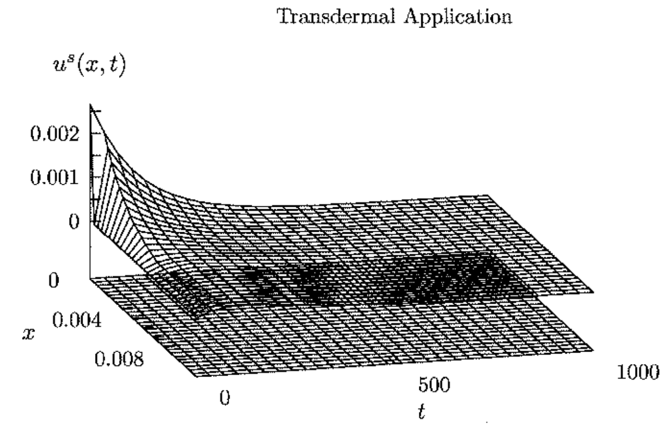

Figure 5.28. Substrate Distribution

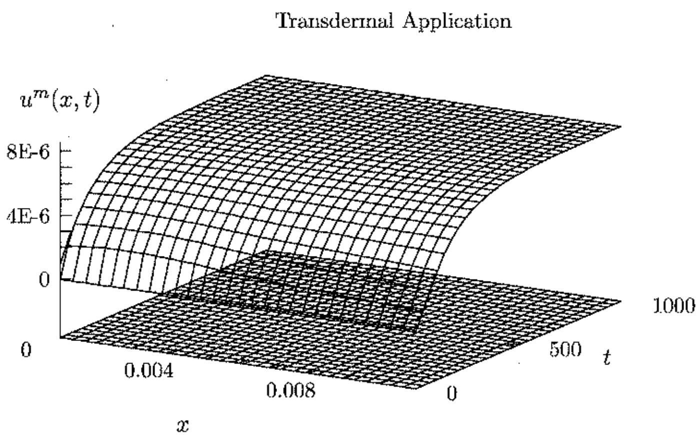

Figure 5.29. Metabolite Distribution

8. Groundwater Flow

The mathematical model describes a tracer experiment that was conducted at the lake Gårdsjön in Sweden, see Andersson and Olsson [5], to investigate acidification of groundwater pollution. To conduct the experiment, a catchment of 1,000 m^2 was covered by a roof. A tracer impulse consisting of lithium-bromide was applied with steady state flow conditions. Tensiometer measurements of the tracer concentration were documented in a distance of 40 m from the center of the covered area.

The diffusion equations proposed by Van Genuchten and Wierenga [454] are chosen by Hoch [200] to analyze the diffusion process and to get a simulation model. A two-domain approach was selected in the form of two equations, to model the mobile and the immobile part of the system. The first one describes the diffusion of the flow through soil by convection and dispersion,

$$\theta_m \frac{\partial c_m}{\partial t}(x,t) + \theta_{im} \frac{\partial c_{im}}{\partial t}(x,t) = \theta_m D_m \frac{\partial^2 c_m}{\partial x^2}(x,t) - \theta_m V_m \frac{\partial c_m}{\partial x}(x,t) \ . \qquad (5.39)$$

A second equation is needed for the so-called immobile part, the mass transfer orthogonal to the flow direction,

$$\theta_{im} \frac{\partial c_{im}}{\partial t}(x,t) = \alpha \left(c_m(x,t) - c_{im}(x,t) \right) \qquad (5.40)$$

for $t > 0$ and $0 < x < L$. Boundary conditions are

$$c_m(0,t) - \frac{D_m}{V_m} \frac{\partial c_m}{\partial x}(0,t) = \begin{cases} a \ , & \text{if } t < t_0; \\ 0 \ , & \text{otherwise} \end{cases} \qquad (5.41)$$

and

$$c_m(L,t) + \frac{D_m}{V_m} \frac{\partial c_m}{\partial x}(L,t) = 0 \qquad (5.42)$$

for $t > 0$, and initial values are given by $c_m(x,0) = 0$ and $c_{im}(x,0) = 0$ for $0 < x < L$. Then we evaluate the fitting function

$$h(t) = c_m(\tfrac{1}{2}L,t) - \frac{D_m}{V_m} \frac{\partial c_m}{\partial x}(\tfrac{1}{2}L,t) \qquad (5.43)$$

defined for $t > 0$.

In the above equations, $c_m(x,t)$ and $c_{im}(x,t)$ denote the tracer concentrations, θ_m and θ_{im} the corresponding water contents, D_m the dispersion coefficient, and α the mass transfer coefficient.

EXAMPLE 5.9 Since we want to investigate the whole process over a length of $L = 80$, experimental measurements are given inside the spatial area, see Figure 5.30. We transform (5.39) and (5.40) into the equivalent system

$$\begin{aligned} \frac{\partial c_m}{\partial t}(x,t) &= D_m \frac{\partial^2 c_m}{\partial x^2}(x,t) - V_m \frac{\partial c_m}{\partial x}(x,t) - p_m(c_m(x,t) - c_{im}(x,t)) \ , \\ \frac{\partial c_{im}}{\partial t}(x,t) &= p_{im}(c_m(x,t) - c_{im}(x,t)) \end{aligned} \qquad (5.44)$$

Table 5.11. Initial Values and Confidence Regions

	initial	*lower*	*final*	*upper*
p_m	1.0	8.681	11.83	14.97
p_{im}	1.0	4.640	6.296	7.950
D_m	100.0	257.9	382.7	507.5

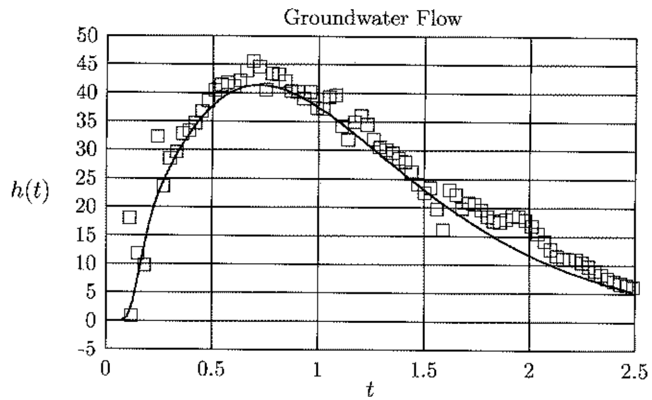

Figure 5.30. Fitting Criterion and Data

for $t > 0$ and $0 < x < L$, with $p_m = \alpha/\theta_m$ and $p_{im} = \alpha/\theta_{im}$. Parameters to be estimated are p_m, p_{im}, and D_m, whereas $t_0 = 0.0104167$, $V_m = 100$, and $a = 5800$ are considered as constants.

The five-point-difference formula is used to discretize first and second derivatives subject to 41 lines. The differential equations are integrated by RADAU5 with error tolerance 10^{-6}. The least squares code DFNLP, executed with termination tolerance 10^{-7}, stops after 34 iterations. Initial and final parameter values are listed in Table 5.11 together with 5 % confidence intervals. Figure 5.30 shows all experimental data and the fitting criterion. The corresponding surface plots for mobile and immobile parts are found in Figures 5.31 and 5.32.

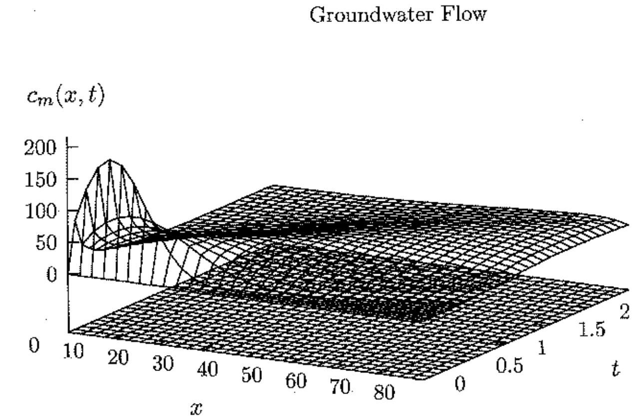

Figure 5.31. Mobile Part

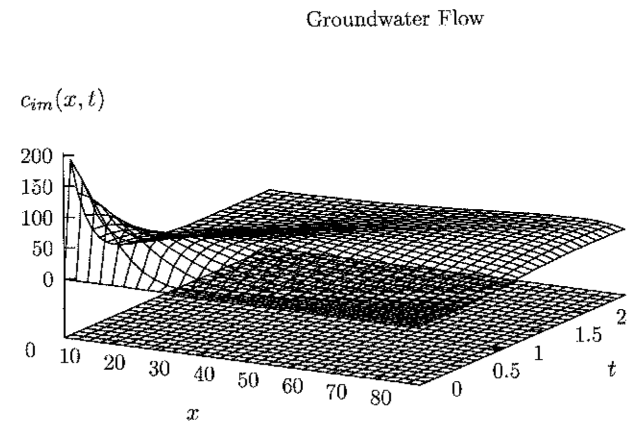

Figure 5.32. Immobile Part