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Characteristic Times and Inverse Problems for Diffusion in Coated Textiles

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Abstract: We study diffusion of active ingredients in coated textiles by a three-scale model. These scales consist of a fiber level representing the fiber with its polymer coating containing an active ingredient, a yarn level, and the level of the room holding the textile. An analysis of the model is carried out using the characteristic times of the different levels. We investigate the influence of the parameters in the model by solving several inverse problems.

Keywords: diffusion, textile modeling, multi-scale modeling, controlled release, characteristic times

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1 Introduction

We study the diffusion of a volatile trapped in a polymer coating on textiles fibers. These fibers are used to construct an intelligent textile. The coating consists of a polymer solution of an active ingredient (AI), e.g. an insect repellent, a perfume or a healing substance. This substance can easily be replaced by other volatiles. The goal is to slow down the release of the AI in order to increase the active lifetime of the textile. We want to investigate how much of the AI has to be present on the textile fiber and which polymer substance to use, to coat the fiber so that the concentration at the outer boundary of the textile stays high enough for as long as required to be effective (e.g. repel or even kill mosquitoes, spread a noticeable odor for humans, have a healing effect ...). Therefore a forward problem is implemented in C-language and an inverse problem is solved using the Levenberg-Marquardt method. The forward model consists of a three-scale approach based upon [6,7,1,4] . The model is given in [2]: a one-dimensional cylindrical diffusion equation on the fiber and yarn levels and a one-dimensional diffusion model for the room. To analyse and simplify the model, its characteristic times are further investigated in this paper. At these times the fiber and yarn model, and the yarn and room model, respectively, tend to reach an equilibrium concentration. The identification of these characteristic times is key in reducing the model to its variously scaled components when simplifying it.

The characteristic times are calculated using Laplace transformation based on [3] and compared to generated outcomes of the model. Implementation of both the forward as the inverse problem was done in C-language using `lsoda` [5] and the `fit` command in `Gnuplot`.

2 Characteristic times for the three-level diffusion

The governing system of equations of the complete three-level model [2] is

$$\begin{cases} \dfrac{\partial C_f(\rho,t)}{\partial t} &= \dfrac{1}{\rho}\dfrac{\partial}{\partial \rho}\left(\rho D_f \dfrac{\partial C_f(\rho,t)}{\partial \rho}\right), \\ \varepsilon\dfrac{\partial C_y(r,t)}{\partial t} &= \dfrac{1}{r}\dfrac{\partial}{\partial r}\left(\varepsilon r D_y \dfrac{\partial C_y(r,t)}{\partial r}\right) + \Gamma_{in}(\Omega,t), \\ \dfrac{\partial C_{\mathrm{r}}(x,t)}{\partial x} &= \dfrac{\partial}{\partial x}\left(D \dfrac{\partial C_{\mathrm{r}}(x,t)}{\partial x}\right), \end{cases}$$

with $\rho \in [R_f, 2R_f]$, $r \in [0, 2R_y]$ and $x \in [R_y, L]$. There is an evaporation flux at the right boundaries for the fiber and yarn model, and a homogeneous Neumann BC at their left boundaries. For the room model a homogeneous Neumann BC is present at the right boundary and an evaporation flux

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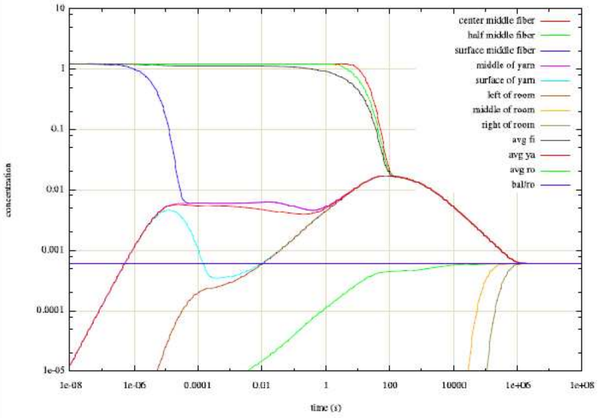


Figure 1: Logarithmic concentration vs logarithmic time with $D_f = 1 \times 10^{-10} \frac{\mathrm{mm}^2}{\mathrm{s}}$, $D_y = 1 \times 10^{-6} \frac{\mathrm{mm}^2}{\mathrm{s}}$ and $D = 1 \times 10^{-5} \frac{\mathrm{mm}^2}{\mathrm{s}}$.

at the left boundary coming from the concentration in the yarn evaporating to the room.

The concentration of the AI is tracked starting in the fiber coating. Once the outer boundary of the coating is reached the AI is evaporating to the yarn air gaps, and further on to the outside of the textile into the room. Plotting the logarithmic concentration against the logarithmic time scale shows that, for standard parameters, after a rather short time (approximately 100 s) the fiber and yarn concentrations coincide and after approximately 10×10^6 s those concentrations coincide with the concentration in the middle of the room, see Figure 1. We will further investigate these moments in time where equilibrium is reached between the different levels to have a better understanding of the interactions in the model and to be able to predict when the concentration of the AI reaches a certain position in the textile and in the room. As a consequence it becomes possible to adjust the textile product to the standards needed.

A way to calculate these characteristic times uses the Laplace transform of the flux. At interesting points of the system we interpret the diffusive flux $\mathscr{F}_T(x)$ as the probability distribution function of the times T when a particle passes a certain position x. The moment-generating function is then related to the Laplace transform of the flux:

$$M_T(-s) = E_T(e^{-sT}) = \int_0^{+\infty} e^{-st} \mathscr{F}_T(t) dt = \mathscr{L}[\mathscr{F}_T(t)](s).$$

A series expansion of this function

$$\mathscr{L}[\mathscr{F}_T(t)](s) = M_0 - M_1 s + M_2 \frac{s^2}{2!} - M_3 \frac{s^3}{3!} + \dots$$

gives the respective moments of the probability distribution function, e.g. the mean M_0 and variance M_1. We also look at the series expansion of the cumulant-generating function $g(-s)$, i.e. the logarithm of the Laplace transform of the flux, where s is in the Laplace domain. The cumulants are given by

$$c_n = \frac{\partial^n}{\partial s^n} g(-s) \bigg|_{s=0}.$$

We are particularly interested in the first and second cumulant. The first cumulant is

$$c_1 = \frac{\partial}{\partial s} [\log(\mathscr{L}[\mathscr{F}_T(t)](s))] \bigg|_{s=0},$$

which is the mean of the probability distribution, i.e. the residence time of the diffusion equation or the average time it takes a particle to pass a certain point. Also the second cumulant or the second derivative of the logarithm of the Laplace transform of the flux in $s = 0$, i.e. the variance of the logarithmic flux, is useful for interpreting the system. All of the characteristic values can be exactly calculated in function of the parameters in the above equations and will help to understand the diffusion in open textile structures.

3 Calculation of the characteristic times

To calculate the exact characteristic times the Laplace transformation of each of the three governing equations is taken. More details can be found in [3].
We use the notation $\mathscr{L}_f = \mathscr{L}[C_f(\rho,t)](s)$, $\mathscr{L}_y = \mathscr{L}[C_y(r,t)](s)$ and $\mathscr{L}_r = \mathscr{L}[C_r(x,t)](s)$ and introduce the function

$$\mathscr{B}_n(x,y) = \frac{I_n(\sqrt{st_f}\, x)}{I_1(\sqrt{st_f}\, y)} + (-1)^n \frac{K_n(\sqrt{st_f}\, x)}{K_1(\sqrt{st_f}\, y)},$$

which is a combination of modified Bessel functions of first and second kind, where $t_f = \frac{\rho_{\max}^2}{D_f}$ is the diffusion time.

For the fiber equation we define

$$X = \left[1 + \frac{p_f}{\sqrt{st_f}} \frac{\mathscr{B}_0(1, \frac{\rho_{\min}}{\rho_{\max}})}{\mathscr{B}_1(1, \frac{\rho_{\min}}{\rho_{\max}})}\right]^{-1}$$
$$= \frac{t_f}{2p_f}\left(1 - \frac{\rho_{\min}^2}{\rho_{\max}^2}\right) s + \cdots.$$

where $p_f = \frac{t_f}{t_{ff}}$ is the Páclet number for the fiber level and $t_{ff} = \frac{\rho_{\max}}{v_f}$ is the transport time.

This dimensionless X makes sure the BC on the right can be written in the form

$$\frac{D_f}{v_f} \frac{\partial}{\partial \rho} \left(\mathscr{L}_f - \frac{C_0}{s}\right) = X \left(\mathscr{L}_y - \frac{C_0}{s}\right),$$

which we can use to calculate $\mathscr{L}_f$ once we have $\mathscr{L}_y$ as

$$\mathscr{L}_f(\rho,r,s) = \frac{C_0}{s} + \left(\mathscr{L}_y(r,s) - \frac{C_0}{s}\right) \cdot \frac{\mathscr{B}_0\left(\frac{\rho}{\rho_{\max}}, \frac{\rho_{\min}}{\rho_{\max}}\right)}{\mathscr{B}_0\left(1, \frac{\rho_{\min}}{\rho_{\max}}\right) + \frac{\sqrt{st_f}}{p_f}\mathscr{B}_1\left(1, \frac{\rho_{\min}}{\rho_{\max}}\right)}.$$

For the yarn level the same strategy is followed taking the Laplace transformed equation and solving it for $\mathscr{L}_y(r,s)$, with

$$S_1 = 2\frac{p_f}{t_f}X = \frac{2v_f X}{\rho_{\max}}, \quad S_2 = 2\frac{p_f}{t_f}XC_0 = \frac{2v_f XC_0}{\rho_{\max}},$$

and

$$Y = \left[1 + \frac{I_0\left(\sqrt{(s+S_1)t_y}\right)}{I_1\left(\sqrt{(s+S_1)t_y}\right)} \frac{p_y}{\sqrt{(s+S_1)t_y}}\right]^{-1} = \frac{1}{2}\frac{t_y}{p_y}\left(2 - \frac{\rho_{\min}^2}{\rho_{\max}^2}\right)s + \cdots,$$

where we use the diffusion time, the Páclet number for the yarn level and the transport time for the yarn equation defined as

$$t_y = r_{\max}^2/D_y, \quad p_y = v_y r_{\max}/D_y = t_y/t_{fy}, \quad t_{fy} = r_{\max}^2/v_y.$$

The BC on the right can again be written as

$$\mathscr{L}_y(R_y,s) - \mathscr{L}_r(0,s) = Y\left(\frac{S_2}{s(s+S_1)} - \mathscr{L}_r(0,s)\right)$$

which allows to solve for $\mathscr{L}_y$ in function of $\mathscr{L}_r(0,s)$. This last term will be calculated by taking the Laplace transformation of the room PDE, which leads to

$$\mathscr{L}_r(x,s) = \frac{p_x \cosh\left(\sqrt{st_x}\left(1-\frac{x}{L}\right)\right) Y \left(\frac{S_2}{s(s+S_1)} - \mathscr{L}_r(0,s)\right)}{\sinh\left(\sqrt{st_x}\right)\sqrt{st_x}}, \tag{$\star$}$$

with S_1, S_2 and Y as above and the diffusion time $t_x = \frac{L^2}{D}$, transport time $t_{fx} = \frac{L}{v_x}$ and the Páclet number for the room level $p_x = \frac{t_x}{t_{fx}} = \frac{v_x L}{D}$. By setting $x = 0$ in ($\star$), we arrive at a linear, thus solvable, equation in $\mathscr{L}_r(0,s)$. Mind that we first need the solution for $\mathscr{L}_r$ to be able to calculate $\mathscr{L}_y$, which, on its turn, is needed for $\mathscr{L}_f$.

To calculate the characteristic times, i.e. the first and second moment, and the residence time of diffusion and the variance of the flux (the first and second cumulant of the system), we look at the fluxes of the solutions found above $\frac{\partial \mathscr{L}_f}{\partial \rho}$, $\frac{\partial \mathscr{L}_y}{\partial r}$ and $\frac{\partial \mathscr{L}_r}{\partial x}$.

For the zeroth, first and second moments we write the fluxes in their series expansion and look for the constant term, the coefficient of $-s$ and the coefficient of s^2 by differentiating and setting s equal to zero. We will do this for the most interesting interfaces in the model, that is the transition from one level to another.

When we look at concentration passing from the fiber level to the yarn level, $\rho = \rho_{\max}$, we can calculate the zeroth moment,

$$M_{0,f} = \frac{1}{4}\left(\frac{(2t_{fx}+t_{fy})C_0}{t_{fx}+t_{fy}}\right)\rho_{\max}.$$

For the yarn and room similar results are achieved. The transition from yarn to room, thus taking $r = R_y$ and $x = 0$ leads to

$$M_{0,y} = \frac{1}{2}\left(\frac{t_{fx}C_0}{t_{fx}+t_{fy}}\right)R_y,$$

where now in the numerator only the transport time in the room appears. For the room flux, which gives an idea of how the particles in the room are distributed, the zeroth moment is

$$M_{0,r} = \frac{1}{2}\left(\frac{t_{fy}C_0}{t_{fx}+t_{fy}}\right)L,$$

where in the nominator the dependence of the flux on the evaporation rate in the air gaps of the yarn becomes clear. Also for the first and second moments the same dependencies appear, but now in a quadratic relation, since a variance has been calculated. For example, for the flux in the room the first moment is

$$M_{1,r} = -\frac{\partial}{\partial s}\left(\frac{\partial \mathscr{L}_r}{\partial x}(-s)\right)\Big|_{s=0} = \frac{1}{2}\left(\frac{t_{fy}C_0}{(t_{fx}+t_{fy})^2}\right)L\left[\frac{(2t_{fx}+t_{fy})}{16}t_f + \frac{t_{fx}}{4}t_y + \frac{t_{fy}}{3}t_x + \frac{(2t_{fx}+t_{fy})}{4}t_{ff} + 2t_{fx}t_{fy}\right].$$

Analogous results are found for the second moments on fiber and yarn level,

$$M_{1,f} = -\frac{\partial}{\partial s}\left(\frac{\partial \mathscr{L}_f}{\partial \rho}(-s)\right)\Big|_{s=0},$$

$$M_{1,y} = -\frac{\partial}{\partial s}\left(\frac{\partial \mathscr{L}_y}{\partial r}(-s)\right)\Big|_{s=0},$$

where we need to stress that for the interesting transition from yarn to room (at $r = R_y$ and $x = 0$) these last two moments can be found in two ways resulting twice in the same expression. We can look at the series expansion of the derivatives of the fluxes $\mathscr{L}_y$ and $\mathscr{L}_r$ and calculate them for the position $r = R_y$ and $x = 0$, or we can look at the derivatives of the difference $(\mathscr{L}_y - \mathscr{L}_r)$, once representing the flux at the right boundary of the yarn $(r = R_y)$ and once representing the flux at the left boundary of the room $(x = 0)$.

In each of these first moments there is an expected dependence on the initial concentration and the denominator each time has the same structure, depending on the distance that should be travelled by the particle.

Even more interesting to look at are the cumulants, which represent the several times were the actual transition from one level to another happens. The cumulants c_1 (the mean of the flux, or thus the mean position in time where a particle passes at a certain position) and c_2 (the variance of the flux) can be found from the above calculated moments, using the chain rule for the cumulant-generating function:

$$\begin{aligned} c_{1,*} &= -\frac{\partial}{\partial s}\left(\log \frac{\partial \mathscr{L}_*}{\partial \bullet}\right)\bigg|_{s=0} = \frac{M_{1,*}}{M_{0,*}}, \\ c_{2,*} &= \frac{1}{2}\frac{\partial^2}{\partial s^2}\left(\log \frac{\partial \mathscr{L}_*}{\partial \bullet}\right)\bigg|_{s=0} = \left(\frac{M_{2,*}}{M_{0,*}}\right) - \left(\frac{M_{1,*}}{M_{0,*}}\right)^2, \end{aligned}$$

where $*$ stands for f, y or r and $\bullet$ for ρ, r or x, respectively.

For the fiber the first cumulant at $\rho = \rho_{\max}$, i.e. the residence time at the position where the AI leaves the fiber coating and evaporates to the yarn air gaps., is

$$\begin{aligned} c_{1,f} = {} & \frac{t_f}{16}\left(\frac{2t_{fx}+t_{fy}}{t_{fx}+t_{fy}}\right) \\ & - \frac{t_y}{4}\left(\frac{t_{fx}\left(2r^2(t_{fx}+t_{fy}) - R_y^2(2t_{fx}+t_{fy})\right)}{R_y^2(t_{fx}+t_{fy})(2t_{fx}+t_{fy})}\right) \\ & + \frac{t_x}{3}\left(\frac{t_{fx}t_{fy}}{(t_{fx}+t_{fy})(2t_{fx}+t_{fy})}\right) + \frac{t_{ff}}{4}\left(\frac{2t_{fx}+t_{fy}}{t_{fx}+t_{fy}}\right) \\ & + \frac{t_{fx}^2 t_{fy}}{(t_{fx}+t_{fy})(2t_{fx}+t_{fy})}. \end{aligned}$$

We get an expected dependence between the residence time and the fiber's diffusion time, or the time for a particle to travel over distance $\rho_{\max}$ via diffusion with diffusion coefficient D_f. In the coefficient of t_f the transport times t_{fx} and t_{fy} (the times it takes a particle to travel via evaporation in the room and yarn air gaps) are also likely to appear, since movement out of the fiber is controlled by the evaporation rate. It is also worth mentioning that the transport time of the room seems to be twice as sensitive as the transport time in the yarn air gaps. This is because of the dimension of the system ($d = 2$), which plays an important role in all coefficients, e.g. the $\frac{1}{16}$ in the first term. The coefficient of t_{fx} is always equal to d.

Also a dependence on t_y and t_x is present. The respective coefficients again show the same linear combination $(2t_{fx} + t_{fy})$ multiplied with the quadratic distance to travel which is present in all the terms. The coefficient of t_y has a factor t_{fy} which is logical when we bear in mind that this is the transport time for a particle to get from the coating to the air gaps by evaporation. The sign is negative because the concentration of AI present in the yarn air gaps inhibits this evaporation and the $\frac{1}{4}$ again comes from the system's dimensions. For the coefficient of t_x we only get both the transport times to travel inside of the yarn and in the room.

There is also a term in t_{ff}, the transport time in the fiber, with the same coefficient as t_f, the diffusion time, but four times as large.

The residence time at the transition point from yarn to room level, at $r = R_y$ and $x = 0$ is

$$\begin{aligned} c_{1,y} = c_{1,r} = {} & \frac{t_f}{16}\left(\frac{2t_{fx}+t_{fy}}{t_{fx}+t_{fy}}\right) + \frac{t_y}{4}\left(\frac{t_{fx}}{t_{fx}+t_{fy}}\right) \\ & + \frac{t_x}{3}\left(\frac{t_{fy}}{t_{fx}+t_{fy}}\right) + \frac{t_{ff}}{4}\left(\frac{2t_{fx}+t_{fy}}{t_{fx}+t_{fy}}\right) \\ & + \frac{t_{fx}t_{fy}}{t_{fx}+t_{fy}}. \end{aligned}$$

Again the same coefficients are present, i.e. $\frac{1}{16}$ for the term in t_f, $\frac{1}{4}$ for the terms in t_y and t_{ff} and $\frac{1}{3}$ for the term in t_y. The coefficient of t_{ff} again is four times as large as the one of t_f. Every term has a positive sign since there can only be a positive effect from each of the underlying levels. The recurring denominator is the combined effect of the transport times in the yarn and the room.

The second cumulants both are of the same form and represent quadratic times since they stand for variances of the flux distribution,

$$\begin{aligned} c_{2,*} = {} & \frac{1}{(t_{fx}+t_{fy})^2}\left[\frac{t_f}{16}\left(\frac{1}{48}a_1 + \frac{1}{2}a_2 t_y + \frac{1}{2}a_3 t_{ff} + 2a_4\right)\right. \\ & + \frac{t_y}{4}\left(\frac{1}{12}a_5 t_y + \frac{1}{2}a_6 t_{ff} + 2a_7\right) \\ & + \frac{t_x}{3}\left(\frac{1}{15}a_8 t_x + \frac{1}{8}a_9 t_f + \frac{1}{2}a_{10} t_y + \frac{1}{2}a_{11} t_{ff} + 2a_{12}\right) \\ & \left. + \frac{t_{ff}}{4}\left(\frac{1}{4}a_{13} + 2a_{14}\right) t_{ff} + t_{fx}^2 t_{fy}^2\right] \end{aligned}$$

The coefficients of the respective terms are completely similar as for the residence times and again can be attributed to the system's dimensions.

For a general pair dimension d the residence time for the room is

$$\begin{aligned} c_{1,r} = {} & \frac{t_f}{a}\frac{dt_{fx}+t_{fy}}{bt_{fx}+ct_{fy}} + \frac{t_y}{e}\frac{t_{fx}}{bt_{fx}+ct_{fy}} + \frac{ct_x}{3}\frac{t_{fy}}{bt_{fx}+ct_{fy}} \\ & + \frac{t_{ff}}{e}\frac{dt_{fx}+t_{fy}}{bt_{fx}+ct_{fy}} + c\frac{t_{fx}t_{fy}}{bt_{fx}+ct_{fy}} \end{aligned}$$

with coefficients a, b, c, and e

$$a = 4(d+2), \quad b = \frac{d^2}{4}, \quad c = \frac{d+2}{4}, \quad e = 4.$$

if d is not divisible by 4, and if d is divisible by 4 the coefficients are twice as large. These coefficients are also present in the other cumulants.

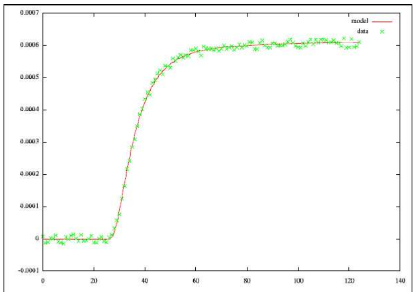
At these residence times the system reaches an equilibrium. In [3] the theoretical values were compared with these numerical solutions of the model. These numerical values are visible in the plot of the logarithmic concentration vs. the logarithmic time scale, Figure 1. The symbolic form calculated above now makes it possible to explain even further the accordance between both.

4 Inverse problem

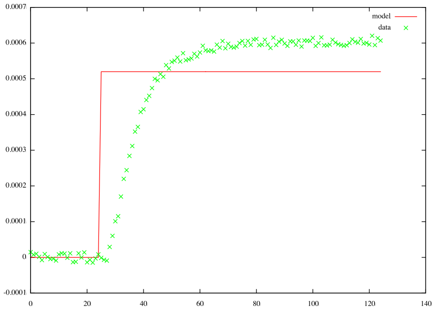
With the programming code utilized it is possible to use Gnuplot's fit command to calculate some inverse problems. Starting from an estimated initial value for the unknown parameter, the model will be fitted to experimental values of the forward problem using nonlinear least squares regression.
In practice measurements of the concentration of the AI in a room can be done, and the model could be fitted to these values. That way the right polymer may be chosen depending on the required diffusion coefficient in the coating and the initial concentration could be determined. It becomes possible to decide on the right composition of the textile, answering the questions of how many fibers are needed to get to the right surface/volume ratio, on its turn determining the needed evaporation rate. The inverse problem is using the same C-code of the 3 level diffusion system as the forward model. Although this does not work for all parameters due to high complexity of some of them and the dependencies between them, it is possible to estimate those of high impact.

For example it is possible to fit the initial concentration C_0 and the diffusion coefficient in the room D (in mm^2/s) starting for C_0 (in $\mathrm{mg}/\mathrm{mm}^3$) at an initial guess of 1.1 and for D at 1.1×10^{-5}. As data points we use the values optioned by the forward model with $C_0 = 1.234$ and $D = 2.345\times10^{-5}$ and a uniform error in $[-\frac{3}{2};\frac{3}{2}]\times10^{-5}$ is superimposed. We want to trace back the values for C_0 and D after fitting the inverse problem.
This is the case after 5 iterations with a root-mean-square of residuals (RMS) of 8.635×10^{-6}. The calculated set of parameters is $C_0 = 1.23401$ with an asymptotic SE of ±0.002 or 0.179% and $D = 2.33142\times10^{-5}$ with an SE of ±0.016 or 0.682%. The data fitting of this problem is shown in Figure 2(a).

However if we start from a very bad initial guess for D at 0.001×10^{-5} the inverse problem does not converge because a singular matrix is encountered, resulting in an estimation of 8388.17 for D. Using the least squares method of Gnuplot thus requires some a priori knowledge about the parameters, but our earlier analysis of characteristic times helps in selecting these. The model plot corresponding to this problem is found in Figure 2(b).



(a) Initial guess of 1.1 for both parameters.



(b) Initial guess of 1.1 for C_0 and 0.001 for D.

Figure 2: Inverse problem for determining initial concentration C_0 and diffusion coefficient in the room model D.

If for example we try to estimate D_f and D from data fitting, the inverse problem does not converge to the correct values. This is because the time frame wherein the AI's particles are moving through the fiber is much smaller than the time these particles are moving through the room. As a consequence we have too little data to be able to trace back the diffusion coefficient in the fiber. The diffusion coefficient in the room is however traceable and the models fit is not too bad after all. After 5 iterations the fit converged with an RMS of 8.816×10^{-6}. The fitted D was 2.34951×10^{-5} with an asymptotic SE of ±0.0145 or 0.616%. Parameter D_f however was fitted as 127.905 with asymptotic SE of ±1994 or 1559%. The correlation between these parameters is -0.048, so it is not responsible for the bad fit. The data fitting can be seen in Figure 3. Fitting can also be done for more than two parameters at a time. For example, it is possible to estimate the three parameters C_0, v_f and D. In the forward problem the values used were 1.234, 1 and 3.456×10^{-5}, respectively. Starting from 1.1, 0.5 and 1.1×10^{-5} it was possible to trace back these values after 5 iterations with an RMS of 9.243×10^{-6}. The estimated model solving the inverse problem is shown in Figure 4.

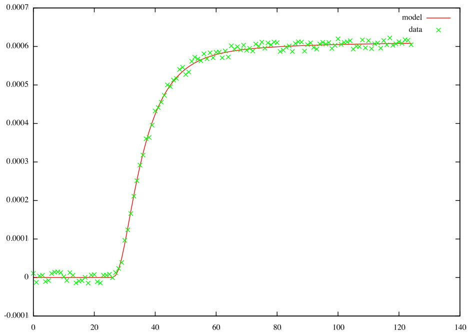


Figure 3: Inverse problem for determining diffusion coefficient in the fiber model D_f and diffusion coefficient in the room model D.

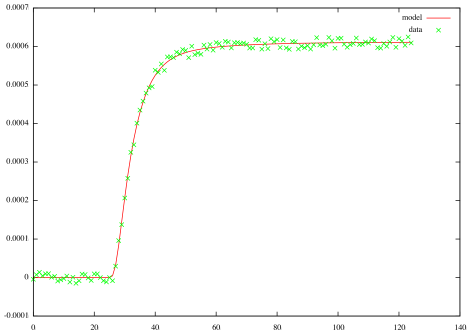


Figure 4: Inverse problem with three parameters for determining the initial concentration C_0, the evaporation speed v_f and the diffusion coefficient in the room model D.

5 Conclusion and future work

The characteristic times for the three level diffusion model were calculated and symbolically analyzed. The present coefficients show the dependence between the several diffusion and transport times and we were able to explain them in a physical way. This gives a proof for the correspondence between the calculated values and the visible transition times on the plot of the logarithmic concentration in function of the logarithmic time in [3].
Several inverse problems were solved using the Levenberg-Marquardt algorithm giving a first approach to use the developed model in practice. Based upon these results we have more knowledge of which parameters can be estimated at the same time, and which rather should be tested via chemical experiments. Especially the fiber diffusion coefficient is hard to estimate because of the small time scale where the AI is present in the fiber only. Experimental values now could be used to answer the question of which textile, coating and AI should be used to give the best practical results.

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