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 prone to errors, 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.

MODELS

The mathematical model behind SiWaPro (Kemmesies 1999) the modeling 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.
Flow Model

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

$$\frac{\partial}{\partial z} \left( k(\theta) \cdot \left( \frac{\partial h_p}{\partial z} + 1 \right) \right) = \frac{\partial \theta}{\partial t} - w_0$$

(1a)

and

$$\frac{\partial \theta}{\partial t} = C(h_c) \cdot \frac{\partial h_p}{\partial t}$$

(1b)

where the independent variables are time t and spatial coordinate z. The dependent variables of equation (1) are the water pressure head $h_p = \rho_w g (h_c = -h_p)$ 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:

$$\theta = A + \frac{\phi - A - B}{1 + (\alpha \cdot h_c)^n}$$

(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 modeled by Mualem (1976) and Luckner et al. (1989) with

$$k(\theta) = k_0 \left( \frac{S}{S_0} \right)^{\lambda} \left[ 1 - \left( \frac{1 - S_0^n}{1 - S^n} \right)^m \right]^{-2}$$

(3)

The parameters of equation (3) are the hydraulic conductivity $k_0(\theta_0)$ at a known degree of water mobility $S_0 = (\theta_0 - \theta_{W,r})/(\phi - \theta_{W,r})$, 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 $\lambda=0.5$.

Transport Model

The well known convection-dispersion-equation (4) is used to describe the transport processes in the unsaturated zone.

$$\frac{\partial}{\partial t} \left( D \cdot \frac{\partial s_{n,m}}{\partial t} \right) - \frac{\partial (u \cdot s_{n,m})}{\partial x} =$$

$$\frac{\partial s_{m}}{\partial t} + \mu_m \cdot s_m + \gamma_m \cdot \theta - q_m$$

(4)

mass storage changes
degradation terms
where is

- \( r \) \( m_R \) Spatial coordinate
- \( t \) \( s \) Time
- \( \theta \) \( m_R^1/m_R^1 \) Water content
- \( D \) \( m_R^2/s \) Dispersion coefficient (\( D = \delta \cdot |v| \))
- \( \delta \) \( m \) Dispersivity
- \( s_m \) \( kg/m_R^3 \) Total specific mass (\( s_m = s_{fl,m} + s_{s,m} \))
- \( s_{fl,m} \) \( kg/m_R^3 \) Specific mass in the liquid phase
- \( s_{s,m} \) \( kg/m_R^3 \) Specific mass in the solid phase
- \( u \) \( m_R/s \) Mean flux
- \( \gamma_m \) \( kg/(m_R^3 \cdot s) \) 0\(^{\text{th}}\) order degradation coefficient
- \( \mu_m \) \( s^1 \) 1\(^{\text{st}}\) order degradation coefficient
- \( q_m \) \( kg/(m_R^3 \cdot s) \) Sinks/sources

\( R, \ fl, \ B \) are indices for the space, the liquid and the soil

The convection term describes the solute transport with the water flux in the unsaturated zone. The dispersion term in equation (4) 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 dispersivity is an empirical parameter, it is a measure of heterogeneity of the soil and therefore depends on the scale. The reasons for dispersion are different velocities in the pore channels
a) different pore sizes and therefore different velocities
b) different flow times because of different flow paths
c) transversal spreading of particles

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).

\[
K_D = (R - 1) \cdot \frac{\theta}{\rho_b}
\]

where \( \rho_b \) is the bulk density of the soil.

Internal reactions (decay and/or degradation) may be described as zeroth or first order process as shown in Figure 1.

\[
\frac{ds_m}{dt} = -\gamma_m \\
s_m = s_{m,0} - \gamma_m \cdot t
\]

\[
\frac{ds_m}{dt} = -\mu_m \cdot s_m \\
s_m = s_{m,0} \cdot e^{-\mu_m \cdot t}
\]

Figure 1: Order and description of degradation processes
SOFTWARE DESCRIPTION

The computer-based decision support system SiWaPro DSS combines the simulation module SiWaPro for numerical modeling of water flow and contaminant transport in variably saturated media with additional simulation and parameter estimation tools, data sources for the simulation and a graphical user interface.

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 2). The software closely follows the concept of modular programming (see Figure 3). 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 behavior of the contaminant (degradation, adsorption, transport).

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**Figure 2: Structure of SiWaPro DSS**

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**Figure 3: Functional schema of SiWaPro DSS**
Development

Since Microsoft Windows is the preferred platform in bureaus and companies in Germany at the present time, 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 to the modeling data during a work session are made in the memory database and are saved to hard disk at the user’s request or the time of 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.

GUI and Help System

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 modeling 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

An example for an input form is shown in Figure 4. The GUI contains an extensive help system consisting of context-sensitive help and online help, as well as data validation checks during data input and the possibility of data input based on recommendations. A version of the online help can be seen in Figure 5. The recommended values can be derived from local and remote databases containing soil and solute parameters for a variety of materials. Overall the structure of the module will resemble those of knowledge-based systems. In addition to the guided data input SiWaPro DSS will also include an “expert-mode” in order to offer the experienced user full access to the modeling parameters.

Figure 4: GUI of SiWaPro DSS
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 the present time the GUI is available in German, English and Spanish. Further languages can be easily implemented.

Mesh Generator

In SiWaPro DSS, the discretization of the modeling area is realized using finite elements with the GALERKIN method. Currently, SiWaPro DSS contains the 2D triangular mesh generator EasyMesh 1.4 (Niceno 1997) and the mesh generator Z88 (Rieg 2003) that is used for generating 2D quadrangular meshes. Both mesh generators allow the generation of meshes with varying element sizes and irregular mesh boundaries. Currently, the generators allow flexible space quantization at modeling time given by the user. 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.

Weather Generator

For a leachate forecast it is very important to know how much seepage is created by rainfall during the simulation time span. Therefore, a tool is needed which allows the prognosis of rainfall for an arbitrary location in Germany. In SiWaPro DSS an already existing weather generator shall be implemented. This generator creates statistical series from series of measurements available from a free database. This database consists of climate data, e.g. temperature, rainfall, snowfall and humidity of 37 locations in Germany since 1950. Using adequate interpolation algorithms the weather generator is able to compute statistical series for any location in Germany. Having access to that tool SiWaPro DSS can give more accurate leachate forecasts to the user.

Database Layer

The database layer consists of different types of databases.

Soil Databases

Soil data used in SiWaPro DSS are derived from UNSODA V2.0 (Nemes et al. 2001) and WISE version 1.1 (Batjes 2002). UNSODA is a widely known database containing 790 soil samples of a variety of compositions and from different climatic regions. It has been developed in order to provide soil hydraulic data for use in numerical models. UNSODA contains textural and soil hydraulic data and has been commonly used not only to derive soil hydraulic data, but also to develop pedotransfer functions. WISE contains 4300 soils from 123 countries worldwide with a variety of textural, compositional and hydraulic parameters. Figure 6 shows a form with the search options available for database access.
Contaminant Databases

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. The contaminant database contains a total of 300 substances including organic contaminants such as PAH, and BTEX, as well as inorganic contaminants such as heavy metals.

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 to derive 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)

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

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

\[
B = e + f \cdot (\%clay)^2 + g \cdot (\%sand)^2 \cdot (\%clay) \quad (6c)
\]

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):

\[
K = 2.778 \cdot 10^6 \{\exp[12.012 - 0.0755 \cdot (\%sand) + 3.8950 + 0.3671 \cdot (\%sand) - 0.1103 \cdot (\%clay) + 8.7546 \cdot 10^{-4} \cdot (\%clay)^2] \cdot (1/\theta)\} \quad (7)
\]
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 7 shows the import mask of the GeODin interface.

Simulation results can be exported in a variety of ways 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 visu-
alization 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 8.

**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 will performed in cooperation with partners of the TU Dresden.

**CONCLUSIONS**

SiWaPro DSS was designed in order to conduct leachate forecast as required by the German soil protection law BBodSchG and BBodSchV. Apart from accurately modeling 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 modeling background.

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

**REFERENCES**


