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Characteristic times for multiscale diffusion of active ingredients in coated textiles

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ABSTRACT

A three-scale approach for textile models was given in [5]: a one-dimensional fiber model and a room model, with a meso-level in between, which is the yarn scale. To analyze and simplify the model, its characteristic times are investigated here. At these times the fiber and yarn model and the yarn and room model, respectively, tend to reach a partial equilibrium concentration. The identification of these characteristic times is key to reducing the model to its variously scaled components when simplifying it.

1. Introduction

We focus on the diffusion of a substance to the outer boundary of textiles. The fibers used to construct this fabric are coated with 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 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…).

The application in mind has the purpose to track the diffusion of an active component released by the fibers of an open textile structure, like a woven scrim, e.g. a gauze bandage. Models and algorithms for this application were based on [1–4] and discussed in [5,6] where a meso-level model that describes the release of the active component in the yarn cross-section is included in between the standard fiber model and the room model. Upscaling from one level to another is done by volume averaging or overlapping domain decomposition (future work). Implementation was done in the C language using lsoda, [7].

2. Characteristic times for the three-level diffusion

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

$$\begin{cases} \dfrac{\partial C_f(\rho,t)}{\partial t} = \dfrac{1}{\rho}\dfrac{\partial}{\partial \rho}\left(\rho D_f \dfrac{\partial C_f(\rho,t)}{\partial \rho}\right), & \rho \in [\rho_{\min}, \rho_{\max}] \quad \text{(a)} \\ \dfrac{\partial C_y(r,t)}{\partial t} = \dfrac{1}{r}\dfrac{\partial}{\partial r}\left(r \dfrac{D_y}{\tau_y}\dfrac{\partial C_y(r,t)}{\partial r}\right) + \dfrac{1}{\epsilon}\Gamma_{\text{in}}(r,t), & r \in [0, R_y] \quad \text{(b)} \\ \dfrac{\partial C_r(x,t)}{\partial x} = \dfrac{\partial}{\partial x}\left(D \dfrac{\partial C_r(x,t)}{\partial x}\right), & x \in [0, L] \quad \text{(c)} \end{cases} \tag{1}$$

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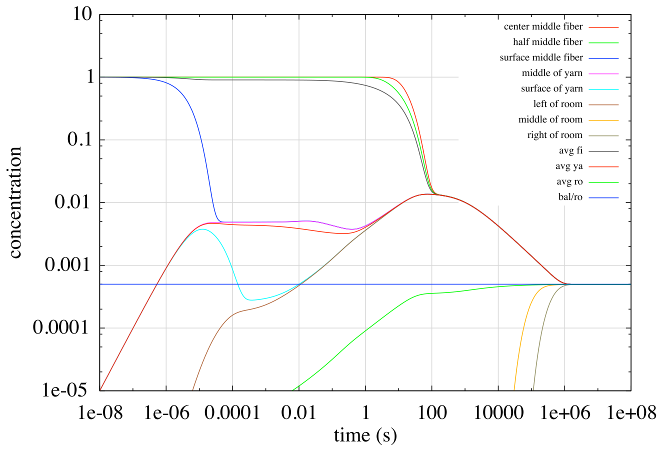

Fig. 1. Log–log plot of the concentrations in function of time for the data (49).

with a homogeneous Neumann BC at the left boundaries and an evaporation flux at the right boundaries for the fiber and yarn model (1)(a) and (b):

$$\frac{\partial C_f}{\partial \rho}(0,t) = 0, \qquad -D_f \frac{\partial C_f}{\partial \rho}(\rho_{\max}, t) = v_f (C_f(\rho_{\max}, t) - C_y(r,t)), \tag{2}$$

$$\frac{\partial C_y}{\partial r}(0,t) = 0, \qquad -D_y \frac{\partial C_y}{\partial r}(R_y, t) = v_y (C_y(R_y, t) - C_r(0,t)). \tag{3}$$

For the room model (1)(c) a homogeneous Neumann BC is present at the right boundary and at the left boundary there exists an evaporation flux coming from the concentration in the yarn evaporating to the room:

$$D\frac{\partial C_r}{\partial x}(0,t) = \alpha_{yr} v_x (C_r(0,t) - C_y(R_y,t)), \qquad \frac{\partial C_r}{\partial x}(L,t) = 0. \tag{4}$$

In the above system of Eqs. (1) the subscripts f, y and r stand for a quantity in the fiber, yarn and room respectively, C represents the concentration of the AI, D is the diffusion coefficient, v is the evaporation speed and α_{yr} is a constant of proportion for the evaporation from yarn to room. The constants τ and ϵ are the tortuosity and porosity of the textile used, respectively. The term Γ_{in} in (1)(b) is the volume averaged condensation/evaporation rate and is calculated as $\alpha_{fy} v_f (C_f(\rho_{\max}) - C_y(r))$ with α_{fy} the surface/volume ratio of the fiber.

At certain points in time equilibrium is essentially reached between the three models. Plotting the logarithmic concentration against the logarithmic time scale (Fig. 1) shows that, for standard parameters, after a rather short time (approximately 5 s) the yarn and room concentrations coincide, the fiber and yarn concentrations coincide at 100 s and after approximately 1×10^6 s all concentrations reach the same value.

As an upscaling method volume averaging is used, the averaged outcome of one model serves as boundary conditions for the other.

These moments in time where equilibria are reached correspond with the systems' characteristic times. These are the time scales τ for a particle to travel over a distance x and on average these are given by $\tau^d \approx x^2/D$ for diffusion and $\tau^e = x/v$ for evaporation.

As a first estimation of these times one may calculate them by this rule of thumb for each of the levels as

$$\begin{cases} \tau_f^d = \dfrac{(\Delta\rho)^2}{D_f}, & \tau_f^e = \dfrac{\Delta\rho}{v_{\text{fiya}}}, \\ \tau_y^d = \dfrac{(\Delta r)^2}{D_y}, & \tau_y^e = \dfrac{\Delta r}{v_{\text{yaro}}}, \end{cases} \tag{5}$$

where v_{fiya} is the evaporation speed for the AI from the fiber surface to the yarn gaps, v_{yaro} is the evaporation speed for the AI from the yarn surface to the room, $\Delta\rho$ and Δr are the thickness of the fiber and yarn cross-section, and D_f and D_y are the respective diffusion coefficients of the first two levels.

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

$$M_x(-s) = E_x(e^{-sT}) = \int_0^{+\infty} e^{-st}\mathcal{F}(x,t)dt = \mathcal{L}[\mathcal{F}(x,t)](s), \tag{6}$$