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COMBESICK - a computer-based decision support system for seepage prognosis

P. Herb & P.-W. Graeber
Institute for Waste Management and Contaminated Site Treatment, TU Dresden, Germany

O. Kemmesies
Dr. Kemmesies und Partner, Gunzenhausen, Germany

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1 INTRODUCTION

With the introduction of the BBSchG in 1999 the need for a standard modeling tool for contaminant transport in the unsaturated zone has become apparent. The BBSchG requires that a seepage prognosis must be conducted in the orienting stage of a contaminated site investigation. This rises a number of requirements for a potential standard modeling tool: firstly the number of available soil parameters in the orienting phase is small which is in contradiction to the number of parameters required by current modeling software. Secondly the modeling software will be commonly used by non-experts in the field of modeling which requires the model to be easy to use but still accurate and correct. In addition to the requirements posed by the BBSchG there are a number of requirements to software that has to become standard: such software should be compatible with the preferential platform of potential users, easy to adapt for the needs of users, it should run stably, and both the mathematical model and the software should be extensively tested for accuracy and correctness.

2 METHODS

The development of a suitable tool for seepage prognosis as specified by the BBSchG imposes a number of requirements on both the mathematical model and the software design.

2.1. The mathematical model

The mathematical model behind SiWaPro (Kemmesies, 1999) the modeling module of COMBESICK, is based on the mathematical model used in SWMS_2D (Šimunek et al 1992), the predecessor of the popular Hydrus_2D. It uses the Richards' equation for calculating variably saturated flow and the advection-dispersion equation for modeling solute transport. Both equations are set up for two dimension. The Richards' equation used in the mathematical model of COMBESICK contains a term for water uptake by plant roots (1):

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

where θ represents the volumetric water content, K the unsaturated hydraulic conductivity function, and S a sink term. The volumetric water content needed in equation (1) is a function of the capillary pressure and the hydraulic conductivity is a function of the water content of a soil. The models to derive these soil hydraulic properties have been developed by Vogel and Císlerová (1988) and Luckner et al (1989) and are based on the popular model of Van Genuchten (1980). According to Luckner et al (1989) the water content function takes the form of equation (2).

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

where θ_w represents the content of the wetting fluid, ϕ the porosity of the soil, and $p_{c,w\text{-}nw}$ the pressure difference between wetting and nonwetting fluid in the capillary. In equation (2) A, B, and n are scaling factors of the water content function. A is a function of the residual water content and B is a function of the residual air content. α represents the magnitude of the capillary pressure at the turning point of the water content function and n characterizes the increase of the water content function at its turning point. The relative permeability which represents the conductivity of the soil is given by Luckner et al (1989) as follows:

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

where $k(\theta_w)$ represents the mobility as function of the water content, and k_0 the mobility at zero water content. $\bar{S}$ and $\bar{S}_0$ are the mobility degrees. Mobilities are used instead of hydraulic conductivities in order to be able to account for the presence of an immobile part of the fluid phase. Kemmesies (1995) defines the mobility degree $\bar{S}_i$ of the phase i as the mobile fluid content θ_i-$\theta_{i,r}$ in its in its area of mobility ϕ-$\theta_{i,r}$:

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

where θ_i represents the phase content of i, $\theta_{i,r}$ the residual phase content of i, and ϕ the porosity of the soil.

The Richards' equation (1) is solved using the Galerkin finite element method with linear basis functions on triangular elements. The model allows for implicit, explicit and Crank-Nicholson methods of time discretization. The resulting matrix is solved iteratively for each time step. After convergence at a specific time step has been achieved, the resulting water content and the fluid flux are handed over to the advection-dispersion equation.

The advection-dispersion equation incorporates terms for linear equilibrium adsorption and for zero-order and first-order degradation (5):

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

where c = concentration of contaminant in solution, s = adsorbed concentration of contaminant, q = volumetric flux, D = dispersion coefficient, μ = first-order rate constants, γ = zero-order rate constants

The Galerkin finite element method is again used to solve the advection-dispersion equation and time quantization can be achieved using implicit, explicit or Crank-Nicholson schemes.

COMBESICK allows for the implementation of various time-dependent and time-independent boundary conditions and it includes the possibility to conduct parameter identification.

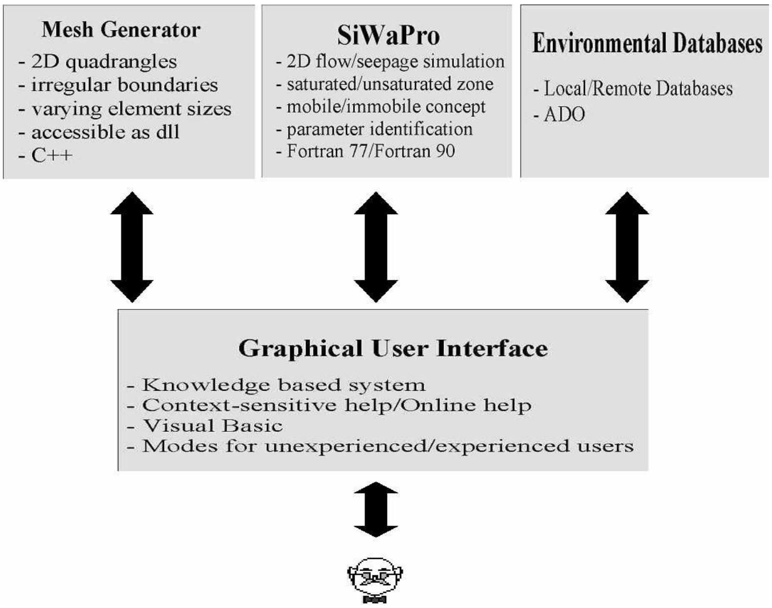
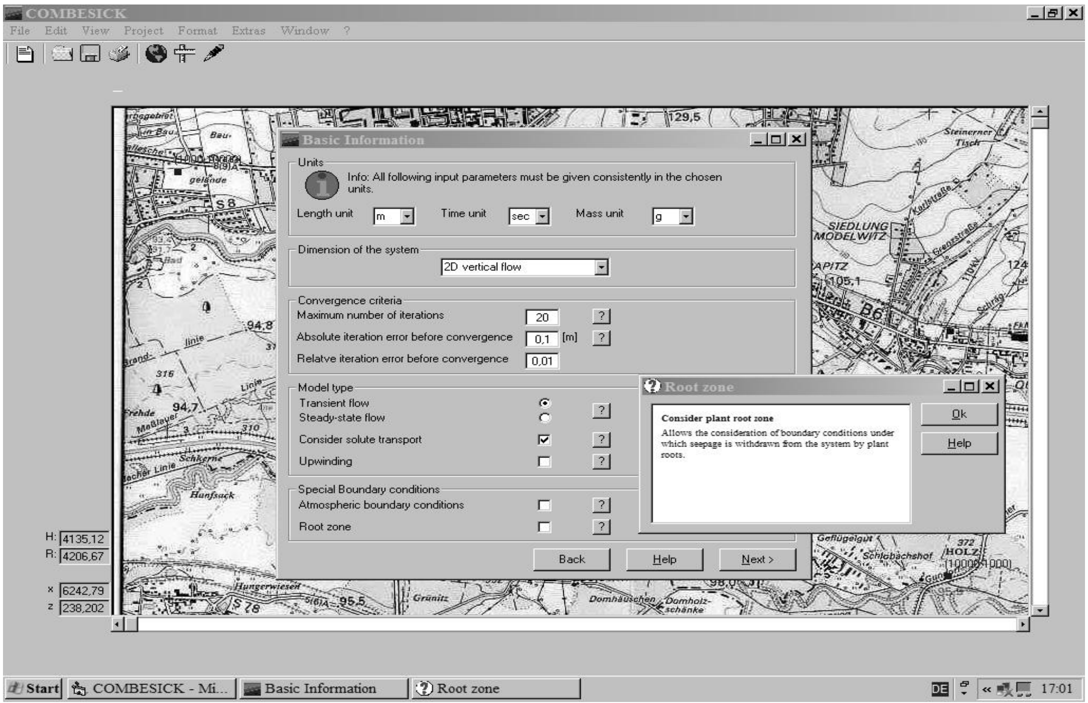


Figure 1. The modules of COMBESICK

It is planned to extend the existing mathematical model by incorporating pedotransfer functions into COMBESICK, in order to derive some of the hydraulic parameters from more easily available parameters like soil texture, composition or grain size distribution. Additionally sensitivity analyses will be conducted on COMBESICK in order to determine which parameters can be safely neglected under which circumstances. The results of the modeling will be given as fuzzy values as accomplished in the decision support system Grumio (Pühl, 2000) in order to account for uncertainties in the mathematical model, and in the soil parameter determination.



Units

Info: All following input parameters must be given consistently in the chosen units.

Length unit: m
Time unit: sec
Mass unit: g

Dimension of the system: 2D vertical flow

Convergence criteria

Maximum number of iterations: 20
Absolute iteration error before convergence: 0,1 [m]
Relatve iteration error before convergence: 0,01

Model type

Transient flow ●
Steady-state flow ○
Consider solute transport ☑
Upwinding ☐

Special Boundary conditions

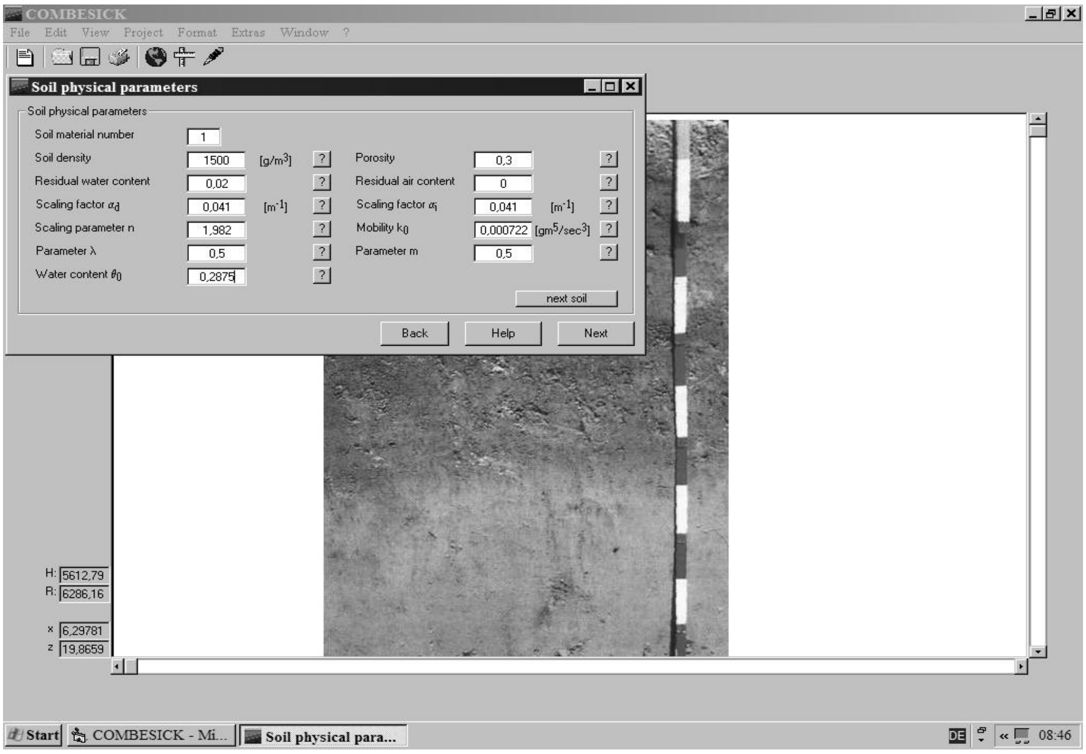
Atmospheric boundary conditions ☐
Root zone ☐

Consider plant root zone

Allows the consideration of boundary conditions under which seepage is withdrawn from the system by plant roots.

H: 4135,12
R: 4206,67
x 6242,79
z 238,202

Figure 2: Form for entering basic modeling parameters with context-sensitive help.



Soil physical parameters

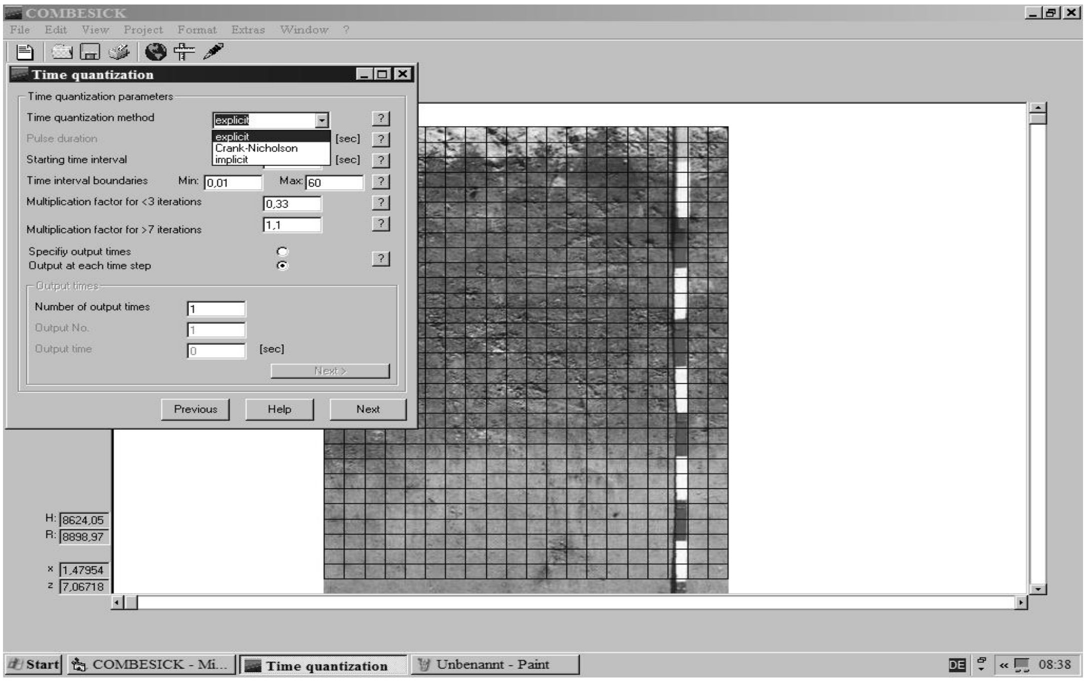
Soil material number: 1
Soil density: 1500 [g/m³]
Residual water content: 0,02
Scaling factor α_d: 0,041 [m⁻¹]
Scaling parameter n: 1,982
Parameter λ: 0,5
Water content θ_0: 0,2875
Porosity: 0,3
Residual air content: 0
Scaling factor α_i: 0,041 [m⁻¹]
Mobility k_0: 0,000722 [gm⁵/sec³]
Parameter m: 0,5

H: 5612,79
R: 6286,16
x: 6,29781
z: 19,8659

Figure 3: Form for entering hydraulic properties of the soil.

2.2 The software design

COMBESICK as a whole closely follows the concept of modular programming. It consists of a simulation module, an adapted mesh generator, modules that regulate access to local and remote databases and a graphical-user interface which behaves similar to knowledge-based systems (Figure 1). The core of COMBESICK is formed by the simulation module SiWaPro (Kemmesies, 1999) which calculates water flow and contaminant transport in two dimensions by solving the Richards' equation and the advection dispersion equation as



Time quantization parameters

Time quantization method: explicit
Pulse duration: [sec]
Starting time interval: [sec]
Time interval boundaries Min: 0,01 Max: 60
Multiplication factor for <3 iterations: 0,33
Multiplication factor for >7 iterations: 1,1
○ Specifiy output times
● Output at each time step

Output times
Number of output times: 1
Output No.: 1
Output time: 0 [sec]

H: 8624,05
R: 8898,97
x: 1,47954
z: 7,06718

Figure 4. Space quantization using mesh generator Z88 (Rieg, 2000) and time quantization in COMBESICK.

described in Section 2.1. A graphical user interface (GUI) guides the user through the process of data input. Parameters required for the simulation include general model options (Figure 2), parameters for describing the soil hydraulic properties (Figure 3), and parameters for describing the behaviour of the contaminant. Furthermore, space relevant data such as boundary conditions have to be entered and time quantization has to be conducted (Figure 4). The GUI contains an extensive help system consisting of context-sensitive help (Figure 2) and online-help, as well as several data validation checks during data input, and the possibility of data input based on recommendations. The recommended values will 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 COMBESICK will also include an "expert-mode" in order to offer the experienced user full access to the modeling parameters. An adapted mesh generator allows flexible space quantization before and during runtime. COMBESICK currently contains the 2D triangular mesh generator EasyMesh 1.4 (Niceno, 1997) and the mesh generator Z88 (Rieg, 2000) used in COMBESICK for generation of 2D quadrangular meshes (Figure 4). Both mesh generators allow the generation of meshes with varying element sizes and irregular mesh boundaries. The simulation module and the mesh generators have been compiled into dynamic link libraries and can therefore be dynamically accessed during runtime. Sample output of seepage spreading in two dimension from a contaminated site is displayed in Figure 5.

3 DISCUSSION AND CONCLUSIONS

COMBESICK attempts to meet the requirements for a standard computer program used for conducting a seepage prognosis according to the BBSchG. These requirements are imposed by the nature of the BBSchG and by the potential users of such a program. COMBESICK tries to resolve the problem of small amounts of available data in the orienting stage of a contaminated site investigation by mathematical and computational methods. Mathematical methos include reducing the number of required parameters based on sensitivity analayses and the use of pedotransfer functions. Computational methods include the connection to environmental databases in order to obtain acceptable estimates for unknown soil parameters. Since these approximations lead to uncertainties in the mathematical model it will be attempted to express the results as fuzzy values.

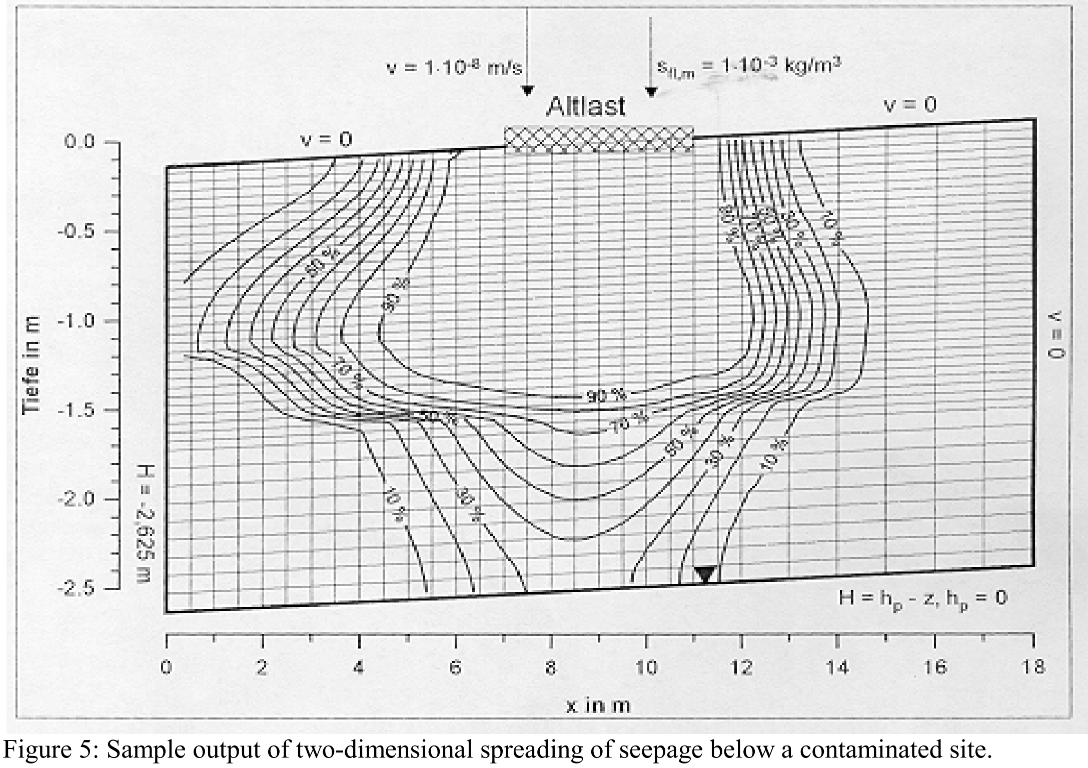


Figure 5: Sample output of two-dimensional spreading of seepage below a contaminated site.

The lack in modeling experience of the potential COMBESICK users is taken into account by implementing a GUI similar to knowledge-based systems, an extensive help system, a large number of error checks, and input value recommendations based on data obtained from local and remote soil databases. Federal environmental bureaus and engineering companies in Germany are the potential users of COMBESICK. Since Microsoft Windows is the preferential platform in bureaus and companies in Germany COMBESICK is being developed for this platform. The modular nature of COMBESICK allows easy adaption to the needs of users or to new governmental regulations. Since the modules of COMBESICK are largely based on popular and extensively tested programs the stability, accuracy and correctness of COMBESICK altogether is also guaranteed. In addition validation of the model by using soil column tests will performed in cooperation with the project partner from TU Dresden.

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Peter-Wolfgang Graeber, Prof. Dr.ing.habil.
Institute of Waste Management and Contaminated Sites, EF: Systems Analysis/Computer Science
Dresden University of Technology
Address: Pratzschwitzer Str. 15, D - 01796 Pirna, Germany
Phone: +49 -(0) 3501 53 00 29 / 21, E-mail: graeber@rcs.urz.tu-dresden.de

Oliver Kemmesies, Dr. ing.
Dr. Kemmesies und Partner, Beratender Ingenieur und Hydrogeologe
Address: Weissenburger Strasse 19, D-91710 Gunzenhausen, Germany
Phone : +49 –(0) 9831 8860-11, E-mail: Oliver@kemmesies.de

Patrick Herb, Dipl.-geol.
Institute of Waste Management and Contaminated Sites, EF: Systems Analysis/Computer Science
Dresden University of Technology
Address: Pratzschwitzer Str. 15, D - 01796 Pirna, Germany
Phone: +49 -(0) 3501 53 00 37, E-mail: Patrick.Herb@mailbox.urz.tu-dresden.de

Herb P., Graeber P.-W., Kemmesies O. COMBESICK – datora programmatūra lēmuma pamatošanai caurplūdes prognozei.

Augsne un pazemes ūdens ir svarīgi dabas resursi. Šie resursi ir ierobežoti, grūti atveseļojami, ja tie ir piesārņoti, un pieprasījums pēc tiem pieaug. Šo apstākļu dēļ resursu aizsardzība ir kļuvusi ļoti nozīmīga. Tāpēc 1999. gadā Vācijas likumdošana ieviesa tā saukto Bundes-Bodenshutzgesetz (BBch6) likumu, kurš regulē augsnes atveseļošanu un aizsardzību Vācijā. Atbilstoši šim likumam, ūdens vertikālās caurplūdis prognoze ir nepieciešama, ja piesārņojuma koncentrācija augsnē pārsniedz likumā pieļauto lielumu. Caurplūdes prognoze nepieciešama, lai noteiktu iespējamo pazemes ūdens piesārņojumu, kuru var izraisīt piesārņojuma avoti virszemē. Datora veikta piesārņojuma transporta modelēšana ir nepieciešama un lēmuma pieņemšanas sistēmu caurplūdes prognozei (COMBESICK). Sistēmu viegli izmantot, tā ir droša pret iespējamām kļūdām salīdzinājumā ar agrāk lietotām caurplūdes modelēšanas programmatūrām.

Herb P., Graeber P.-W., Kemmesies O. COMBESICK - A computer-based decision support system for seepage prognosis.

Soil and groundwater are important natural resources. Due to increasing demand for soil and groundwater, their limited capacity, and the difficulties of remediating these resources once contaminated, their protection has become increasingly important. As a result, in 1999 the German legislator introduced the so-called Bundes-Bodenschutzgesetz (BBSchG) – a law regulating the protection and remediation of soil in Germany. According to the BBSchG a seepage prognosis has to be conducted if contaminant concentrations in the soil exceed values specified in the BBSchG. The purpose of the seepage prognosis is to determine potential groundwater contamination originating from surfecial contaminated sites. Computer-based simulation of contaminant transport in the unsaturated zone is an indispensable, cost-effective method of conducting a seepage prognosis. We suggest a decision support system for seepage prognosis (COMBESICK) which will be easy to use, widely available, and less error-prone than previous seepage modeling software.

Герб П., Грабер П.-В., Кеммесис О. COMBESICK - программатура для обоснования решеня по прогнозу просачивания.

Почва и подземные воды являются важными ресурсами природы. Эти ресурсы ограничены, их трудно оздоровить, если они загрязнены. Потребноть в этих ресурсах возрастает, поэтому их защита очень важна. Это послужило тому, что в 1999 году законодательство Германии внедрило так называемый Bundes-Bodenschutzgesetz (BBSchG) закон, который определяет порядок оздоровления и защиты почвы в Германии. Согласно этому закону необходим прогноз вертикального просачивания подземной воды, если концентрация загрязнений в почве превышает допустимую величину. Прогноз просачивания необходим для определения возможного загрязнения подземных вод, которое могут вызвать источники на поверхности земли. Компьютерная программа для моделирования транспорта загрязнений является необходимым и дешевым методом прогнозирования просачивания. Мы предлагаем систему принятия решения по прогнозу просачивания (COMBESICK). Эту систему можно легко использовать, она более надежна относительно возможных ошибок по сравнению с ранее применяемыми программами для прогноза просачивания.