1 Introduction

Leachate forecasts are claimed to evaluate the hazard to the groundwater caused by contaminations in the subsurface. The source is described by a concentration either in the leachate or in the soil vs. time. The hazardous material is subjected to retardation and in some cases also to degradation or decay during its transport as solute through the unsaturated zone to the saturated or groundwater zone.

Because of the complex nature of soils and their transport properties it is recommended to use computer models for the leachate forecast. But quite a lot of parameters are needed to describe the properties of the source, of the transport through a heterogeneous unsaturated zone and also of the climatic boundary conditions and the fluctuating groundwater table. The assessment of these parameters is expensive and, additionally, the uncertainty of the values is very high.

A useful tool which allows easing parameter estimation required for leachate forecast is the computer software SiWaPro DSS developed by the authors. SiWaPro is an acronym standing for the German word “Sickerwasserprognose” and DSS for Decision Support System. This software tool is used for leachate forecasts with respect to the German soil protection law (“Bundes-Bodenschutzgesetz” (BBodSchG) and “Bundes-Bodenschutz- und Altlastenverordnung” (BBodSchV)). SiWaPro DSS can handle water flow and contaminant transport processes including degradation under steady-state or transient conditions.
2 Models

The mathematical model behind SiWaPro (Kemmesies 1999), the modelling module of SiWaPro DSS, is based on the mathematical model used in SWMS_2D (Šimunek et al. 1994). The theoretical basics of the processes taking place in the unsaturated soil layer will be explained in the following section.

2.1 Flow model

The flow model describing unsaturated one dimensional vertical water flow in the unsaturated zone is given by the RICHARDS equation (1)

\[
\frac{\partial}{\partial z} \left( k(\theta) \left( \frac{\partial h_p}{\partial z} + 1 \right) \right) = \frac{\partial \theta}{\partial t} - w_0 \tag{1a}
\]

and

\[
\frac{\partial \theta}{\partial t} = C(h_c) \cdot \frac{\partial h_p}{\partial t} \tag{1b}
\]

whereas the independent variables are time \( t \) and spatial coordinate \( z \). The dependent variables of equation (1) are the water pressure head \( h_p = p_w/\rho_w \cdot g \) \((h_c = -h_p)\) and the water content \( \theta \). \( w_0 \) is the sink/source term. The capillary capacity function \( C(h_c) \) is the first derivative of the hysteretic soil water retention curve. The unsaturated hydraulic conductivity \( k(\theta) \) depends on the water content in the soil.

The hysteretic parametric model of soil water retention curve is given after van Genuchten (1980) and Luckner et al. (1989) by:

\[
\theta = A + \frac{\phi - A - B}{\left[ 1 + \left( \frac{\alpha \cdot h_c}{n} \right)^n \right]^{-1}} \tag{2}
\]

The parameters of equation (2) are the porosity \( \phi \), the residual water content \( \theta_{W,r} \), the residual air content \( \theta_{A,r} \), the scaling factor \( \alpha \) and the slope parameter \( n \).

The function of unsaturated hydraulic conductivity was modelled by Mualem (1976) and Luckner et al. (1989) with

\[
k(\theta) = k_0 \left( \frac{\bar{S}}{\bar{S}_0} \right)^{\lambda} \cdot \left[ \frac{1 - \left( 1 - \frac{1}{\bar{S}} \right)^{m}}{1 - \left( 1 - \frac{1}{\bar{S}_0} \right)^{m}} \right]^{2} \tag{3}
\]

The parameters of equation (3) are the hydraulic conductivity \( k_0(\theta_0) \) at a known degree of water mobility \( \bar{S}_0 = (\theta_0 - \theta_{W,r})/(\phi - \theta_{W,r}) \), the parameter \( \lambda \) and the transformation parameter \( m \).

The parameters \( \phi, k_0 \) and \( \theta_0 \) must be estimated in advance using lab and/or field tests. The parameter \( \lambda \) in the model may range between 0<\(\lambda<1\), but it is kept fixed at \( \lambda = 0.5 \).
2.2 Transport model

The well known convection-dispersion-equation is used to describe the transport processes in the unsaturated zone.

The convection term describes the solute transport with the water flux in the unsaturated zone. The dispersion term is the sum of the molecular diffusion and the hydrodynamic dispersion. Both processes are caused by concentration gradients. The hydrodynamic dispersion is always bound to convection, but molecular diffusion is independent from it and may appear without any convection.

The reason for retardation is sorption. The parameter describing the linear distribution function between the solute in the liquid and at the solid phase is the distribution, or Henry coefficient $K_d$. The distribution and the retardation coefficient $R$ are related to each other through equation (5).

$$K_d = (R - 1) \cdot \frac{\theta}{\rho_b} \quad (5)$$

whereas $\rho_b$ is the bulk density of the soil.

In practice, further sorption models have found a wide spread application. Therefore, in SiWaPro DSS models according to Freundlich and Langmuir were additionally implemented, which provide a nonlinear description of the interaction between fluid and solid phase. The computation of retardation factor related to the sorption models in SiWaPro DSS is performed in compliance with equations (6) – (8).

$$R = 1 + \frac{\rho_b \cdot \theta}{\theta} \cdot K_d \quad \text{HENRY-isotherm} \quad (6)$$

$$R = 1 + \frac{\rho_b \cdot q \cdot K_d \cdot \rho_{fl,m}^{q-1}}{\theta} \quad \text{FREUNDLICH-isotherm} \quad (7)$$

$$R = 1 + \frac{\rho_b}{\theta} \cdot \frac{s_{b,max} \cdot K_L \cdot \rho_{fl,m}}{1 + K_L \cdot \rho_{fl,m}} \quad \text{LANGMUIR-isotherm} \quad (8)$$

3 Software description

The program SiWaPro DSS combines the simulation module SiWaPro for numerical computation of water flow and contaminant transport in variably saturated media with additional simulation and parameter estimation tools, data sources for the parameters and a graphical user interface.

3.1 Layout and structure

The structure of the software SiWaPro DSS closely resembles that of a typical three-layer framework with separation into a data layer, an application layer, and a presentation layer (see Figure 1). The software closely follows the concept of modular programming. It consists of a simulation module, 2 different mesh generators, modules regulating access to local and remote databases and a graphical user interface (GUI), which behaves similarly to knowledge-based systems. The GUI guides the user through the data input process. Parameters required for simulation include general model options, parameters for describing the soil hydraulic properties, and parameters for describing the behaviour of the contaminant (degradation, adsorption, transport).
3.2 Development

Since Microsoft Windows is the preferred platform in bureaus and companies in Germany at present, SiWaPro DSS is being developed for this platform under the usage of Microsoft’s .NET framework. This framework provides a number of advantages to computer programmers and users of the software. E.g., the data processing speed can be significantly increased, due to the usage of the computer’s memory as a database. Therefore, all modifications of the modelling data during a work session are made in the memory database and are saved to hard disk at user’s request or at program shut down. Object-oriented programming and the substitution of the Windows API classes for .NET built-in functions are advantages which result in a fast and less susceptible software coding. Finally, the .NET framework is a future-proof technology because Microsoft provides it as the programming base for current and future windows systems.

3.3 Graphical user interface

Space relevant data such as boundary conditions have to be entered, and time quantization has to be conducted. The GUI consists of several input masks where the user can specify different necessary data concerning the model to be created. Only the most important data should be mentioned here:

- model options (kind of flow, solute transport, units)
- geometry (profile of the modelling area)
- coordinate system (dimension – 1D, 2D)
- soil properties (conductivity, pressure head, porosity, water content, …)
- transport properties (dispersivity, diffusion, degradation)
- iteration options (error level, number of steps, …)
- time parameters (quantization method, time step increment, …)
- parameters for evapotranspiration
3.4 Assistant for leachate forecasts

For an easy accomplishment of leachate forecasts, an assistant was implemented in SiWaPro DSS who leads the user in 5 steps to meaningful prognosis results. These steps include the following information:

- Specification of the model domain: automatic geometry setup and Finite-Element-Generation
- Definition of the soil parameters: estimation from database (DIN 4220), van Genuchten parameters, soil hydraulic properties
- Assigning the flow boundary conditions: constant or time-variable flow rate using the implemented weather generator
- Setting the transport parameters: estimation of diffusion coefficient, sorption parameters (Henry, Freundlich, Langmuir) and degradation rates from database (organic and/or inorganic matters)
- Definition of the transport boundary conditions: constant or transient pollutant infiltration rates using step function, Dirac impulse or source term functions

With respect to the expected amendment of the BBodSchG and its input for an EU-wide soil protection law, the GUI of SiWaPro DSS is designed in multiple languages with the ability to switch between languages during application runtime. At present, the GUI is available in 8 different languages: German, English, Spanish, French, Polish, Japanese, Vietnamese and Arabic. Further languages can be easily implemented.

3.5 Mesh Generator and boundary conditions editor

In SiWaPro DSS, the discretisation of the modelling area is realized using Finite Elements with the GALERKIN method. Currently, SiWaPro DSS contains the 2D triangular mesh generator EasyMesh 1.4 (Niceno 1997). The mesh generator allows the generation of meshes with varying element sizes and
irregular mesh boundaries. The further development aims at accomplishing the optional usage of adaptive mesh generating at simulation runtime. This feature provides the possibility to respond very flexibly to numerically fluctuating solutions, e.g. mass balance failures.

![Mesh generator and boundary conditions editor](image)

Figure 3  Mesh generator and boundary conditions editor

### 3.6 Weather generator

On the soil surface, precipitation, root water uptake and potential evaporation as atmospheric boundary conditions have to be taken into the calculation to provide more accurate simulation results using transient flow conditions. Background for the generation of synthetic time series for those variables in daily values is the analysis of available long term series from climate gauging stations (for example of the DWD (German Weather Service)). The characteristic of the real time series is described with statistic parameters. These parameters allow firstly a generation of time series for unknown locations via regional interpolation and secondly a generation of time series of any length. After a validation and a trend test, for example the precipitation is described through Markov-chains first order (for the precipitation condition of a day) and a Weibull distribution (for the amount of precipitation of a day). These parameters are then determined for a 14-day time period respectively, so that seasonal changes can be displayed. Using the synthetic time series, daily evapotranspiration can be calculated with the method of TURC-WENDLING. Further modules for correction of the evapotranspiration with data for declination, orientation and the value for Albedo value of the surface, for modelling the interception reservoir and for modelling root water uptake reduce the available potential evapotranspiration to the required parameters root water uptake, potential soil evaporation and ground level precipitation (Nitsch, 2007).

### 3.7 Database layer

The database layer consists of different types of databases.

#### 3.7.1 Soil database

The definition of the soil parameters requires the specification of quite a few values. To ease up the input for the user, the software provides the possibility to search in a database. This database contains parameters of about 37 different soil types according to the standard DIN 4220.
3.7.2 Contaminant database

The contaminant database was developed in order to ease up the process of data input by allowing inexperienced users to find required contaminant parameters quickly. Currently, the contaminant database contains parameters for 37 substances including organic contaminants such as PAH and BTEX, as well as inorganic contaminants such as heavy metals.

3.8 Pedotransfer functions

Pedotransfer functions have been predominantly developed in order to derive soil hydraulic properties that are difficult to obtain – such as parameters describing the $K$-$\theta$-$h$ relationship from more easily available soil properties – such as soil texture, porosity, bulk density, and organic matter content. The relationship between easily available soil parameters and parameters that are difficult to obtain is usually established using soil databases and mathematical methods such as linear and nonlinear regression analysis, artificial neural networks, the group method of data handling (GMDH) and classification and regression trees (CART). The implementation of pedotransfer functions in SiWaPro DSS is still in its initial stages. So far, three PTFs relating textural data with soil hydraulic data have been implemented. The equations of (Saxton et al. 1985) allow deriving the complete soil water retention curve from 0 kPa to 1500 kPa. The soil water retention curve in the range of 10 kPa to 1500 kPa, for example, can be described using the empirical equation (6):

$$H = A \cdot \theta^B \quad (6a)$$

$$A = \exp[a + b \cdot (%) + c \cdot (%)^2 + d \cdot (%)^2 \cdot (%)] \cdot 100 \quad (6b)$$

$$B = e + f \cdot (%)^2 + g \cdot (%)^2 \cdot (%) \quad (6c)$$

where $H$ is the soil water potential, $\theta$ is the water content, and $a$, $b$, $c$, $d$, $e$, $f$, and $g$ are constants. An empirical equation for the $K$-$\theta$ relationship is equation (7):
K = 2.778 \cdot 10^{-6} \{\exp[12.012 - 0.0755 \cdot (\%sand) + 
+(-3.8950 + 0.03671 \cdot (\%sand) - 0.1103 \cdot 
\cdot (\%clay) + 8.7546 \cdot 10^{-4} \cdot (\%clay)^2] \cdot (1/\theta)]\} \quad (7)

3.9 Import and export interfaces

Connection to other popular software for data exchange is important for a simulation tool. Currently, SiWaPro DSS supports an import interface to the software GeODin developed by the FUGRO CONSULT GMBH company. GeODin is designed to handle drilling profiles. With SiWaPro DSS, it is possible to import these drilling profiles and to create a model in a semi-automated manner. The interface generates a 1D finite element mesh and assigns all available and useful drilling data to the model, e.g. soil layers, boundary conditions for the mesh nodes and dump times. For the user of SiWaPro DSS, this provides a time-saving method for data input. Figure 5 shows the import mask of the GeODin interface.

![GeODin interface form for data import](image-url)
Simulation results can be exported in different formats for further processing. Files can be exported with either the typical ASCII files or as Excel or Access files. Excel and Access are well known products of the Microsoft company. Another possibility is the output to the software Surfer – a tool for visualization and plotting of different kind of maps by the Golden Software company. A sample output of two dimension spreading of leachate below a contaminated site is shown in Figure 6.

3.10 Validation and application

The potential users of SiWaPro DSS in Germany are federal environmental bureaus and consulting companies. The modular nature of the software allows easy adaptation to the needs of users or to new governmental regulations. Since the modules of SiWaPro DSS are largely based on popular and extensively tested programs, the stability, accuracy and correctness of SiWaPro DSS altogether is also guaranteed. In addition, validation of the model by using soil column tests is performed in cooperation with partners of the TU Dresden.

4 Conclusions

SiWaPro DSS was designed in order to conduct leachate forecasts as required by the German soil protection law BBodSchG and BBodSchV. Apart from accurately modelling, the contaminant transport SiWaPro DSS must also be able to provide simulation results if only few data are available. The software has to offer both, full access to all corresponding parameters for experienced users and support for data input to users who don’t have an extensive modelling background.

The flexible manner of data input and the implemented interfaces to soil and contaminant databases allow modelling and simulation of a wide variety of contaminants. The modular design of SiWaPro DSS and the usage of well tested components provide stable and easily adaptable software.
5 References


