

MATHEMATICAL CONCEPTUAL MODELLING AND SIMULATION OF MIGRATION PROCESSES IN SOIL WATER ZONES

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Migration models for the unsaturated soil water zone are of great importance not only for the control of the industrial crop production but also for the protection of groundwater resources against contaminants. System describing models are used in the GDR most at all to investigate migration processes by simultaneous measuring and theoretical analysing and naturally to formulate and to adjust conceptual block models.

MATHEMATICAL CONCEPTUAL MODELLING

Flow Model

We use for homogeneous soils the eq. (1)

$$\frac{\partial}{\partial z} \left( k \frac{\partial h}{\partial z} \right) = k \frac{\partial^2 h}{\partial z^2} + \frac{\partial k}{\partial z} \frac{\partial h}{\partial z} = c \frac{\partial h}{\partial t} + aet \quad (1)$$

with  $h = \frac{p}{\rho} + z = z - \gamma$  and  $c = \partial w / \partial h \Big|_z = const.$

and for infiltration processes in very dry soils eq. (2)

$$\frac{\partial^2 U}{\partial z^2} - G(U) \frac{\partial U}{\partial z} = F(U) \frac{\partial U}{\partial t} + aet \quad (2)$$

with  $U = \int_0^{\gamma} k(\gamma) d\gamma$  ;  $F(U) = c(\gamma) / k(\gamma)$  ;

and  $G(U) = \partial k(\gamma) / (k(\gamma) d\gamma)$ .

The model of the specific evapotranspiration rate aet has the form

$$aet = PET \cdot r(w) \cdot f(z). \quad (3)$$

For the potential evapotranspiration PET we use the model from T u r c /2/ in the summer periode (from May to October) and constant rates from November to April /2/. For the function f (z) we use /1/

$$f(z^*) = \frac{c(2z^* - L) + L}{L^2} \quad \text{with } 1 \geq c \geq -1 \quad (4)$$

z\* - depth under the soil surface

and for the reduction function r (w) /2/

$$r(w) = \begin{cases} (4,4 - pF)/\beta & \text{for } pF > 4,4 - \beta \\ 1,0 & \text{for } 1,7 \leq pF \leq 4,4 - \beta \\ 0,0 & \text{for } pF < 1,7 \end{cases} \quad (5)$$

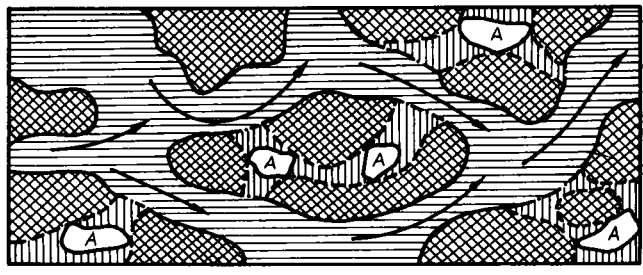
with  $\beta \approx 0.2$  PET in mm/day  $\approx 2 \cdot 10^{-9}$  PET in m/s  
 ( $\beta$  is here undimensioned;  $pF = \log(\psi \text{ in cm})$ )

Quality Model

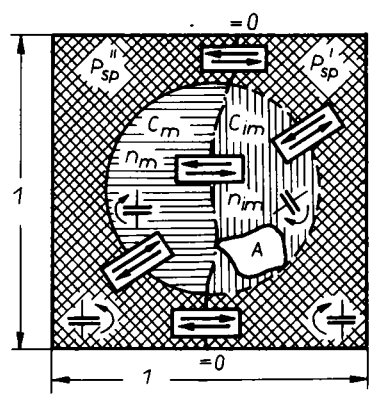
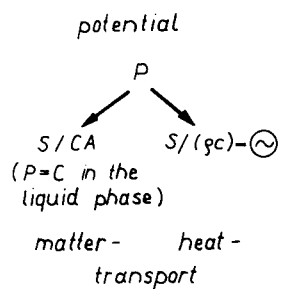
For the water quality model we use eq. (6)

$$\underbrace{\frac{\partial}{\partial z} (\delta v_z \frac{\partial C_m}{\partial z}) - v_z \frac{\partial C_m}{\partial z}}_{\text{Transportation process}} = \underbrace{\frac{\partial (C_m (n_m + k_3))}{\partial t}}_{\text{storage process}} + \underbrace{(Z - A)}_{\text{exchange between the phases}} + \underbrace{C_{im} a e t}_{\text{external transfer}} \quad (6a)$$

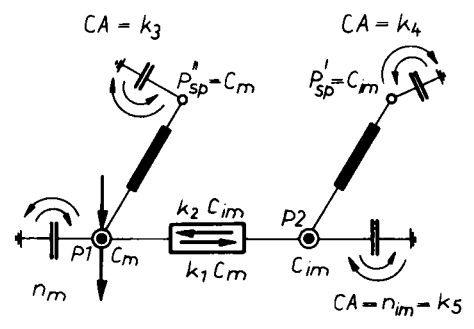
As shown in figure 1 this model describes the migration of pollutants in the mobile (6a) and in the immobile phase (6b) of soil water. The transportation (hydrodynamic dispersion and convection) is only considered in the mobile liquid phase. Between the liquid and solid phase we assume two equilibrium reactions, so that we can regard the storage capacity of the mobile liquid phase as the summe of  $(n_m + k_3)$  and of the immobile liquid phase as  $(n_{im} + k_4)$ . The coefficients  $k_3$  and  $k_4$  may be constant (H e n r y - isotherme), proportional to  $C^{q-1}$  (F r e u n d l i c h - isotherme) and so on /1/. We normally describe the exchange process between the mobile and the immobile liquid phase  $(Z - A)$  by first-order reactions, especially by reversible lineare or nonlineare reactions and also by bilineare reversible reactions /1/. Last not least we assume, that the evapotranspiration takes place only from the immobile soil water phase.



a)



b)



c)

- |  |  |  |                                      |
|--|--|--|--------------------------------------|
|  | rock (solid phase)                                       |  | interface: rock-mob. liquid phase    |
|  | mobile liquid phase                                      |  | rock-immob. liquid phase             |
|  | immobile liquid phase with blocked air                   |  | immob. liquid ph.-mob. liq. ph.      |
|  | symbol of the transportation process internal of the ph. |  | fictive interface in the solid phase |
|  | symbol of the storage process internal of the phase      |  |                                      |
|  | symbol of the exchange process between two phases        |  |                                      |

Fig. 1: First steps of the modelling of migration processes

ANALYTICAL SOLUTION AND NUMERICAL UTILIZATION

Analytical Solution

With the restriction, that

- $v_z, n_m, k_1, k_2, k_3, n_{im}$  and  $k_4$  are constant in space and time,
- the exchange process between the parts of the soil water follows the mathematical model of a linear reaction of first order with constant velocity rates  $k_1$  and  $k_2$ ,
- the internal conversion is not considered and
- the evapotranspiration is neglected

we get from eq. (6) eq. (7).

$$D \frac{\partial^2 C_m}{\partial z^2} - v_z \frac{\partial C_m}{\partial z} = (n_m + k_3) \frac{\partial C_m}{\partial t} + k_1 C_m - k_2 C_{im} \tag{7}$$

$$0 = (n_{im} + k_4) \frac{\partial C_{im}}{\partial t} - k_1 C_m + k_2 C_{im}$$

with the boundary conditions

$$\lim_{z \rightarrow 0^+} (v_z C_m - D \frac{\partial C_m}{\partial z}) = \begin{cases} v_0 C_{max} & 0 \leq t \leq t_1 \\ 0 & t \geq t_1 \end{cases} \tag{8a}$$

$$\lim_{z \rightarrow \infty} C_m(z, t) = 0 \tag{8b}$$

$$C_m(z, 0) = C_{im}(z, 0) = C_{min} \tag{8c}$$

we found the solution /4/:

$$C_m^*(f, T) = C_1^*(f, T) + C_2^*(f, T) + C_3^*(f, T) \tag{9}$$

$$C_1^*(f, T) = \frac{2B}{\sqrt{\pi}} f \exp(2Bf - K_2 T) \int_0^{\sqrt{T/F_3}} \frac{1}{t^2} g(f, t) f_1(\tilde{T}, t) dt \tag{10a}$$

$$C_2^*(f, T) = -\frac{2}{\sqrt{\pi}} \exp(2Bf - K_2 T) \int_0^{\sqrt{T/F_3}} g(f, t) f_2(\tilde{T}, t) dt \tag{10b}$$

$$C_3^*(f, T) = \begin{cases} -C_1^*(f, T - T_1) - C_2^*(f, T - T_1) & \text{für } T \geq T_1 \\ 0 & \text{für } 0 \leq T < T_1 \end{cases} \tag{10c}$$

$$f_1(\tilde{T}, t) = \int_{\tau=0}^{\tau=\tilde{T}} I_0(4t\sqrt{BK_1 K_2 \tau}) h_1(\tilde{\tau}) d\tau; \tilde{T} = T - F_3 \cdot t^2; \tilde{\tau} = \tilde{T} - \tau \tag{11a}$$

$$f_2(\tilde{T}, t) = \int_{\tau=0}^{\tau=\tilde{T}} I_0(4t\sqrt{BK_1 K_2 \tau}) h_2(\tilde{\tau}) d\tau + D_7 I_0(4t\sqrt{BK_1 K_2 \tilde{T}}) \tag{11b}$$

$$h_1(T) = (D_1 T + D_2) \exp(K_2 T) + \frac{D_3}{1+K_3} \exp\left(-\frac{K_1}{1+K_3} T\right); h_2(T) = (D_4 T + D_5) \exp(K_2 T) + \frac{D_6}{1+K_3} \exp\left(-\frac{K_1}{1+K_3} T\right) \tag{12}$$

$$g(f, t) = \exp\left(-\frac{f^2}{4t^2} - F_2 t^2\right) \tag{13}$$

with the undimensioned parameters

$$\begin{aligned}
 c_m^* &= \frac{c_m - c_{min}}{c_{max} - c_{min}} & \gamma &= \frac{z}{L} & B &= \frac{v_2 L}{4D} & K_3 &= \frac{k_3}{n_m} & K_4 &= \frac{k_4}{n_m} \\
 K_5 &= \frac{n_{im}}{n_m} & K_1 &= \frac{k_1 L}{v_2} & K_2 &= \frac{k_2 L}{v_2 (n_{im} + k_4)} & T &= \frac{v_2 t}{L n_m} & s &= s' \frac{L n_m}{v_2} \\
 D_1 &= -\frac{K_2^2}{(K_1 + (1+K_3)K_2)} & D_2 &= -\frac{2K_1 K_2 + (1+K_3)K_2^2}{(K_1 + (1+K_3)K_2)^2} & D_3 &= -\frac{K_1^2}{(K_1 + K_2 (1+K_3))^2} \\
 D_4 &= 4B^2 D_1 & D_5 &= -4BK_2 + 4B^2 D_2 & D_6 &= 4B^2 D_3 & D_7 &= -4B & \begin{aligned} F_2 &= 4B(B \cdot K_1 - K_2(1+K_3)) \\ F_3 &= 4B(1+K_3) \end{aligned} & (14)
 \end{aligned}$$

The analytical solutions from van Genuchten and Wierenga /7/ as well as from Cameron and Klute /8/ are special cases for  $k_1 = k_2$  respectively for  $k_4 = 0$ .

Of course the math. structure of eq. (7) doesn't depend on the value of  $k_4$  but our analytical solution (9) with (10) and (11) gave us better numerical possibilities for a faster computer program as the analytical solution of Cameron and Klute.

#### Numerical Utilization of the Analytical Solution

For the numerical utilization of eq. (9) we wrote FORTRAN program ALSUB 3. We applied the procedure of Runge - Kutta - Fehlberg of fourth order for the integration of the function  $g(\gamma, t)$  in connection with a minimum limitation. The average computer time consumption amounted to about 30 seconds CPU using computer BESM-6 for each example.

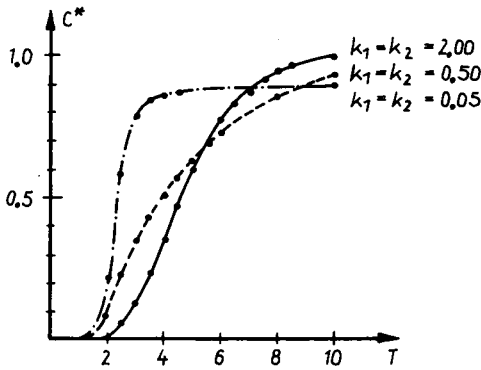
The computer tests gave us a very good coincidence with a computer program based of the analytical solution of van Genuchten and Wierenga for  $k_1 = k_2$  as well as a program based of the analytical solution of Cameron and Klute for  $k_4 = 0$ .

Fig. 2 shows results, received with our program ALSUB 3.

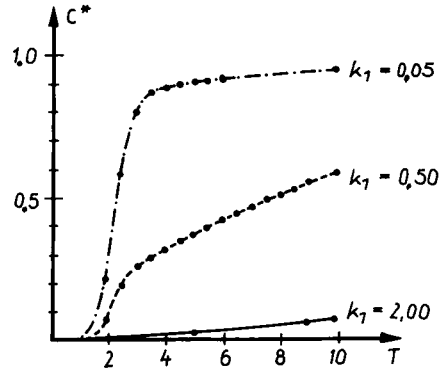
It demonstrates the sensibility of the break-through curves in connection with the parameters  $k_1$ ,  $k_2$ ,  $k_3$ ,  $n_{im}$  and  $k_4$  respectively  $n_m$ .

Of course we can expand the possibilities of the utilization of the analytical solution (9) by means of the convolution procedure for problems with a time variable boundary condition.

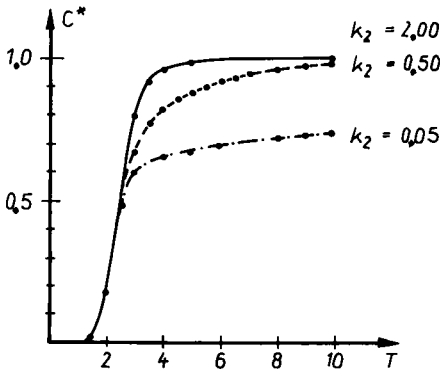
The solution (9) last not least posses also a great importance for checking various digital solutions.



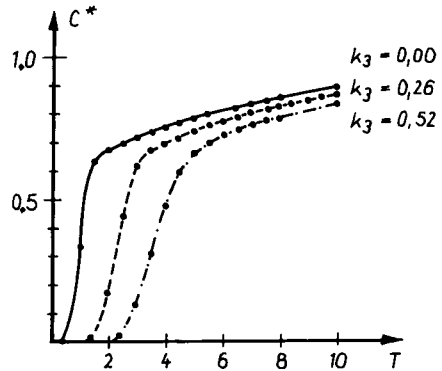
a: influence of  $k_1=k_2$  with  $k_3=0,26$ ,  $k_4=0,29$ ,  $k_5=0,20$ ,  $n_m=0,20$



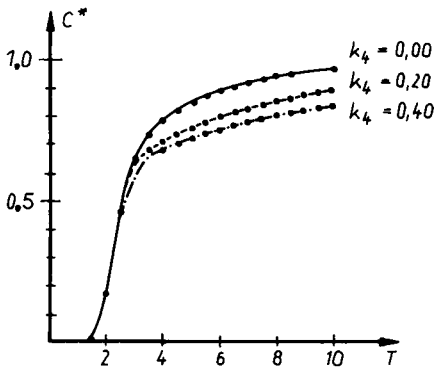
b: influence of  $k_1$  with  $k_2=0,15$ ,  $k_3=0,26$ ,  $k_4=0,29$ ,  $k_5=0,20$ ,  $n_m=0,20$



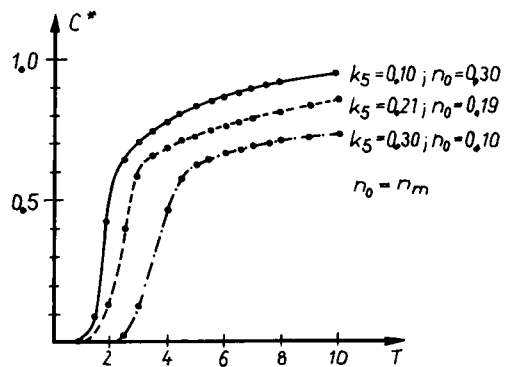
c: influence of  $k_2$  with  $k_1=0,15$ ,  $k_3=0,26$ ,  $k_4=0,29$ ,  $k_5=0,20$ ,  $n_m=0,20$



d: influence of  $k_3$  with  $k_1=k_2=0,15$ ,  $k_4=0,29$ ,  $k_5=0,20$ ,  $n_m=0,20$



e: influence of  $k_4$  with  $k_1=k_2=0,15$ ,  $k_3=0,26$ ,  $k_5=0,20$ ,  $n_m=0,20$



f: influence of  $k_5$  and  $n_m$  with  $k_1=k_2=0,15$ ,  $k_3=0,26$ ,  $k_4=0,29$

Fig. 2 : Break - through curves for various parameters  $k_1$ ,  $k_2$ ,  $k_3$ ,  $n_{im}$ ,  $k_4$  respectively  $n_m$ . For all exemples is applied:  
 $v_2 = 10 \text{ cm/d}$  ;  $L = 30 \text{ cm}$  ;  $f = 1,0$  ;  $D = \delta v_2 = 6 \text{ cm}^2/\text{d}$

## DIGITAL SIMULATION

Discretisation of the Flow Model

We recommend for eq. (1) the predictor-corrector scheme of Douglas and Jones /5/:

$$\nabla^2 h_i^{t+\Delta t/2} + (1/k_i^t) \nabla k_i^t \nabla h_i^t = \frac{c_i^t}{k_i^t} \cdot \frac{h_i^{t+\Delta t/2} - h_i^t}{\Delta t/2} + aet_i^t \quad (15a)$$

$$\begin{aligned} 0,5 \nabla^2 (h_i^t + h_i^{t+\Delta t}) + \left( \frac{1}{k_i^{t+\Delta t/2}} \right) \nabla k_i^{t+\Delta t/2} \nabla h_i^{t+\Delta t/2} = \\ = \frac{c_i^{t+\Delta t/2}}{k_i^{t+\Delta t/2}} \cdot \frac{h_i^{t+\Delta t/2} - h_i^t}{\Delta t} + aet_i^{t+\Delta t/2} \end{aligned} \quad (15b)$$

and for eq. (2)

$$\nabla^2 U_i^{t+\Delta t/2} - G_i^t \nabla U_i^t = F_i^t \frac{U_i^{t+\Delta t/2} - U_i^t}{\Delta t/2} + aet^t \quad (16a)$$

$$0,5 \nabla^2 (U_i^t + U_i^{t+\Delta t}) - G_i^{t+\Delta t/2} \nabla U_i^{t+\Delta t/2} = F_i^{t+\Delta t/2} \frac{U_i^{t+\Delta t} - U_i^t}{\Delta t} + aet^{t+\Delta t/2} \quad (16b)$$

Discretisation of the Quality Model

We also recommend for the discretisation of eq. (6) the predictor-corrector scheme from Douglas and Jones /5/:

*predictor step :*

$$\begin{aligned} (k_4 + k_5)^t \frac{C_{im,i}^{t+\Delta t/2} - C_{im,i}^t}{\Delta t/2} + \left[ C_{im} \frac{\partial k_5}{\partial t} - (Z-A) - C_{im} aet \right]_i^t = 0 \\ \frac{D_{i,i+1}^t}{\Delta Z} \cdot \frac{C_{i+1}^{t+\Delta t/2} - C_i^{t+\Delta t/2}}{\Delta Z} - \frac{D_{i,i-1}^t}{\Delta Z} \cdot \frac{C_i^{t+\Delta t/2} - C_{i-1}^{t+\Delta t/2}}{\Delta Z} = \\ = (n_m + k_3)^t \frac{C_i^{t+\Delta t/2} - C_i^t}{\Delta t/2} + \left[ v_i \frac{C_{i+1} - C_{i-1}}{2 \Delta Z} + C_i \frac{\partial n_m}{\partial t} + (Z-A) \right]_i^t \end{aligned}$$

*corrector step :*

$$\begin{aligned} (k_4 + k_5)^{t+\Delta t/2} \frac{C_{im,i}^{t+\Delta t} - C_{im,i}^t}{\Delta t} + \left[ C_{im} \frac{\partial k_5}{\partial t} - (Z-A) - C_{im} aet \right]_i^{t+\Delta t/2} = 0 \\ \frac{D_{i,i+1}^{t+\Delta t/2}}{\Delta Z} \cdot \frac{(C_{i+1}^{t+\Delta t} + C_{i+1}^t) / 2 - (C_i^{t+\Delta t} + C_i^t) / 2}{\Delta Z} \cdot \quad (17) \end{aligned}$$

We used other methods, too /1/, especially  
 - the method of characteristics (MOC) and  
 - the method from S t o y a n /6/.

### Numerical Tests

The numerical tests were carried out with our FORTRAN - program AERGUE containing the simultaneous solution of the mathematical models (15) or (16) and (17).

Fig. 3 shows the results which we got with this computer program in comparison with our program ALSUB 3 utilizing the analytical solution (9) - see also Fig. 3.

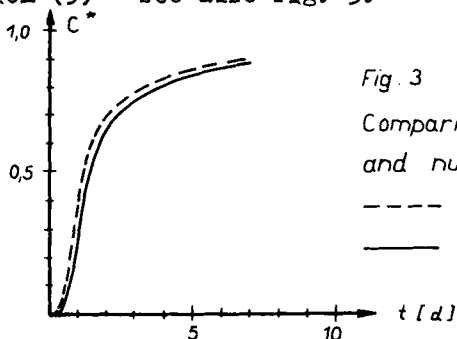


Fig. 3

Comparison between analytical  
and numerical solution

----- numerical solution for  $Pe = 1.0$

———— analytical solution

### LABORATORY TESTS

For these tests we used columns with a length of 1.20 m and a diameter of 0.20 m. For example  $Ca = 45$  of a  $CaCl_2$  - solution was used as migrant. The water content  $w$  in the column was discovered by means of a  $\gamma$ - ray measurement. In additional tensiometers are used for the measurement of  $\psi$ . At that time we try to calibrate the parameters of the used mathematical model by solving the inverse problem.

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