018530 - SWITCH

Sustainable Water Management in the City of the Future

Integrated Project
Global Change and Ecosystems

D5.3.3: Criteria for the assessment of the feasibility of BF and ARR as a pre-treatment or "Total water treatment system" under given conditions

D5.3.4. Tools for prediction of selected water quality parameters of BF and ARR treated water under given conditions

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PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
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SWITCH WP 5.3 - Maximizing the use of natural systems in urban water management

D5.3.3: Criteria for the assessment of the feasibility of BF and ARR as a pre-treatment or "Total water treatment system" under given conditions

D5.3.4. Tools for prediction of selected water quality parameters of BF and ARR treated water under given conditions

The research in work package 5.3 aimed at maximizing the exploitation of natural systems and processes for the effective management of municipal water resources, of water supply and sanitation services, and of the municipal water cycle as a whole.

An important component has been the (applied) research and innovation in terms of "Natural systems for drinking water (pre)treatment". This research consisted of the following sub-tasks:

- **Task 2a** To perform a literature survey and collect operational data from existing Bank Filtration (BF) and Artificial Recharge and Recovery (ARR) water treatment systems. The work will include the analysis of factors influencing the feasibility of BF and ARR for drinking water treatment for centralised (for urban water supply) and decentralised applications (for small towns and rural water supply). Furthermore the potential of BF and ARR as a 'Total Water Treatment System' (i.e. avoiding disinfection) under different conditions will be explored.
- **Task 2b** To perform soil column studies. Laboratory scale soil column studies will be conducted to evaluate the effect of redox conditions (aerobic and anoxic), and biotic and abiotic conditions on removal of different contaminants (particulate, dissolved, microorganisms), by BF and ARR. Based on the experimental results, residence time-distance relationships will be developed for each category of contaminants.
- **Task 2c** To develop and apply models describing BF and ARR processes. Based on the literature review, experimental results and field data collected, models will be developed to estimate the removal of selected contaminants by BF and ARR under given conditions. This will help in the effective design, operation and optimisation of BF and ARR schemes in conjunction with subsequent treatment processes (if any).

The results of this research have mainly been published as PhD and MSc research, and are therefore reported under Deliverable 5.3.12. Theses produced within this topic include:

- A. Maeng, Multiple Objective Treatment Aspects of Bank Filtration, UNESCO-IHE PhD thesis
- M.O. Ibrahim, Organic matter characterisation and EDCs removal during riverbank filtration, UNESCO-IHE MSc thesis
- S. Devkota, Endocrine Disrupting Chemicals removal during river bank filtration, UNESCO-IHE MSc thesis
- C. Abel, Impact of Biodegradability of Natural Organic Matter and Redox Conditions on Removal of Pharmaceutically Active Compounds during Riverbank Filtration, UNESCO-IHE MSc thesis
- H.W. Simarmata, QSAR-Based Model for Assessment and Prediction of Organic Micropollutants Removal during Bank Filtration, UNESCO-IHE MSc thesis

A main outcome of this task has been the development of a Prediction tool for removal of organic micropollutants during bank filtration called SOMA: "SWITCH Organic Micropollutants Assessment". It is an Excel-based tool that facilitates the design and operation of BF systems in the reduction of selected groups of OMPs. The manual follows after this summary document.

One journal publication resulted from the research of task 2:

S. K. Maeng, S. K. Sharma, A. Magic-Knezev and G. Amy (2008). Fate of effluent organic matter (EfOM) and natural organic matter (NOM) through riverbank filtration. Water Science and Technology, 57(12), 1999-2007.

Next to presentations at the various SWITCH consortium meetings, one external conference presentation was given:

Maeng. S.K., Sharma, S.K. and Amy, G. (2010) Modelling of Removal of Wastewater-derived Organic Micropollutants during Managed Aquifer Recharge. Proceedings of the IWA World Water Congress 2010, (19-25 September 2010), Montreal, Canada.

Maeng, S.K., Ameda, E., Sharma, S.K. and Amy, G. (2009) Framework for assessment of pharmaceutically active compounds removal during managed aquifer recharge and recovery. Proceedings of the NATO Workshop (24-27 October 2009), Luxor, Egypt.

Prediction tool for removal of organic micropollutants during bank filtration (SOMA)

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SWITCH

Prediction tool for removal of organic micropollutants during bank filtration (SOMA)

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Abstract

Bank filtration (BF) is a relatively low cost natural treatment technology that has been proven to be an excellent option for the attenuation of organic micropollutants (OMPs) often found in surface waters. However, there are no guidelines to facilitate design and operation of these systems for optimal efficiency in the removal of OMPs. The main goal of this study was to analyse the performance of various bank filtration systems in the removal of OMPs. Focus was also on the derivation of relationships between the removal efficiencies of these pollutants with the key influencing factors namely; retention time, travel distance and redox conditions, among others. This was geared towards the development of a SWITCH Organic Micropollutants Assessment (SOMA) tool that would facilitate design and operation of BF systems in the reduction of selected groups of OMPs. The methodology of the study consisted of a desk study that was used in the compilation of a database on the removal of OMPs from soil column and field studies. Supplementary to this, was a comprehensive database from the NASRI project on OMPs detected in BF and artificial recharge (AR) sites at the Lake Tegel in Berlin, Germany. These datasets were analysed using MS-Excel, SPSS, Slidewrite and SigmaPlot to establish generalised relationships between the variables and the selected trace organics. The methods employed in the analysis were multiple regression analysis and clustering of data.

The BF site generally showed better removal rates for x-ray contrast agents, while the AR site indicated higher removals for selected PhACs. The derived rate constants generally showed more rapid removals at the recharge site, with this being mainly attributed to the aerobic microbial activity taking place beneath the pond. Bi-variate kinetic models for the removal of trace organics with residence time, distance, and redox potential were developed for selected compounds. A multi-regression expression modelling the removal of carbamazepine was also estimated. Predictive guidelines for the removal of groups of OMPs, were developed and together with the regression and kinetic models, incorporated into a water quality prediction tool/spreadsheet. This tool enables preliminary estimation of removal efficiencies of selected compounds and groups of OMPs. In conclusion, the SOMA can be useful for the preliminary estimation of the removal of selected OMPs and groups of compounds (e.g., X-ray contrast agent, endocrine disrupting compounds, pesticides, volatile organic compounds, pharmaceutically active compounds, benzene, and aromatic compounds). However, some background knowledge on the behaviour of some of the target compounds would be necessary to effectively use this tool. Quantitative Structure Activity Relationship (QSAR) model is also developed to support SOMA, and the model development was based on influent data carried out in laboratory scale experiment.

1. Introduction

The need for quality drinking water is growing rapidly worldwide especially with increased urbanisation and population growth. This need is greatest in the developing world where more than one billion people have no adequate water (Pimentel et al., 2004). Furthermore quality of the most of the water resources especially surface waters in industrialized and urban areas are deteriorating rapidly as a result of pollution waste discharges into receiving waters, which may also serve as drinking water sources. This, therefore, creates the possibility for the occurrence of potentially harmful pollutants such as organic micropollutants (OMPs), in drinking water treatment systems and ultimately in drinking water.

Recently, there has been growing concern over the increased detection of OMPs in surface and ground water and this has resulted in increased research and use of advanced technologies to maintain supply of quality potable water (Mechlinski and Heberer, 2005). The development of better analytical techniques of detection to much lower concentrations has contributed to the growing concern due to increased detections.

The removal of OMPs from water is relatively costly in both conventional and advanced water treatment technologies, thus creating a high unit t cost of water treatment rendering the water unaffordable especially for the poor in developing countries. Bank filtration (BF), that has been applied for over a century in some parts of Central Europe, especially Germany, is a relatively low cost natural based treatment technology that has been proven to be an excellent option for the attenuation of OMPs often found in surface waters (Amy, 2007; Schmidt et al., 2007).

This technology has several advantages over surface water abstractions and other treatment methods because of its relatively low costs, capability to eliminate suspended solids, biodegradable compounds, bacteria, viruses, parasites, part elimination of adsorbable compounds, through the main beneficial natural attenuation processes like mixing, biodegradation and sorption processes (Hiscock and Grischek, 2002). Furthermore, BF has been applied mainly as a pre-treatment step and thus saves on treatment costs due to lower chemical and energy requirements for removal of contaminants like bacteria, suspended matter, micro-pollutants, etc. It is also very attractive for its protective multi-barrier treatment of potentially harmful pollution that may occur especially during chemical spillover or accidents. All these benefits make this natural treatment technology a promising one especially for developing countries where clean water is desperately needed.

Despite the long experience in the use of this technology, the complex degradation processes under the various aquifer conditions are yet to be understood (Hiscock and Grischek, 2002). Of particular interest is the fate of emerging OMPs during BF and the processes and conditions under which they can best be attenuated; with attenuation being refered to as removal that has been mainly influenced by biodegradation and adsorption processes, and not a result of dilution.

The detection of some of these compounds especially pharmaceutically active compounds (PhACs) and endocrine disrupting compounds (EDCs), personal care products (PCPs) among others, in BF systems have raised further concern which has led to more intensive research in their fate and removal (Heberer et al., 2001). This raises the need for the development of guidelines and models to predict the removal of trace organics.

2. Research Objectives

The main goal of this study was to analyse the removal of OMPs in various BF systems with specific focus on the key influencing factors of travel time and well distance among other relevant ones, so as to develop a SWITCH Organic Pollutant Assessment (SOMA) tool which could be used for prediction of r the removal or reduction of OMPs during BF, in the form of a guideline. This goal was achieved through the following specific objectives:

1. Analysis of removal of OMPs under different travel distance/times at various study sites.

2. Establishment of relationships/patterns in the removal of OMPs with respect to selected variables of travel time/distance using statistical tools.

3. Development of a QSAR model that will support SOMA used to predict removal efficiencies of OMPs and to aid design of BF systems for selected groups of OMPs.

3. Methodology

Data Collection

A desk study was carried out through a comprehensive literature review on BF systems and their capacities to attenuate OMPs. Understanding of the underlying active mechanisms and processes was sought in this review. The major groups/categories of OMPs were identified and information on the removals of OMPs from BF and laboratory-based studies was compiled. Supplementary to this literature data, was a comprehensive database from the NASRI project in Berlin, Germany on OMPs that were detected and measured at the transects of Lake Tegel BF and AR sites. Hence, the literature survey and the NASRI database served as the two sources of data for this analytical study of OMPs removal in BF. This comprehensive data was then analysed using a combination of software packages which included; SPSS 14.0, MS-Excel, SlideWrite 5.0 and SigmaPlot 10.0. These tools were used to ultimately develop a prediction tool for the removal of organic micropollutants.

Literature sources

A literature survey of previous studies was carried out on the fate and transport of organic micropollutants in BF systems and column studies. The total number of literature sources and the corresponding type of studies are summarised in Table 1.

Table 1. Literature sources and study types used to compile database

Type of Bank Filtration Study	No. of Literature Sources
Column	15
Field Sites (20 No. sites)	27
Total	**42**

Data Analysis and interpretation

The two databases (NASRI and literature-based) were analysed using MS-Excel, the statistical package SPSS 14.0 and graphical softwares SlideWrite 5.0 and SigmaPlot 10.0. SPSS 14.0 is a very versatile and widely used tool for advanced statistical analysis hence its selection; while Slidewrite 5.0

and SigmaPlot 10.0 are powerful tools for transforming data into technical charts, graphs, curve-fitting.

The obtained information from the literature sources (literature-based database), was used to estimate water quality guidelines that could be used to predict the performance of bank filtration systems. This was done by means of scatter plots and clustering techniques. The two NASRI data sets were analysed for the extent of removal of these compounds along the transects. Their relationships with the travel distance and residence time and some cases oxygen, were also analysed and where they existed, expressions describing them were estimated using regression and correlation analysis.

Assumptions made in prediction tool/model development

(1) The predicted values or guidelines for removal of OMPs are applicable only within the stated influent and effluent ranges of the specific compound group considered.

(2) Other factors influencing the performance of BF on OMPs removal were not considered (e.g., soil types, mixing from local groundwater, temperature and redox conditions).

4. SOMA

The water quality prediction tool (SOMA) which predicts the removal performances of BF systems for different OMPs are incorporated into a simple Microsoft Excel spreadsheet to enable preliminary estimation of the removal of the different groups of OMPs; X-ray contrast agents, PhACs, EDCs, pesticides and volatile organic compounds. The tool is comprised of several worksheets that compute the guidelines (or estimated range of effluent concentrations under given conditions) based on either a known residence time or well distance from surface water sources (e.g., lake, river and infiltration basin) (Figure 1, Figure 2 and Figure 3). The removal efficiencies estimated by the spreadsheet are however limited to the influent and effluent ranges for which these guidelines were developed (i.e., boundary conditions). The tool was also developed to give preliminary guidelines for the removal of dissolved organic carbon and six selected groups of OMPs: phenazone (PhACs), propyphenazone (PhACs), acetylaminoantipyrine (AAA) (transformation product), formylaminoantipyrine (FAA) (transformation product), adsorbable organic bromide (AOBr) and carbamazepine. These removals were based on a first-order kinetics model estimated in the analysis of the NASRI data and can be applied under similar site conditions as that at the NASRI project sites (Figure 4).

Layout of the prediction tool

The SOMA tool has been designed in the form of interlinked spreadsheets for easy use. The introduction/home page, typical computation worksheets and references of the water quality prediction tool are as shown in Figure 1, Figure 2 and Figure 3, respectively. The Introduction Page of the tool (Figure 1) shows eight buttons for different classes of OMPs and two additional buttons ABOUT and NOTES. Eight buttons consist of X-ray contrast agent, Endocrine disrupting compounds, Pesticides, Volatile organic compounds, Pharmaceutically active compounds, Benzene and Aromatic compounds. On each computation sheet for the removal of groups of OMPs, the limits of the guidelines are clearly indicated and a hyperlink is provided for the full display of the guidelines and literature references used in their compilation.

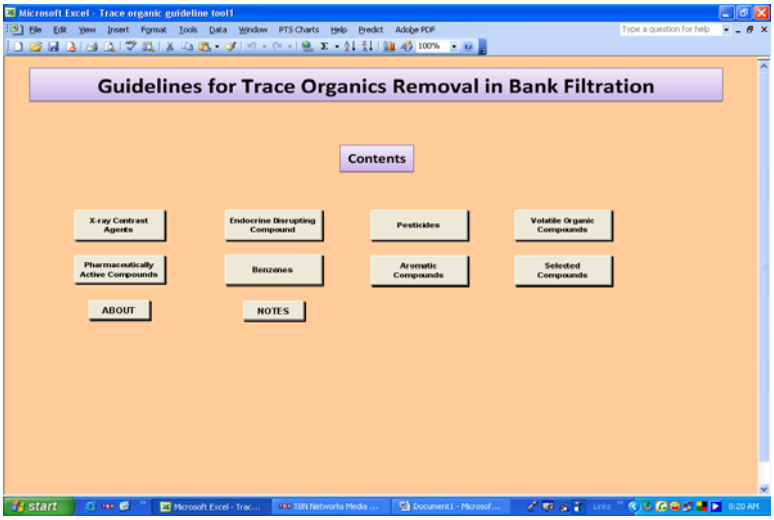


Figure 1. Introduction page of the water quality prediction tool

Input Parameters

The input parameters for the preliminary estimation of the removal of groups of OMPs are:

1. *Influent concentration*: The influent concentration of the surface water source is required mainly to confirm if the parameter fell within the stated influent range. This input is linked to a message cell that provides feedback on whether the organic micropollutants are within the range or not.

2. *Well distance from the surface water source (travel distance*) – The expected/known distance of a well from the surface water source is a required input, especially if the residence time is not known. For a planned/non-existent MAR system, it is most likely that the residence/travel

time at the site may not be known. The spreadsheet estimates are computed based on either the well distances or the residence times. If both inputs are available, then two sets of results would be expected, which could then be compared.

3. *Travel time:* The travel time of water from the surface water source to a given well location, is required as one of the inputs. This input requirement may be preferred to the previous variable as it is more representative of the actual flow path of contaminants.

As may be noted in Figure 2, the input requirements are indicated by yellow cells in the spreadsheet, while the outputs are indicated by blue cells. The green cells show instructions to be followed especially with regard to the influent concentration range.

Output Parameters

The output parameters of the estimation of removal of OMPs is basically a range of removal efficiencies, which were either based on the travel times or well distances. For the selected OMPs, outputs were given as both removal efficiencies and effluent concentrations. It should be noted that in both cases the removal efficiencies estimated are based on either travel times or travel distances. Hence, if both inputs are available/known, then the two sets of results can simply be compared, whereas if only one is known, at least one result would be expected. These outputs are simply a guide of the anticipated removals for a given MAR site.

HOME is for when a user wants to go back to the main menu and Guidelines is for the complete references for a target compound or class.

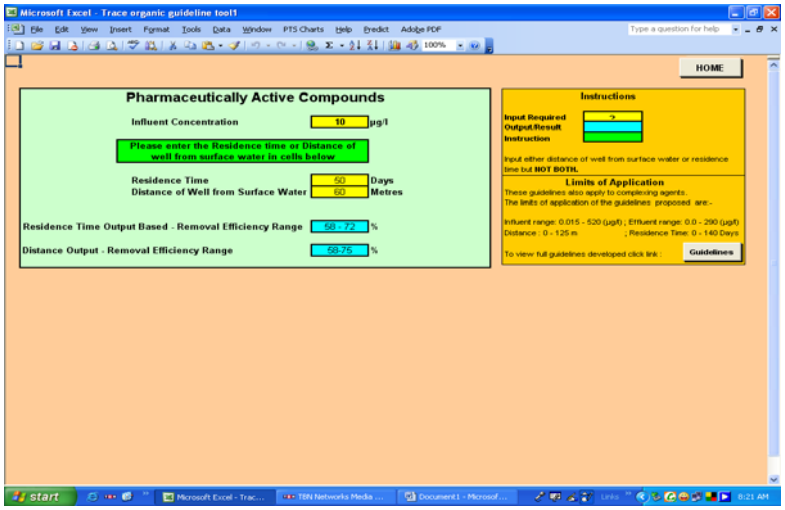


Figure 2. Typical computation worksheet for guidelines of a group of OMPs

Guidelines lead to a list of references used for guidelines development. Top of Page lead to NOTES screen which shows a list of guidelines in SOMA and single compound (e.g., dissolved organic carbon (DOC), AAA, Phenazone, FAA, AOBr, Propyphenazone and Carbamazepine) that can be investigated from SOMA. Moreover, there are Introduction and Assumptions sections for users to explain about SOMA.

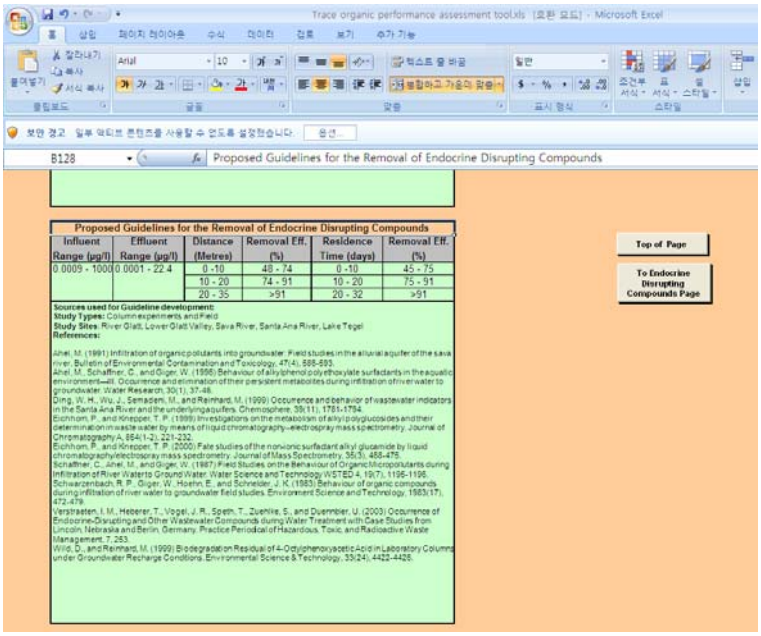


Figure 3. A list of references used for guideline developments

The guideline for single compound described above is based on kinetic models, and the models were developed from data collected from field site of a BF system equipped with several monitoring (different depths and travel distances). Rate constants from proposed guidelines are based on the first-order kinetics.

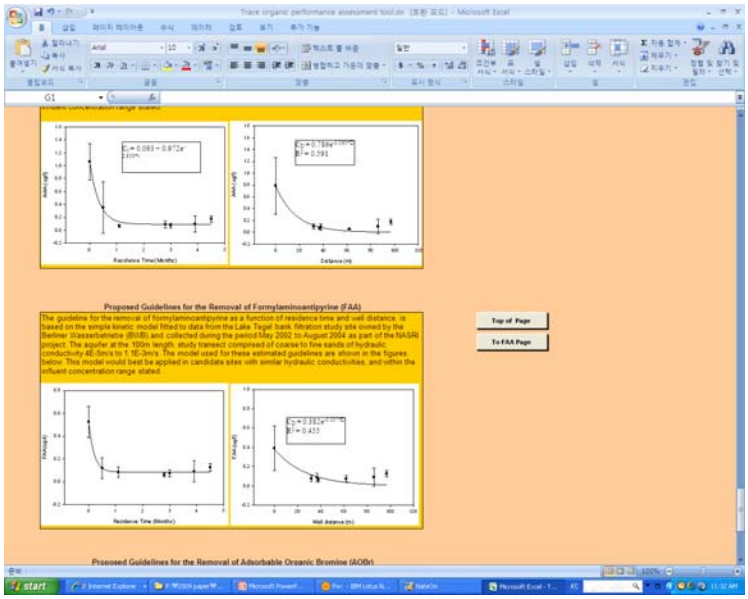


Figure 4. A list of references and rate constants used for guidelines development

Procedure for SOMA

1. Make sure you give a permission to enable macro function in MS Excel program. In Excel 2010, please ignore the security message

2. After you get the Introduction Page (Figure 1), click on the class of compound you want to investigate for bank filtration or click SELECTED COMPOUNDS to select individual compound available from SOMA. Each compound may ask different input data. For example, carbamazepine needs more than just residence time. It requires redox potential and temperature in order to predict the concentration in the riverbank filtrate and the removal efficiency.

3. The input requirements are by yellow cells, and outputs are indicated by blue cells. Enter influent concentration within the range given in the right menu box.

4. Enter residence time (travel time) and distance of well from the river. These values have to be in given range in right box. This input is linked to a message cell that provides feedback on whether the OMPs are within the range or not.

5. Removal efficiencies based on residence time and travel distance will appear in boxes located below

6. To see the complete references of a prediction tool or full guidelines in SOMA, click Guidelines

7. If you want to go back to the main menu (HOME) screen, click HOME.

8. In the main menu, click NOTES to see referenced that used to develop the prediction tool.

The predictive removal guidelines were tested on using Lake Tegel BF data to assess its performance and the reliability of the estimates. Compounds from the following groups of OMPs were selected and used in the example summarised in Table 2; PhACs, X-ray contrast agents, and pesticides. In the example shown in Table 2, two trials were carried out for each compound and in each trial different well-distances and corresponding residence times were used. The prediction errors were then computed.

It can generally be noted that predictions made using the residence times showed lower error than those made using the well-distances. This could be likely because, residence times are more representative of the flow than the well-surface water distances. Nevertheless, apart from the large prediction error noted in the compound FAA, the deviations of the ranges of removal efficiency from the actual values is not so high (0-16%), since these are supposed to serve as preliminary guidelines. It is noted that in the second trial of bentazone the prediction error could not easily be established. This was because the pesticides group had narrow limits of the residence times and well-distances, a problem which could have been caused by limited number of cases used during the development of the guidelines.

Table 2. Example showing the application of the water quality predictive guidelines

Compound	Compound Group	Mean Influent (µg/l)	Trial 1						
			Well Distance (m)	Distance-based Predicted Removal Efficiency (%)	Prediction Error (%)	Residence Time (Days)	Time-based Predicted Removal Efficiency (%)	Prediction Error (%)	Actual Removal at Field Site (%)
AAA	PhAC	1.06ug/l	0	-	-	30	45-58%	-13%	67%
FAA	PhAC	0.53ug/l	38	54 - 58%	-35%	84	80-93%	0%	89%
AOBr	X-ray Contrast Agent	12ug/l	0	-	-	30	56-67%	0%	63%
Diclofenac	PhAC	0.077 ug/l	86	87-89%	4%	117	93->96%	14%	84%
Bentazone	Pesticide	0.018ug/l	37	38-58%	19%	33	67-86%	0%	72%
Compound	Compound Group	Mean Influent (µg/l)	Trial 2						
			Well Distance (m)	Distance-based Predicted Removal Efficiency (%)	Prediction Error (%)	Residence Time (Days)	Time-based Predicted Removal Efficiency (%)	Prediction Error (%)	Actual Removal at Field Site (%)
AAA	PhAC	1.06ug/l	97	87 - 89%	4%	135	93 - >96%	11%	84%
FAA	PhAC	0.53ug/l	97	87 - 89%	13%	135	93 - >96%	21%	77%
AOBr	X-ray Contrast Agent	12ug/l	32	53-77%	0%	90	76-80%	4%	73%
Diclofenac	PhAC	0.077 ug/l	37	54-58%	16%	33	45-58%	16%	69%
Bentazone	Pesticide	0.018ug/l	0	-	-	30	67-86%		0%

Example: Phenazone: Influent 1 ug/L, Travel time: 0.5 and 1 month, Acetylaminoantipyrine: Influent 1 ug/L, Travel time: 1 and 4 months

	Influent concentration (ug/L)	Residence time (month)	Effluent concentration (ug/L)	Removal (%)
Phenazone	1	0.5	0.13	87
Phenazone	1	1	0.05	95
Acetylaminoantipyrine	1	1	0.14	86
Acetylaminoantipyrine	1	4	0.09	91

5. Quantitative Structure Activity Relationship Model

Beside SOMA, a quantitative structure activity relationship (QSAR) based model was proposed to predict the removals of OMPs. A QSAR approach links compound properties (i.e., structure) to the removals (activity). Furthermore, it is important to have reliable datasets in order to develop a QSAR model because there are many factors that can influence the removal of OMPs during soil passage. The QSAR approach is especially useful for compounds with little information about their fate during soil passage. Such an assessment framework for OMP removal is useful for adapting BF as a multi-objective (-contaminant) barrier and understanding the fate of different classes of compounds during soil passage and the determination of post treatment requirements for BF systems. The QSAR model developed in this study predicts the fate of PhACs during soil passage and is useful for compounds with limited information such as a new PhACs. In other words, QSAR is another way to check the proposed guideline developed in this study and should be as a screen tool for BF systems.

Model Development

Reliable data of PhACs are needed to develop a model that can be explained in a mechanistic manner. Having results under different spatial and hydrogeochemical conditions (i.e, field studies) will easily lead to a model with limited applicability. Experimental data from column studies using four different classes of PhACs including lipid regulators, psychostimulants, analgesics and anticonvulsants (13 selected PhACs) were used for developing a QSAR model. Adding more cases from the different therapeutic usages of PhACs (e.g., antibiotics) would certainly increase the applicability of the model. Genetic algorithm was used to select the best descriptors followed by an ordinary least squares (OLS) method to develop the QSAR model. Genetic algorithms (GA) are an evolutionary method which often used in several fields such as chemistry and QSAR (Goldberg,

1989). GA selects descriptors by considering populations of models generated through a reproduction process and optimized according to a given objectives (Todeschini et al., 2003). The model was selected based on the correlation coefficient (R^2) and the external predictivity. The following QSAR model based on 4 variables was selected among 247 molecular descriptors.

% removal of PhACs = 174.8(±11.6) nImidazoles + 158.4(±19.8) AR – 98.1(±5.8) nCONN – 1830.3(±193.2) ME + 1851.1(±188.3)

R^2 = 0.84, Q^2 = 0.81 and Q^2_{ext} = 0.64

Number of cases in the training set = 65, number of cases in the testing set = 26 cases (external validation)

As shown in Table 3, there are four variables selected in the model (NImidazloles, AR, nCONN and ME) to estimate the removal of PhACs tested in the column studies. Selected descriptors with positive coefficients indicate that those descriptors contribute positively to the removal of PhACs, whereas descriptors with negative coefficients lead to an inverse effect on PhACs removal. During soil column experiments, ionic PhACs were not effectively removed under abiotic conditions using sodium azide (abiotic conditions where only sorption is influential) but were significantly removed under biotic conditions. Moreover, physicochemical properties associated with sorption and electrostatic forces (e.g., dipole moment, K_{ow}, etc.) had little or no impact on the model. Therefore, it is believed that the selected descriptors may correlate to biodegradation. The significance of the selected descriptors can be determined using standardized regression coefficient values; ME (Mean atomic Sanderson Electronegativity) (-0.8) and AR (aromatic ratio) (0.8) in the model are relatively low compared to nCONN (-1.6) and nImidazoles (2.5). All variables have different units of measurements, and these variables were standardized by subtracting the mean and dividing by the standard deviation. ME was selected in the model because it indicates the negative influence of electronegativity of PhACs. On the other hand, an increase in the number of Imidazole groups (i.e., functional groups) leads to an increase in biodegradation. According to Organization for Economic Co-operation and Development (OECD) Screening Information DataSet (SIDS) report, imidazole is a readily biodegradable compound that degrades between 90 and 100% (OECD, 2003). nCONN was probably selected because carbamazepine, the most persistent compound during the soil passage, contains urea derivatives. Table 4 shows an example of estimated descriptors for some PhACs.

Table 3. Summary of selected descriptors

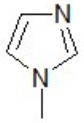
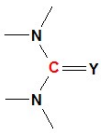
	Descriptors	Type	
NImidazloles	Number of Imidazole groups	Functional groups	
AR	Aromatic ratio (number of aromatic bond over the total Number of non-H bonds)	Constitutional descriptors	
nCONN	number of urea (-thio) derivatives	Functional group	
ME	Mean atomic Sanderson electronegativity (scaled on carbon atom)	Constitutional descriptors	

Table 4. Example of descriptor estimations

		NImidazoles	AR	nCONN	ME
Analgesics	Ibuprofen	0	0.4	0	0.9
Blood lipid regulators	Gemfibrozil	0	0.3	0	0.9
Anticonvulsants	Carbamazepine	0	0.6	1	1

Model validation

R^2 is often used as a measure of goodness-of-fit of a QSAR model. However, validation has to be carried out to determine the robustness and predictivity of the model. LOO cross validation, the most commonly applied for an internal validation, was used to predict the reliability of the model (Gramatica, 2007). Thus, if the cross validation coefficient Q^2 is greater than 0.5, then the model can be attributed a high predictive power (Ghasemi et al., 2009). The developed QSAR model presented a Q^2 of 0.81. Therefore, the model was acceptable by analyzing LOO cross validation. External data collected from

various field studies were used for external validation of the QSAR model. According to Gramatica (2007), only externally validated models are applicable to both external prediction and regulatory purposes. A Q^2_{ext} value of 0.64 was obtained, suggesting the prediction power of the model by external validation was lower than that of internal validation.

6. Limitations of the Tool

Some of the limitations in the use of this spreadsheet model/tool are listed below:

- It can only be used within the specified influent ranges, hence if a given site has influent concentrations outside this range, no preliminary estimates of removal can be determined.
- The predicted removal efficiencies of OMPs were based on only travel times and well-surface water distances (travel distances), whereas there are several other important factors such as redox conditions, flow velocity, transmissivity, etc, which, if known and incorporated in the tool would improve the estimates.
- The treated water quality estimated for the selected OMPs, were based on kinetic models and a multi-regression model fitted to data from the Lake Tegel LBF site, which makes them quite specific. Hence, their use would be best applied in cases where site conditions such as aquifer material, transmissivity, redox conditions, etc, are generally similar.
- For a more fruitful use of this water quality prediction tool, general knowledge on the removal/persistent nature of a compound may be necessary, so as to avoid misinterpreting the predicted guidelines. This is because not all compounds falling in a given group of OMPs may actually follow the predicted guideline/trend.Some guidelines were developed with a relatively limited number of data points, hence narrowing the limits of the distances, residence times and influent ranges.

7. Recommendations

The following recommendations are made regarding the results obtained in this study:

1) The prediction tool or developed guidelines for the groups of OMPs can be further improved to increase their reliability, by including more literature sources than what was used to create the

guidelines in this study.

2) The computation spreadsheet can be made more accurate and user-friendly through the adoption of the following approach:

- Use of JAVA programming platforms to design a more user-friendly interface

- Combination with a groundwater model (i.e., transport model) to have a complete package that would include the fate of organic micropollutants

3) The developed guidelines should be used along with some general background information on the target organic micropollutants, so that the obtained removal efficiencies are more meaningful and better interpreted, otherwise for persistent compounds falling within a given group, a wrong impression could be made of any high removals that may be predicted.

8. Publications Related to the Tool Developed

International referred journals

Maeng, S.K., Sharma, S.K., Amy, G.L., Magic-Knezev, A., 2008. Fate of effluent organic matter (EfOM) and natural organic matter (NOM) through riverbank filtration. Water Science & Technology, 57(12), 1999–2007.

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