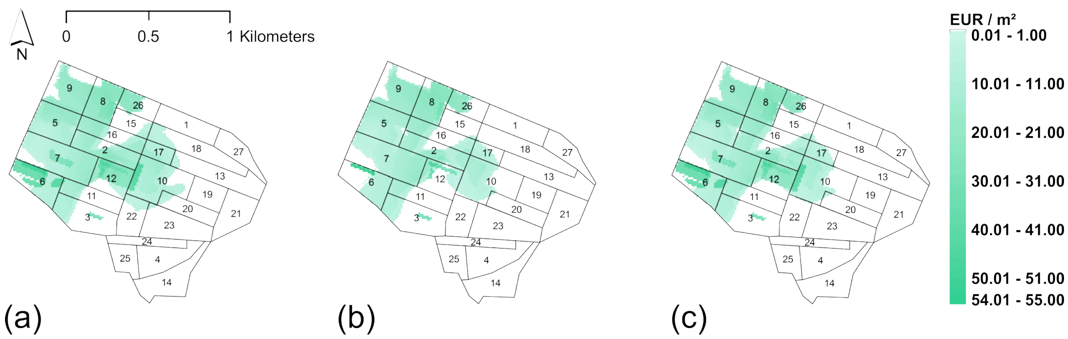

Figure 6.3: Remediation costs c_l per sq.m for uniform land use with (a) residential, (b) commercial, (c) recreational use-type.

Figure 6.4 depicts the market value for the considered land-use class $v_{l,i,j}$ according to Eq. 6.6, divided by the cell's area (i.e. EUR/m^2). The pattern in the $v_{l,i,j}$

depiction stems from location quality correction factor matrix Q (cf. Table 6.4), where the according discount or surcharge factors $q_{l,i,j}$ were defined patch wise (i.e. on the basis of the planning units).

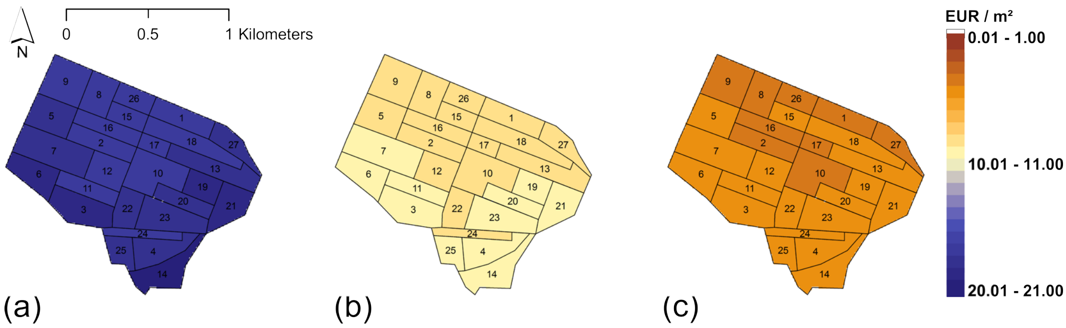

Figure 6.4: Market value v_l per sq.m for uniform land use with (a) residential, (b) commercial, (c) recreational use-type.

Figure 6.5 illustrates the remaining value $r_{l,i,j} = v_{l,i,j} - c_{l,i,j}$ for uniform allocation of the considered land-use classes. Assuming the land-use allocation will be done on the basis of planning units, the market values and remediation costs were summed up and averaged for each planning unit. The arithmetic mean of remaining value $r_{l,i,j}$ for each planning unit is illustrated in Figure 6.6. For land-use class 'residential', all planning units except no. 6, 8, and 12 yield a positive remaining value. In contrast, land-use class 'commercial' yields a slightly positive remaining value on planning units 6 and 12, while on planning units no. 2, 5, 9, and 26 remediation costs are considerably higher than the calculated market value. For recreational land-use class, remediation costs exceed the market value for almost all planning units located on the central and for all planning units on the north-western part of the site.

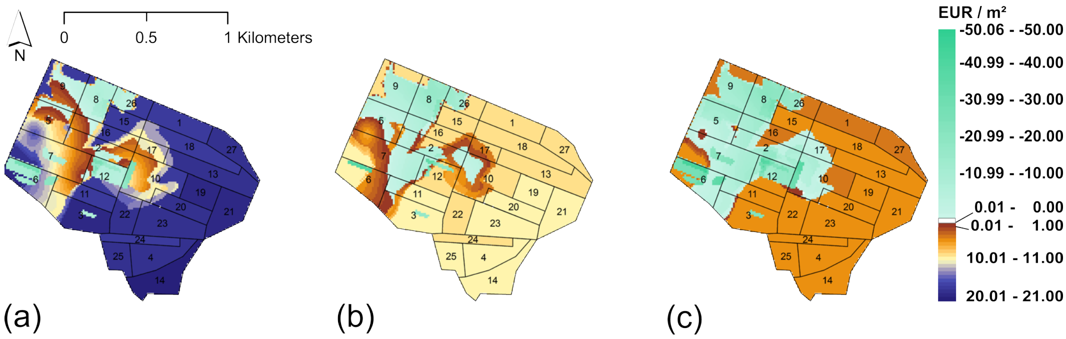

Figure 6.5: Remaining value R per sq.m depicted per raster grid cell for uniform land use with (a) residential, (b) commercial, (c) recreational use-type.

The overall remediation costs C_{tot}, market value V_{tot} and remaining value R for the land-use classes are summarized in Table 6.5. The high market value for 'resi-

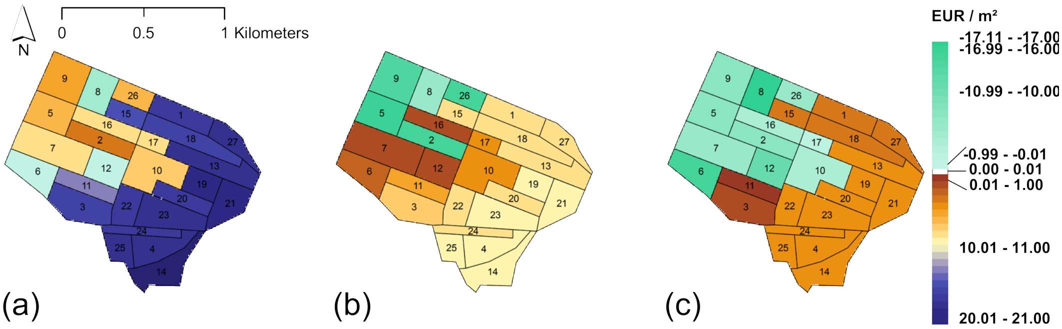

Figure 6.6: Remaining value R per sq.m, arithmetic mean for each planning unit.

dential' outweighs the remediation costs for almost all patches. Since 'recreational' has a lower market value, but comparable sensitivity to subsurface quality, the remaining value R becomes significantly lower than for uniform 'commercial', or 'residential' use.

Table 6.5: Remediation costs C_{tot}, market value V_{tot}, remaining value R, and sustainability potential E_{tot} assuming uniform use options and for the initial land-use layout i.e. configuration M_{init} (values for a raster grid resolution of 50m and – in brackets – for 10m) [n.c. = not calculated].

	Land use option (uniform)			Initial layout
	Residential	Commercial	Recreational	M_{init}
C_{tot}	6.82	**4.56**	6.01	5.02
[Mio. EUR]	(7.06)	(4.65)	(6.26)	(n.c.)
V_{tot}	**20.91**	10.25	4.76	12.05
[Mio. EUR]	(20.78)	(10.18)	(4.73)	(n.c.)
R	**14.09**	5.69	-1.25	7.03
[Mio. EUR]	(13.72)	(5.53)	(-1.35)	(n.c.)
E_{tot}	-10.21	**+9.39**	-25.00	+0.59
[-]	(n.c.)	(n.c.)	(n.c)	(n.c.)

For comparison, Table 6.5 also lists the values of C_{tot}, V_{tot}, and R of the initial layout M_{init} (Figure 6.2).

6.3.4 Sustainability evaluation settings

The evaluation of the sustainability indicators is based on the parameters given in Table 6.2. Indicators no. 1–4, 11, 14, and 19 were evaluated on the basis of spatial queries. For the remaining indicators, a global default answer 'True' or 'False' was predefined (i.e. indicator evaluation function 'Global'). The location of public bus stations, relevant for spatial query of indicator no. 11, is indicated in Figure 6.1. The decision to select only a subset of indicators for spatially explicit evaluation was based on the reason to keep the results more transparent and traceable for discussion within the scope of this paper.

To allow comparison to sustainability results of the OR presented further below, the degree of suitability for sustainable development E_{tot} was calculated for the uniform land-use classes, and for the initial layout M_{init}. Table 6.6) shows the single indicator results for uniform land-use compositions and M_{init}. Uniform land-use composition 'commercial' has the highest suitability for sustainable development, followed by the initial scenario M_{init}. 'Residential' is evaluated slightly worse, whereas a uniform composition consisting of 'recreational' use has a significantly lower suitability for sustainable development. This is because for 'recreational', only four of 23 indicators have a relevance for evaluation, from which two result in a score of $e_x = -1$ (and of $E_{x,s} = -457$, respectively).

Please note that, the uniform land-use compositions are not affected by indicators 1, 2, and 3 because these need a second land-use type being present for evaluation (cf. zero values in Table 6.6 and columns 'Affected use type' and 'Evaluation use-type' in Table 6.2).

Table 6.6: Sustainability results of relevant indicators x for uniform land-use compositions and M_{init}. Matrix sums of the positive and negative scores of $E_{x,s}$, and E_{tot} acc. to Eqs. 6.8 and 6.9. Indicators 4, 7, 8, 10, 12, 19,and 23 do not affect the land-use types assigned to the land-use classes used in this case study or receive zero values due to global default answers.

No.	**Uniform land-use compositions**						**Initial land-use map** M_{init}					
x	Residential		Commercial		Recreational		Residential		Commercial		Recreational	
	$E^+_{x,s}$	$E^-_{x,s}$	$E^+_{x,s}$	$E^-_{x,s}$	$E^+_{x,s}$	$E^-_{x,s}$	$E^+_{x,s}$	$E^-_{x,s}$	$E^+_{x,s}$	$E^-_{x,s}$	$E^+_{x,s}$	$E^-_{x,s}$
1	0	0	0	0	0	0	0	0	144	0	156	0
2	0	0	0	0	0	0	157	0	0	0	0	0
3	0	0	0	0	0	0	157	0	0	0	0	0
5	0	0	0	-457	457	0	0	0	0	-144	156	0
6	0	-457	0	-457	0	0	0	-157	0	-144		0
9	0	-457	0	0	0	0	0	-157	0	0	0	0
11	221	-236	221	-236	0	0	60	-97	76	-68	0	0
13	457	0	457	0	457	0	157	0	144	0	156	0
14	0	-457	0	0	0	0	0	-157	0	0	0	0
15	457	0	0	0	0	0	157	0	0	0	0	0
16	0	-457	0	-457	0	0	0	-157	0	-144	0	0
17	457	0	457	0	0	-457	157	0	144	0	0	-156
20	457	0	457	0	0	0	157	0	144	0	0	0
21	0	-457	0	0	0	-457	0	-157	0	0	0	-156
22	0	0	457	0	0	0	0	0	144	0	0	0
$\sum_x E^+_{x,s}$	2049		2049		914		1002		796		468	
$\sum_x E^-_{x,s}$		-2521		-1607		-914		-882		-500		-312
E_s	-10.21		9.39		-25.00		-0.55		5.40		-4.27	
E_{tot}	-10.21		9.39		-25.00				0.52			

6.3.5 Objectives and settings of optimization runs

Purely economically driven optimization runs (OR) were conducted with single and weighted aggregate objective functions (OF) as defined in Chapter 6.2.7. The single goals were minimization of remediation costs (Eq. 6.11, $w_1 = 1$ in Eq. 6.18) and maximization of market value (Eq. 6.13, $w_2 = 1$ in Eq. 6.18). OR with multicriteria OF were conducted with $w_1 > 0$ and $w_2 > 0$ at different weighting combinations, aiming at the highest possible remaining value R. The objective of compact land-use pattern (Eq. 6.16) was evaluated in combination with the economic objectives ($w_1 = w_2 = w_4$).

To search for options with maximum suitability regarding sustainable development, OR with single OF were conducted ($w_3 = 1$). Additionally, multiobjective OF were used to trade off economical and sustainability goals ($w_1 = w_2 = w_3$).

All OR were ran with varying values of constraint c_1, (0.2, 0.5, 0.9, and 1.9), whereas deviations of the total land-use classes area ratio are allowed in positive ($A_l(M(g)) > A_l(M_{init})$), as well as in negative direction ($A_l(M(g)) < A_l(M_{init})$) (cf. Eq. 6.20). Note that the highest c_1 value of 1.9 was chosen such that a land-use class cannot disappear completely, i.e. to ensure mixed land-use options. Uniform land-use compositions' results were already presented in the previous sections.

Some OR were repeated with a finer grid resolution of $d = 10$m to investigate the influence of grid scale to optimization. The majority of OR were conducted with a coarser grid resolution of 50m to obtain acceptable response times of the optimization, especially for the evaluation of F_3.

Because of the stochastic nature of heuristic optimization techniques such as GA, it cannot be guaranteed that their algorithms will find the optimum in a single optimization attempt (i.e. optimization run OR). As a consequence, several OR need to be conducted to increase the probability of success. Here (at least) 6 attempts were made for each objective function, and constraint c_1, considered in this case study. The obtained series of multiple solutions give an indication of the reliability and reproducibility of the optimization result.

The optimization parameters were tuned manually during test runs until a reasonable performance was achieved. The optimization parameters used in the framework presented in this paper are listed in Table 6.7. The settings were kept for all runs presented in this paper, except for the weighting and constraint parameters.

6.4 Results and Discussion

6.4.1 Economical optimization

The results of all economically directed OR are summarized in Figure 6.7. The dash-dotted lines indicate equal remaining land value (R). Each marker represents the respective values for the best individual of an OR for one of the objectives that has been considered. A total number of 204 OR were conducted with a purely economic objective, either $\min C_{tot}$, $\max V_{tot}$, or $\max R$ (16 runs per objective-constraint

Table 6.7: Parameters used for the optimization runs.

Parameter	Value	Description
popSize	200	number of individuals in population
pAU	0.5	probability p_{au} of changing areal units
pCross	0.95	probability of cross-over p_{Cross}
pMut	0.01	probability of mutation p_{Mut}
pRepl	0.75	proportion of replacement in next generation p_{Repl}
nGen	4000	maximum number of generations
pConv	0.99	proportion of convergence
nConv	50	number of generations to be compared for convergence criterion
alleleset_area	100, 200, 300	land use classes used for building allele-set of genome
area_change_except		land-use patches not to be changed
AREA_IDMAP	id_area	id-map with predefined planning units
areaID_cat	100, 200, 300	land-use ids in initial map that should be considered
neighborhood	4	type of cell neighborhood (4 or 8 neighbors)
min_area	10	minimum patch/planning unit area to be considered in GA (here: grid cell size)
weightings	0.25, 0.25, 0.25, 0.25	w_i, weighting factor for objective function F_i
constraints	0.5	c_i
landusemap	lu_map	initial land-use configuration from which the population of individual is generated
inputmaps	ROCO100, ROCO200, ROCO300, MV100, MV200, MV300, pubtrans	evaluation maps
LUTblp	1 ,4, 3	Relation between occurring land-use classes and sustainability use types in Table 6.1

combination on a 50m by 50m grid discretization and one additional run using a 10m by 10m grid discretization). As could be expected, the results differ remarkably, depending on the specified goal that has been targeted with the optimization, as well as on the value of constraint c_1 used in the OR. The OR runs using finer discretization delivered similar results and, therefore, are not further differentiated here. Green asterisks mark the best OR for each objective – constraint combination and are illustrated as maps in Figures 6.8, 6.9, and 6.10, respectively. Summary statistics of the results are presented in Table 6.8.

Table 6.8: Best, worst and arithmetic mean results for economically directed OR.

c_1	Result	Objective								
	Mio. EUR	$\min C_{tot}$ Best	Mean	Worst	$\max V_{tot}$ Best	Mean	Worst	$maxR$ Best	Mean	Worst
0.2	C_{tot}	**4.69**	4.90	5.33	6.08	5.74	5.46	4.96	5.19	5.78
	V_{tot}	11.55	11.61	11.97	**13.31**	13.18	13.04	13.22	13.02	13.02
	R	6.86	6.71	6.64	7.23	7.44	7.58	**8.27**	7.83	7.24
0.5	C_{tot}	**4.57**	4.62	4.71	5.58	5.94	6.01	4.86	5.03	4.65
	V_{tot}	10.85	10.43	10.37	**14.94**	14.78	14.69	14.62	14.42	13.17
	R	6.28	5.81	5.66	9.36	8.83	8.69	**9.76**	9.39	8.51
0.9	C_{tot}	**4.56**	4.60	4.68	6.07	6.17	6.25	4.98	5.03	4.66
	V_{tot}	10.61	9.84	11.23	**17.07**	16.98	16.85	17.11	16.45	15.05
	R	6.05	5.24	6.55	11.00	10.82	10.60	**12.13**	11.42	10.39
1.9	C_{tot}	**4.56**	4.56	4.65	6.71	6.69	6.26	5.56	5.39	4.65
	V_{tot}	11.02	9.76	10.06	**20.42**	20.04	19.26	19.07	17.72	15.10
	R	6.46	5.20	5.41	13.71	13.35	13.00	**13.51**	12.33	10.44

The objective $\min C_{tot}$ yields the lowest remediation costs. For $c_1 = 0.2$, 4.69 Mio. EUR are achieved, whereas higher c_1 (indicated by different marker colors in Figure 6.8) yield lower C_{tot}, since the ratio of less sensitive land-use class ‘com-

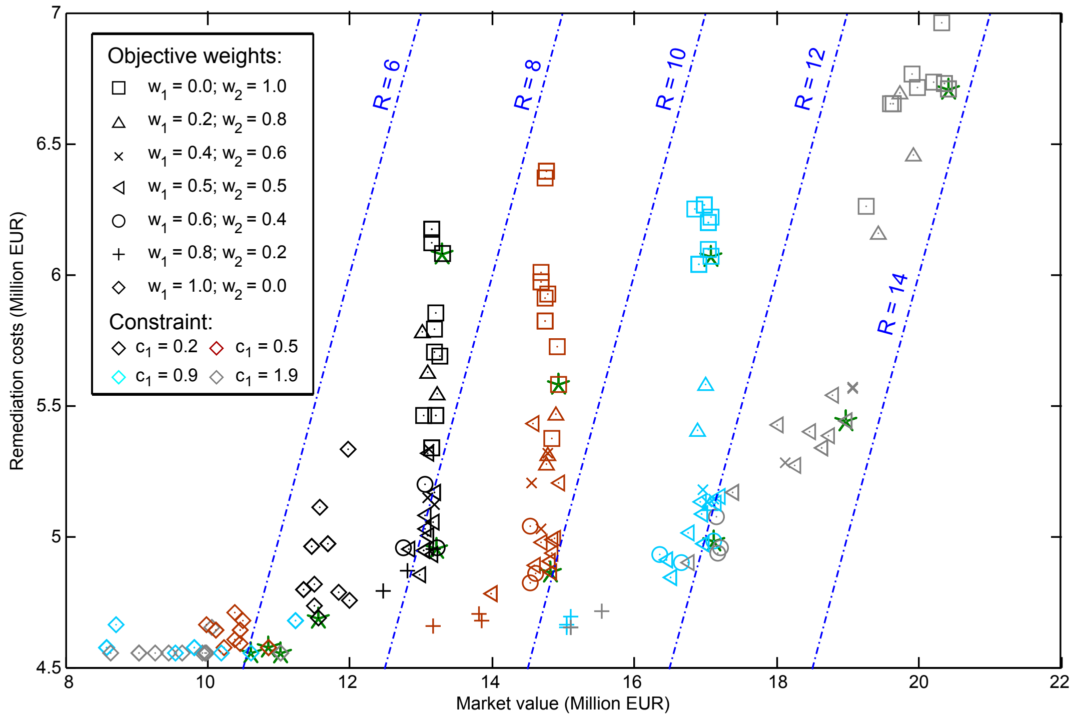

Figure 6.7: Remediation costs (w_1) vs. market value (w_2): Best individuals of each OR. Dash-dotted lines represent isolines of equal remaining value R (in Million EUR). OR results marked with green asterisk are depicted in Figures 6.8, 6.9, and 6.10.

mercial' can be raised. Note that the lowest possible C_{tot} of ca. 4.56 Mio. EUR (compare Table 6.5) is almost realized at $c_1 = 0.5$. Less strict (i.e. higher) c_1 values yield only a marginal improvement because a certain areal ratio of sensitive land-use classes can be assigned to the uncontaminated southeastern part of the site (cf. Figure 6.3). Depending on the allocation of land-use classes in this part of the site, market values differ at equal remediation costs. Please note further that the reproducibility of multiple OR increase with increasing c_1, as indicated by the more and more narrowed range of results.

The maximum achievable market value strongly depends on the constraint c_1. When only little deviation from the initial land-use class ratio is allowed ($c_1 = 0.2$), the market value is limited to a maximum of 13.31 Mio. EUR. For a maximum degree of freedom, values are beyond 20 Mio. EUR. Higher V_{tot} values are achieved by higher ratio of land-use class 'residential' (cmp. Figure 6.4 and Table 6.5). Thus, the best OR result in land-use maps showing the maximum allowed ratio of land-use class 'residential' (Figure 6.9). The small range of V_{tot} values resulting from multiple OR indicates a high reliability of each single OR.

In order to determine the maximum remaining value R_{max}, the trade off of both goals, $\min C_{tot}$ and $\max V_{tot}$, was examined using weighted aggregates. Different weighting sets (w_1, w_2) were applied (see marker symbols for both, $w_1 > 0$, and

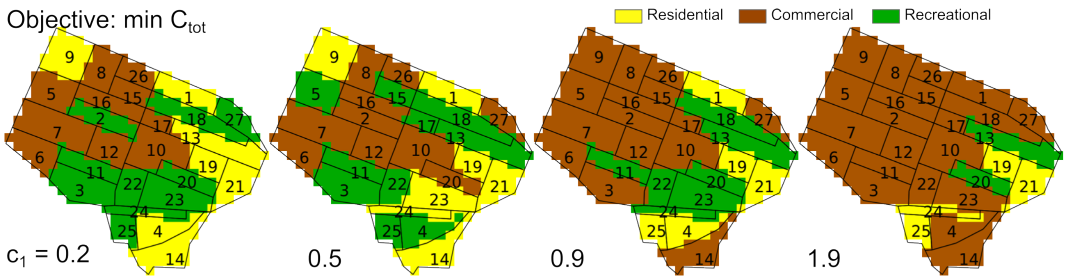

Figure 6.8: Best individuals of OR to minimize remediation cost for different c_1 values.

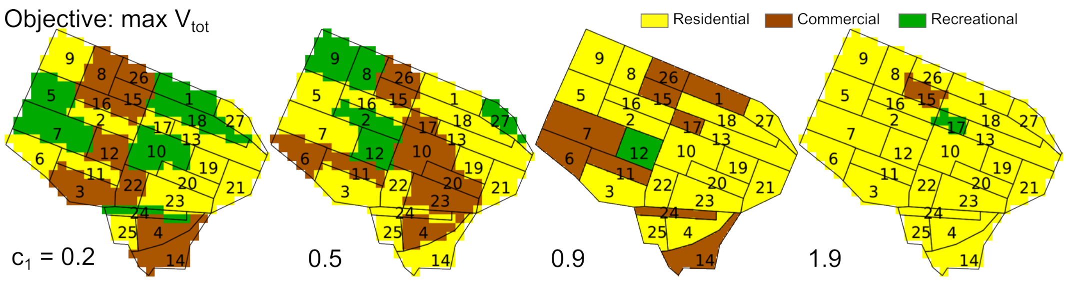

Figure 6.9: Best individuals of OR to maximize the market value for different c_1 values.

$w_2 > 0$, in Figure 6.7). Depending on the given value of constraint c_1, the optimal result R_{max} varies between 8.27 Mio. EUR and 13.71 Mio. EUR (see also Table 6.8). For low c_1 values from 0.2 to 0.9, best results are achieved with weightings between 0.4 and 0.6 for w_1 or w_2. For $c_1 = 1.9$, OR with $\max V_{tot}$ ($w_1 = 0$, $w_2 = 1$) yield better results than any of the OR with weighted aggregate OF that were examined. This is due to high values of V_{tot} that can be achieved by increasing the residential area if areal ratios of land-use classes are only a little constrained, and which cannot be outweighed by lowering C_{tot}, a goal being included in the aggregate OF of maximizing R. Exceptions are the patches no. 6 and 12, which pose a higher R for land-use class 'commercial', (cf. also Figure 6.6). These patches get assigned the land-use class 'commercial' in the best outcomes of all OR at all c_1 values considered (Figure 6.10).

OF with an additional objective to maximize the compactness of land-use patches ($w_1 = w_2 = w_4$) were used, but those OR did not yield significantly different results with respect to neither the economical values nor the configuration of shapes and, therefore, are not separately illustrated in this paper.

It is important to note that similar values of R may be achieved with different ratios of C_{tot} and V_{tot} contributing to the aggregated value of R. The higher the C_{tot} value on an R-isoline (Figure 6.7), the higher the portion of remediated area will be, if the land-use configuration shall be implemented (i.e. preference of risk reduction). In contrast, the same, or similar R could be achieved by solutions where

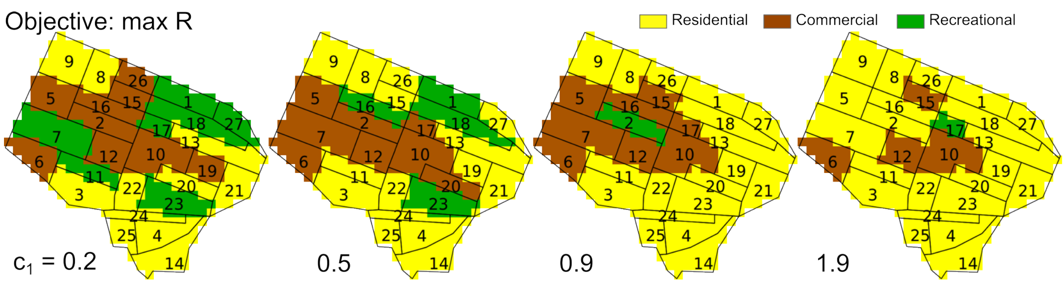

Figure 6.10: Best individuals of OR to maximize the remaining market value R for different c_1 values.

less site remediation is needed due to allocation of less sensitive land-use classes (preference of least possible remedial action). This range of similar R-values gets wider, the higher the c_1 value is set.

6.4.2 Optimizing suitability for sustainable development

OR using F_3 (max E_{tot}) as single criterion result in a E_{tot} range between +7.122 and +14.133, as illustrated in Figure 6.11 by triangle markers. Again, the relaxation of the constraint c_1 yields better results i.e. higher values of E_{tot}. The small range of E_{tot} is caused by the (i) relatively large amount of indicators the value of which is determined globally (default 'true' or 'false'), and (ii) the relatively large threshold distance in comparison to the site's extent. Please note that, for the case study site, mixed use-type scenarios in general gain relatively high E_{tot} values, as opposed to most of the uniform land-use scenarios [also see Schädler et al., 2011b,a]. This is due to the possibly higher numbers of indicators that are relevant for evaluation at the given mixed-use configurations as opposed to uniform land-use composition and thus possibly yields a higher impact in the evaluation (cmp. Table 6.6). Only the uniform land-use composition of 'commercial' had a slightly higher E_{tot} than M_{init} (Table 6.5).

The maps of the best results of all OR conducted for each c_1 are shown in Figure 6.12. It can be seen that patches are successively replaced by land-use class 'commercial' with increasing c_1 value. However, the remaining patches of 'residential' and 'recreational' use, even if they only contribute by a few percent to E_{tot}, raising its value beyond that of uniform 'commercial' use (10.205 to 14.133 for c_1 values of 0.5 to 1.9 vs. 9.39 for uniform 'commercial').

The allocation of the land-use classes 'residential' and 'commercial' is preferably set to planning units with a distance smaller than 500m to the bus stations (cf. Figure 6.1), controlled by indicator number 11. Consequently, land use class 'recreational' is situated rather in the northern part of the site. With higher c_1, the areal fraction of the 'recreational' and 'residential' land-use classes gradually decrease but still have their positive impact for the evaluation of indicators 1, 2, and 3, respectively. The economical parameters have rather low values in all land-use

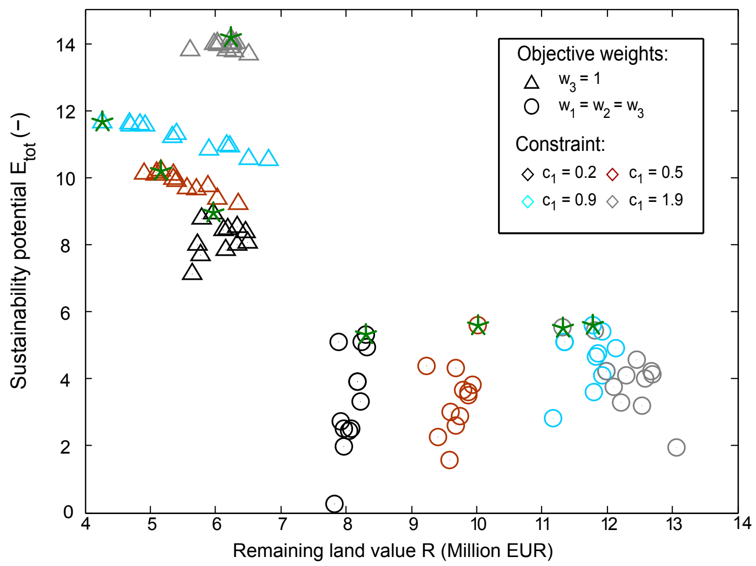

Figure 6.11: Remaining land value vs. sustainability potential E_{tot}: Best individuals of OR. Best individuals marked with green asterisks are depicted in Figures 6.12 and 6.13.

Table 6.9: Sustainability evaluation results for each objective with given constraint c_1. Values for C_{tot}, V_{tot}, and R in Mio. EUR.

c_1	Result	Objective					
		max $E_{tot}(w_3 = 1)$			max equally weighted		
		Best	Mean	Worst	Best	Mean	Worst
0.2	E_{tot}	**8.926**	8.186	7.122	**5.308**	3.345	0.253
	C_{tot}	5.89	5.58	5.09	4.85	4.95	5.28
	V_{tot}	11.86	11.66	11.45	13.10	13.03	12.79
	R	5.97	6.08	5.64	8.30	8.08	7.83
0.5	E_{tot}	**10.205**	9.846	9.211	**5.589**	3.429	1.559
	C_{tot}	5.09	5.31	5.29	4.84	4.94	5.12
	V_{tot}	10.24	10.80	11.65	14.86	13.97	14.70
	R	5.16	5.49	6.36	10.02	9.70	9.58
0.9	E_{tot}	**11.652**	11.193	10.512	**5.586**	4.611	2.833
	C_{tot}	5.39	5.05	4.88	5.12	4.95	4.87
	V_{tot}	9.65	10.53	11.70	16.91	16.66	16.05
	R	4.26	5.48	6.81	11.79	11.71	11.17
1.9	E_{tot}	**14.133**	13.918	13.669	**5.543**	4.035	1.938
	C_{tot}	4.79	4.76	4.69	4.76	5.14	5.40
	V_{tot}	11.02	10.92	11.20	16.07	17.45	18.46
	R	6.23	6.16	6.51	11.31	12.31	13.06

configurations that resulted from optimizing the suitability for sustainable development.

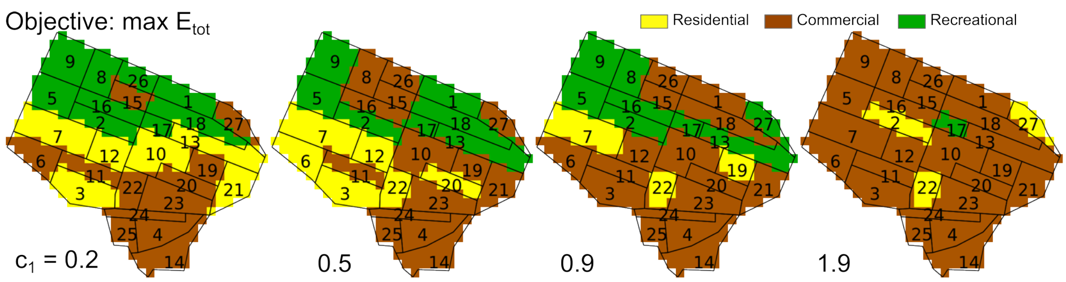

Figure 6.12: Best individuals of the OR to maximize sustainability potential for different c_1 values.

6.4.3 Trading off economically favorable and sustainable land-use configurations

Optimizing the re-use of the site from an integrated perspective using an OF that includes economic criteria (F_1 and F_2), as well as the sustainability criterion (F_3) with a set of equal weightings ($w_1 = w_2 = w_3$), leads to land use configurations that show a mixture of patterns that were observed in the unidirectional OR investigated previously. While the latter resulted in configurations dominated by one single land-use class ('residential' and 'commercial', respectively), the integrated optimization suggests a fairly balanced allocation of these two land-use classes, as is shown in Figure 6.13. Though 'commercial' areas, having a relatively low reference land value, are not preferred from a strictly economic point of view (cf. Figure 6.10) they are obviously a good compromise, as they contribute to a good sustainability grade and, due to their relative insensibility, minimize remediation costs in the northwestern part of the site.

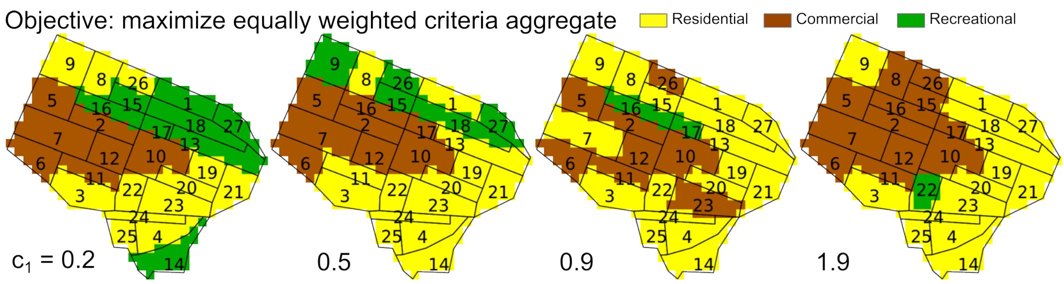

Figure 6.13: Best individuals of OR to maximize the aggregate objective of economic and sustainability criteria, with equal weights ($w_1 = w_2 = w_3$) for different c_1 values.

On the basis of the resulting land-use pattern, it can be inferred that the integrated optimization based on an aggregation of normalized evaluation functions is satisfactory in the trade-off between economic and non-economic objectives. However, a closer inspection of Figure 6.11 reveals that, independent of the values of

c_l, best individuals have a R value close to the optimum (cf. to Table 6.13) while E_{tot} values are relatively low. The fact that for E_{tot}, in contrast to R, hardly any improvement can be observed with increasing scope of planning (i.e. larger c_l values) further supports the impression that sustainability may be considered to a minor extent (see Figure 6.11 and Table 6.9 for a summary). This might be due to the fact that normalization of suitability for sustainable development (Eq. 6.15) can not be done in a case-specific way, as opposed to the economic criteria. This is because the maximum value of E_{tot} that can be achieved within the given planning scope cannot be calculated a priori. The normalization of E_{tot} with respect to the absolute maximum (which is, most likely, not achievable in the given case) may also contribute to the relatively small ranges of E_{tot} compared to the possible variations in R for a given range of land-use class compositions (defined by c_1). Changes in the evaluation of remediation costs and market value, therefore, seem to have a larger impact on the resulting fitness of the individual under evaluation, giving preference to individuals gaining a high R.

6.4.4 Computational considerations

The number of generations were set high ($n_{Gen} = 4000$), in order not to compromise the convergence, i.e. stopping, criterion in ending the OR before near-optimal results were achieved. OR stopped after about 60 to 125 generations, when there was no significant improvement (less than 2 percent increase of the objective score) over the last tenths of generations. Using an OF excluding the sustainability evaluation function F_3 (i.e. $w_3 = 0$), one OR took roughly 4 to 5 hours on a Pentium IV 3,2 GHz processor for the fine grid discretization. OR including sustainability assessment using evaluation function F_3 ($w_3 > 0$) on the fine grid were discarded due to the expected large calculation times. For the coarse grid, the runtime for one OR took between 15 and 20 minutes (excl. evaluation of F_3) or between 40 minutes to 1 hour (incl. evaluation of F_3).

6.4.5 Conclusions

The proposed integrated planning, assessment and optimization framework is intended to support decision making for brownfield restoration projects. The framework allows to determine mixed land-use options that are preferable from an economic perspective, as well as regarding their suitability with respect to sustainable development. On basis of spatial evaluation functions that assess the appropriateness (i.e. fitness) of land-use configurations, the framework creates spatial configurations of a set of predefined land-use classes, which represent a near-optimum, according to the given objectives (e.g. to meet stakeholders' demands with respect to the number and ratio of individual land-use types), and which cannot be found intuitively.

The discrete consideration of the two economic variables remediation costs (C_{tot}), and market value (V_{tot}), provides more useful information than would be available if only the aggregated economic value in terms of the remaining land value R (market value minus remediation costs) were evaluated. It could be shown that similar values of R can be achieved by various land-use configurations having quite different evaluation results for C_{tot} and V_{tot}. For the optimization, this differentiation between costs and benefits allows to follow two strategies: the maximization of R at a minimum of costs C_{tot}, or the maximization of R at a maximum of market value V_{tot}. Though both strategies will maximize the economic outcome, their consequences for the environmental system in terms of remaining contamination may be significantly different. Even if not mandatory, the differentiation will become more important if uncertainty shall be properly taken into account, which can be very different in accordance with their particular governing parameters and factors for C_{tot} and V_{tot}.

Pattern metrics were not further discussed in this paper, although implemented in the optimization approach, because they showed not much impact in the particular case study presented. Pattern metrics would be a matter of concern for land-use planning problems including brownfield redevelopment projects, where the given 'planning units' are e.g. different in shape or size than the typically required sizes for implementation of land-use classes under discussion [e.g. Herold et al., 2005, for discussion of urban landscape metrics], or in cases where they are not defined at all (i.e. size of planning unit equals the grid cell size in this approach).

Furthermore, it could be demonstrated that sustainability issues can be conveniently considered within a spatial optimization framework for land use planning by means of a fully quantitative scheme. Although such a scheme can not replace a detailed and expert-based evaluation of sustainability measures, it may strongly improve the basis for transparent and stakeholder friendly discussions on the re-use of brownfields. Nevertheless, several issues need to be investigated and elaborated in more detail, namely the role of the method of normalization in combination with the weighting and the influence of assumptions made regarding threshold distances, and with respect to the evaluation of individual indicators (e.g. globally or spatially explicit).

Finally, it should be pointed out that the results obtained in the presented case study certainly depend on the assumptions made therein and on the specific characteristics of the site. The parameters used to characterize the land-use classes, namely the clean-up targets and reference land values, but also the attributed type of land use according to the classification used in the sustainability assessment, govern the evaluation of individual land-use configuration's fitness, and can differ from those presented here in other cases. Moreover, type, level, and spatial distribution of subsurface contamination of the brownfield, may have a strong impact on the outcome of the optimization, as they determine the extent and costs of remedial activities required to make the implementation of a particular re-use plan possible.

6.5 Software availability and supplementary data

The adapted version of LUPOlib called MOOL can be requested free of charge as windows binary or source code. The megasite management tool suite, including a simplified version of the presented optimization framework, can be requested via contact address on its website http://www.safira-mmt.de.

6.6 Acknowledgments

The authors gratefully acknowledge the support of the German BMBF research priority program REFINA (contract no. 0330757C) and of the Helmholtz Centre for Environmental Research - UFZ in Leipzig (contracts no. 4500029698 and 4500050981) and the EC research project TIMBRE (project no. 265364). Thanks go to Ksenia Voronina for language editing.

6.7 Algorithms

Algorithm 4 Sustainability indicator evaluation function ‘Distance’

```
Read sustainability indicator table {CSV-ASCII file, cf. to Table 6.2}.
Relate occurring land-use classes of L in actual map M to sustainability land-use types {cf. Table
6.1} according to assignment given in configfile (cmp. Table 6.7, parameter ‘lutBLP’).
Read affected and evaluation land-use types and grids
Read land-use type specific positive and negative indicator values
Assign default positive and negative value for indicator to matrix
Get class area of evaluation land-use types
for rows i of actual map do
    for cols j of actual map do
        for no. of affected types do
            for no. of evaluation types do
                if s(M_{i,j}) = s of affected type then
                    Calculate minimum distance between i, j and evaluation type cells
                    if minimum distance < dThresh AND class area of evaluation use type > aThresh
                    then
                        Assign positive indicator value to e_{x,s,i,j}
                    else
                        Assign negative indicator value to e_{x,s,i,j}
                    end if
                else
                    Assign zero indicator value to e_{x,s,i,j}
                end if
            end for
        end for
    end for
end for
Return land-use type specific indicator value matrices E_{x,s}
```

Algorithm 5 Optimization routine, changed after Holzkämper et al. [2006]

Initialization of population:
while individuals in population < population size **do**
  genome initialization $\rightarrow g$
  genome to map transformation $\rightarrow M(g)$
  objective function evaluation $\rightarrow J(M)$ {cf. section 6.2.7}
end while
Evolution:
while generation < final number of generations n_{gen} **do**
  Select parent genomes from population acc. to $J(M)$ values (roulette wheel selection)
  Crossover between parents with probability p_{cross}
  Mutation of new genomes with probability p_{mut}
  while individuals n_{pop} **do**
    Genome to map transformation $\rightarrow M(g)$
    objective function evaluation $\rightarrow J(M)$
  end while
  Resize population by deleting the overlapping proportion of the population p_{repl}
  if generation / outputincrement == round(no. of generation / outputincrement) **then**
    Best individual in generation: genome to map, write output map, write score and single evaluation parameters to score file
  end if
end while
Select the best genome of final generation
Genome to map transformation $\rightarrow M(g)$
Write output map, score and single evaluation parameters to scores file.

Chapter 7

Summary and conclusions

Integrated brownfield revitalization projects include economic as well as social aspects. Decision support systems that include these different aspects enhance the assessment of re-use scenarios and can foster transparent decision making. Stakeholder participation and integrated evaluation of re-use scenarios may yield different land-use configurations than only looking at a single criterion like e.g. minimization of remediation costs.

There is still a demand for holistic, integrated DSS that includes all relevant aspects of brownfield revitalization assessment. Spatially explicit DSS aids the evaluation process by integrating data management, processing, modeling, analysis, and visualization of all relevant data and information.

Within this thesis, several methods were presented to improve the integrated assessment of re-use scenarios:

Regarding input data preparation for spatial DSS, a new flow guided interpolation (FGI) method was introduced to generate spatially continuous concentration distributions in groundwater contaminant plumes. It improves decision making especially at early stages of site assessment, where only limited amounts of physical samples are available. The FGI method utilizes additional information on groundwater flow and the contaminant source zone size and concentration to enable segment wise interpolation of contaminant concentration point data. This approach delivers an improved performance and robustness in comparison to standard interpolation methods for determining the contaminant solute distribution in a plume. Application of FGI at different investigation stages and coupling to conflict analysis and remediation cost models showed that the uncertainty about expected remediation costs for re-use scenarios may be reduced by using FGI during the assessment process.

The identification of remediation requirements in order to avoid or reduce risks for receptors (human health and environment) being present in the re-use scenario is seen as an important point in brownfield assessment. GIS based conflict analysis reveals contaminant, land-use and site specific needs for remediation. Different land-use types in a re-use scenario can have different sensitivities and demands with respect to subsurface quality. Therefore, conflict analysis is proposed as a site-and land-use specific method that gives valuable input for spatially explicit cost modeling. This method shows the local relation of expected costs and therefore aids cost-optimized planning of reuse layouts. Conflict analysis is embedded in the DSS by utilizing spatial data modeling.

It was shown that brownfield re-use, especially at large sites that allow for many different scenarios, could be optimized with respect to their spatial configuration by analyzing the possible layouts and determining the consequences of the specific configuration of a re-use plan. Integrated brownfield assessment was complemented by heuristic optimization methods in order to generate better land-use layouts with respect to different criteria marked as relevant for future site use. These criteria include economic aspects (i.e. minimization of remediation costs and maximization of market value) and the suitability for sustainable development (e.g. based on a context-specific indicator system), which are formulated as a multi-criterial objective function of a spatial optimization framework. Multi-criteria optimization allows for trade-off of conflicting interests and supports the identification of near-optimal planning alternatives based on preference weights of single criteria. Especially at larger sites with more planning options, optimization embedded in a brownfield DSS can aid the identification of favorable land-use options and feasible layouts that are evaluated on the basis of different criteria.

Within a case-study application, it was shown, that multi-criteria optimization can determine land-use configurations that contain trade-offs of economical aspects like expected remediation costs and the goal of maximized market value, yielding a more beneficial re-use layout than manual planning could achieve. The case-study also reveals that economically beneficial scenarios and layouts do not necessarily contradict layouts preferable for sustainable development. A trade-off of these aspects is supported and an emphasis can be given to compromises that might have to be made with respect to the stakeholders' differing perspectives.

The experience from years of work on integrated DSS showed that demand to support practical decision making with scientific methods can only be fulfilled, if researchers are allowed not only to understand the societal demands, but also work on the transfer of scientific knowledge into applied decision making, which is an abiding challenge.

Appendix A

Publications related to brownfield and megasite management

A.1 Peer reviewed papers

- Morio, M., Schädler, S. & M. Finkel (**submitted**): A multi-criteria genetic algorithm framework for the identification of holistically optimum brownfield redevelopment options, submitted to Environmental Modelling & Software. **Part of this thesis**

- Schädler,S., Finkel, M. , Bleicher, A., Morio, M. & M. Gross (**submitted**): Systematic improvement of sustainable brownfields redevelopment by automated quantitative spatial assessment of sustainability indicators. submitted to Landscape and Urban Planning.

- Schädler, S., Morio, M., Bartke, S. & M. Finkel (2012): Integrated planning and spatial evaluation of megasite remediation and reuse options, in Journal of Contaminant Hydrology 127(1–4), 88–100.

- Schädler, S., Morio, M., Bartke, S., Rohr-Zänker, R., Finkel, M. (2010): Designing sustainable and economically attractive brownfield revitalization options using an integrated assessment model. Journal of Environmental Management, 92(3), 827-837. **Part of this thesis**

- Schädler, S., Finkel, M., Morio, M., Bartke, S., Schwarze, R., Rohr-Zänker, R., Bittens, M., Bielke, A. & M. Freygang (2009): Integrierte Bewertung von Wiedernutzungsoptionen für vornutzungsbedingt belastete Brachflächen, altlastenspektrum, 18(6), 273-279.

- Morio, M., Finkel, M. & E. Martac (2010): Flow guided interpolation – A GIS-based method to represent contaminant concentration distributions in groundwater, Environ. Model. Softw. 25(12), 1769-1780. **Part of this thesis**

A.2 Book chapters

- Finkel, M., Bartke, S., Rohr-Zänker, R., Morio, M., Schädler, S. & R. Schwarze (2010): Ganzheitliche Evaluation von Nutzungsstrategien für Brachflächen, in Frerichs, S., Lieber, M. & T. Preuß (eds.), Flächen- und Standortbewertung für ein nachhaltiges Flächenmanagement, Methoden und Konzepte. Beiträge aus der REFINA-Forschung, Reihe REFINA Band V, S. 97-109.

A.3 Conference Proceedings

- Morio, M. & M. Finkel (2010): A screening level method to derive contaminant distributions in groundwater for early stage assessments of brownfields. In: Ground-water Quality Management in a Rapidly Changing World. - IAHS Publ. no. 324, 189-193. **Part of this thesis**

- Schädler, S., Finkel, M. & M. Morio (2010): Integrated Screening Level Evaluation of Megasite Redevelopment. In: Groundwater Quality Management in a Rapidly Changing World. - IAHS Publ. (accepted).

- Morio, M., Martac, E. & M. Finkel (2008): Enhancing brownfield revitalisation strategies by analysing future land use scenarios, contamination and clean-up costs: A holistic multi-method approach. In: Proc. of ConSoil 2008: 10th International UFZ/TNO Conference on Soil-Water Systems, Milano, Italy, June 3-6, F177-F186.

- Morio, M., Finkel, M., Schädler, S., Hartmuth, G. & H. Rügner (2008): Improving mega-site revitalisation strategies by trading off benefits from future land use and clean-up costs. Groundwater Quality: Securing Groundwater Quality in Urban and In-dustrial Environments.- IAHS Publ. no. 324, 555-562. **Part of this thesis**

- Schädler, S., Morio, M. & M. Finkel (2008): Land use related cost estimates for contaminated site development: consequences of uncertainty to planning and investment decisions. Groundwater Quality: Securing Groundwater Quality in Urban and Industrial Environments.- IAHS Publ. no. 324, 539-546.

A.4 Project reports

A.4.1 BMBF project REFINA–SINBRA

For further information and additional documents to those listed below, please cf. to http://www.sinbra.de

- Martac, E., Peter, A., Morio, M. & M. Finkel (2009): SINBRA Methodenkatalog – 4. Modellgestützte Untersuchungen und Methoden, pp. 87–95.

- Morio, M, Schädler, S. & M. Finkel (2009): SINBRA Methodenkatalog – 3.3. Konfliktanalyse, Kostenschätzung und ganzheiltliche Bewertung mit dem Entscheidungsunterstützungstool EUGEN, pp. 125–151.

- Bartke, S., Morio, M. & S. Schädler (2009): BMBF Forschungsvorhaben SINBRA – Strategien zur nachhaltigen Inwertsetzung nicht wettbewerbsfähiger Brachflächen am Beispiel der ehemaligen Militär-Liegenschaft Potsdam-Krampnitz: Abschlussbericht der Teilvorhaben 1 und 3, http://www.sinbra.de , 53pp.

A.4.2 SAFIRA II - Megasite Management System

For further information and additional documents to those listed below, please cf. to http://www.safira-mmt.de

- Morio, M. & M. Finkel (2009): SAFIRA II Managementsystem (MMS): Modellbasierte Interpretation von Grundwassererkundungsdaten – Prozeduren für das Geographische Informationssytem ArcGIS, 28pp.

- Schädler, S., Finkel, M, Pulsani, B.R. & M. Morio (2009): SAFIRA II Managementsystem (MMS): Interactive Land Use Map (ILUM) – Dokumentation und Handbuch, 13pp.

- Finkel, M., Morio, M., & S. Schädler (2010): SAFIRA II Managementsystem (MMS): Verbesserung der Schätzung von Bodensanierungskosten: Kurzbeschreibung, 9pp.

- Finkel, M., Morio, M., & S. Schädler (2010): SAFIRA II Managementsystem (MMS): Implementierung eines alternativen Ansatzes zur Nachhaltigkeitsbewertung, 19pp.

- Finkel, M., Justen, A., Morio, M., & S. Schädler (2010): SAFIRA II Managementsystem (MMS): Allgemeine Verbesserungen der MMT, 14.12.2010, 28pp.

- Morio, M., Finkel, M. & A. Srinivasan (2010): SAFIRA II Managementsystem (MMS): Automatische Optimierung der räumlichen Verteilung der Landnutzungen (MOOL: Multi-Objective-Optimisation of Land Re-Use), Handbuch / Dokumentation zu Methodik und Anwendung innerhalb der Megasite Management Toolsuite (MMT), 77pp.

- Morio, M. & Finkel, M. & (2011): SAFIRA II Managementsystem (MMS): Probabilistische Konfliktanalyse, 15.01.2011, 14pp.

A.5 Software manuals

Manuals of decision support software systems, developed within the BMBF research projects REFINA–SINBRA and SAFIRA II:

- Handbuch zur Anwendung des Entscheidungshilfesystems EUGEN (for further information cf. to http://www.sinbra.de)
- Morio, M., Schädler, S., Finkel, M., Justen, A., Bleicher, A., Bartke, S. & M. Gross (2010): MMT - Megasite Management System - User's Guide , v.1.2.0, March 2011, http://www.safira-mmt.de, 131pp.

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