COMBESICK – A new tool for seepage modelling in early stages of contaminated site investigations

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ABSTRACT

With the introduction of the Bundes-Bodenschutzgesetz (BBSchG) need has arisen for a seepage modelling tool in early stages of contaminated site investigations. Hydrologic modelling in these early stages is usually difficult due to lack of reliable soil hydraulic data. Particularly the numerical models which are applicable to a wider range of settings than analytical models require a large number of input parameters. Reliable experimental determination of input parameters such as the θ-h-k relationship is both time-consuming and expensive. Apart from experiments the estimation of soil hydraulic parameters can also be achieved by deriving measured parameters of similar soils from soil databases or by calculating the missing parameters from more easily available soil data through pedotransfer functions. However, there is currently no modelling tool that combines simulation with soil databases and parameter estimation. The modelling software COMBESICK which is developed at Dresden University of Technology combines a simulation module with soil databases and pedotransfer functions in order to provide reliable estimates for missing soil hydraulic parameters. The validity of COMBESICK will be validated against experimental data from soil column experiments.

INTRODUCTION

In 1999 the German legislator introduced the Bundes-BodenschutzGesetz (BBSchG) in order to emphasize the importance of soil as a natural resource and to regulate its protection and remediation. The BBSchG demands the carrying out of seepage modelling in the early stage of the contaminated site investigation in order to determine whether expected contaminant concentrations reaching the groundwater surface will be higher than values imposed by the BBSchG. In case the model yields higher values than those imposed by the BBSchG more detailed and expensive investigations of the contaminated site will be necessary. Thus there is a need for a seepage modelling tool for early stages of investigation where little data about the contaminated site is available. It would therefore be useful to combine a simulation tool with soil databases and parameter estimation tools in one computer program. The Dresden University of Technology is currently developing COMBESICK, a computer program that consists of the seepage simulation tool SiWaPro (Kemmesies 1999) which numerically solves the Richards equation and the advection-dispersion equation, combined with the soil databases UNSODA (Nemes et al. 2001) and WISE (Batjes 2002) and with a variety of pedotransfer functions for estimation of input parameters of the numerical model.

METHODS

COMBESICK follows the concept of modular programming in order to make the program easier to adapt to needs of users, to new requirements imposed by law, or to new developments in science. COMBESICK contains the simulation module SiWaPro (Kemmesies 1999) written in Fortran 77 and two mesh generators for space quantization, namely EasyMesh (Niceno 1997) and Z88 (Rieg and Hackenschmidt 2000) both written in C. These modules have been compiled into dynamic link libraries for flexible access during runtime. They are well known and have been extensively tested for stability and validity. The soil database part of COMBESICK consists of UNSODA 2.0 (Nemes et al. 2001) and Wise 1.1 (Batjes 2002). A graphical user interface guides the user through the process of data input. The graphical user interface is written in Visual Basic and contains access to the dynamic link libraries, as well as to the soil databases and to the pedotransfer functions (Figure 1).

The simulation module SiWaPro

SiWaPro (Kemmesies 1999) is based on SWMS_2D (Šimunek et al. 1992). SiWaPro calculates water flow by numerically solving the Richards equation for variably saturated flow in two dimensions (Equation 1).

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left[K(K_{ij}{}^{A}\frac{\partial h}{\partial x_j} + K_{iz}{}^{A})\right] - S \qquad (1)$$

In Equation 1, θ represents the volumetric water content, K the unsaturated hydraulic conductivity function, and S a sink term. Water content and hydraulic conductivity needed

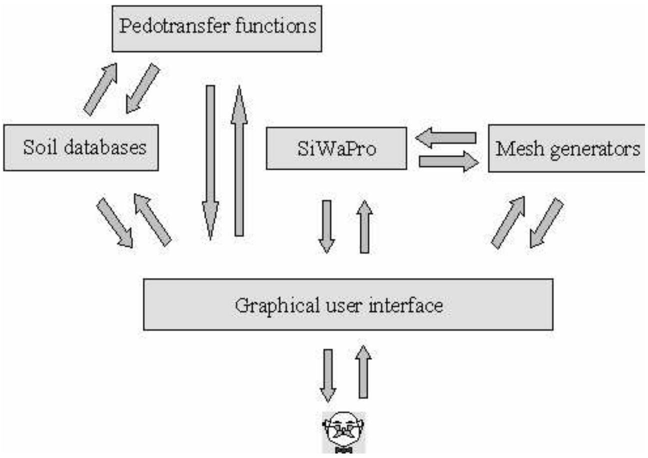

Figure 1: The modules of COMBESICK.

to solve the equation are derived from equations based on the Van Genuchten model (1980). According to Luckner et al. (1989) the water content as a function of the capillary pressure during the wetting process can be calculated using equation 2.

$$\theta_w = A + \frac{\phi - A - B}{\left[1 + (\alpha p_{c,w-nw})^n\right]^{1-\frac{1}{n}}} \quad (2)$$

In equation 2 θ_w represents the content of the wetting fluid, ϕ the porosity of the soil, and $p_{c,w-nw}$ the pressure difference between wetting and nonwetting fluid in the capillary. A and B are functions of the residual air content and the residual water content, respectively. α and n define the shape of the water retention curve with α representing the magnitude of the capillary pressure at the inflection point and n characterizing the increase of the water retention curve at its inflection point. In addition to the water content equation 1 needs the hydraulic conductivity of the soil as input. According to Luckner et al. (1989) The hydraulic conductivity can be represented as the relative permeability and is a function of the water content of the soil (Equation 3).

$$K_r(\theta_w) = \frac{k(\theta_w)}{k_0} = \left(\frac{\overline{S}}{\overline{S}_0}\right)^{\lambda} \left[\frac{1-\left(1-\overline{S}^{\frac{1}{m}}\right)^m}{1-\left(1-\overline{S}_0^{\frac{1}{m}}\right)^m}\right]^2 \quad (3)$$

In equation 3 mobilities are used instead of hydraulic conductivities in order to be able to take immobile parts of the fluid located at grain margins into account. $k(\theta_w)$ represents the mobility as function of the water content during the wetting process, and k_0 the mobility at zero water content. $\overline{S}$ and $\overline{S}_0$ are the mobility degrees. λ and m are empirical fitting parameters. Kemmesies (1995) defines the mobility degree $\overline{S}_i$ of the phase i as the mobile fluid content θ_i-$\theta_{i,r}$ in its in its area of mobility ϕ-$\theta_{i,r}$ (Equation 4).

$$\overline{S}_i = \frac{\theta_i - \theta_{i,r}}{\phi - \theta_{i,r}} \quad (4)$$

In equation 4 θ_i represents the content of phase i, $\theta_{i,r}$ the residual phase content of i, and ϕ the porosity of the soil. The Richards equation is solved numerically using the Galerkin Finite Element method with linear basis functions on triangular elements. The resulting water content is then used as input for the advection-dispersion equation (Equation 5) in order to calculate contaminant transport.

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial c}{\partial x_j}\right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - Scs \quad (5)$$

In equation 5 c represents the concentration of a contaminant in solution, s the adsorbed concentration of contaminant, q the volumetric flux, D the dispersion coefficient, μ and γ first- and zero-order rate constants, respectively.

The advantage of numerically solving the Richards equation and the advection dispersion equation over analytical solutions of both equations is the wide range of applicability of the numerical solution. However, the disadvantage of the numerical solution is the large number of required input parameters. COMBESICK tries to approach this problem through soil databases and parameter estimations using pedotransfer functions.

The soil database

The soil database of COMBESICK consists of soil data 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 (e.g. Arya et al, 1999a, b). WISE contains 4300 soils from 123 countries worldwide with a variety of textural, compositional and hydraulic parameters. The graphical user interface of COMBESICK allows access to data from both databases. Figure 2 shows the form for entering soil hydraulic parameters with the option for access to soil databases and pedotransfer functions.

Pedotransfer functions

Pedotransfer functions have been predominantly developed in order to derive soil hydraulic properties from more easily available soil properties such as soil texture, porosity, bulk density, and organic matter content among others. Earlier pedotransfer functions have been developed using linear and nonlinear regression analysis (e.g. Rawls and Brakensiek 1985). More recently pedotransfer functions have been developed using other mathematical techniques such as artificial neural networks (AAN) (Koekkoek and Bootlink 1999), the group method of data handling (GMDH) (Pachepsky et al. 1998) and Classification and Regression Trees (CART) (McKenzie and Jacquier 1997).

Figure 2: Form for entering soil parameters with access to soil databases and pedotransfer functions in COMBESICK.

Some pedotransfer functions have been derived for specific soil texture classes – the so-called class pedotransfer functions – while others have been developed for use with any type of soil – the so-called continous pedotransfer functions.
In COMBESICK a variety of pedotransfer functions have been implemented and can be accessed through the graphical user interface (Figure 2).

DISCUSSION AND CONCLUSIONS

COMBESICK is a new modelling tool for early investigation stages of contaminated site investigations as required by the BBSchG. The numerical model of the simulation module SiWaPro allows to model a wide variety of settings. The lack of parameters for the numerical models is approached by combining the simulation module with soil databases and pedotransfer functions. The validity of COMBESICK will be tested against soil column tests.

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