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Characteristic times in a three scale model with overlapping domain decomposition

Tineke Goessens *, Denis Constales

Department of Mathematical Analysis, Research Group NaM², Faculty of Engineering and Architecture, Ghent University, Krijgslaan 281 - S22, Ghent, Belgium

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ABSTRACT

A three-scale diffusion model for textiles was given in Goessens et al. (2015): consisting of a fiber, yarn and room model. To analyze and simplify the model, its characteristic times were investigated in Goessens et al. (2015) [8, 9]. At these times the fiber and yarn model, and the yarn and room model, respectively, tend to reach a partial equilibrium concentration. Here an addition will be made to the model based upon the previous work. An overlap zone is considered between the yarn and room level. Then the overlapping domain decomposition technique is used to calculate the exchange of active ingredient from one level to another in this zone. The mass balance for the system with the overlap zone is calculated and tested in C-language.

1. Introduction

We consider textiles wherein the fibers 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 that first diffuse to the outer boundary of the textile and from there on evaporate to the surrounding air. 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 [5–7]. The model consists of three levels, starting from the micro level of the fibers. Next the AI is diffusing to the yarn meso-level, considering the concentration build up in a cross section of a yarn made out of fibers. Afterwards the AI is moving further to the outer boundary of the textile and to the surrounding air represented by the room level. Upscaling from one level to another can be done using volume averaging and/or the overlapping domain decomposition technique. In [8,9] the characteristic times were calculated for a model where only volume averaging was used for upscaling. Now an addition is made using an overlap zone where the exchange of AI from one level to another is happening. Solving the standard diffusion equations we know which concentration is coming into this overlap zone at the left boundary, and we want to know how much is going to the next level after upscaling in the overlap zone. Therefore we will investigate the relation between the Laplacian of both the concentration and the flux at the left and right boundary of the overlap zone. That way we can express the characteristic times, i.e. the moments and cumulants of the system in the overlap zone where concentration is averaged out in one level in function of the other level. This gives an idea of how a perfect exchange of AI would look, or which properties of the textile can influence this movement of substances to go faster or slower. Also it will be possible to implement the relation between the left and right boundary of the overlap zone in the already existing C-code, which is using `lsoda` to solve the system. The original C-code will be extended with the possibility of using domain decomposition for upscaling. For test purposes the conservation of mass is recalculated for the new setting.

* Corresponding author.
E-mail address: tineke.goessens@ugent.be (T. Goessens).

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We will calculate the relation between the left concentration and flux in function of the concentration and flux at the right boundary. First we will do this for the simple one-dimensional case, afterwards for general dimensions d_1 and d_2 of the two levels. Furthermore we will calculate these relations for a specific concentration function.

Based upon this, it becomes possible for future research to investigate what will happen if the setting is changing, e.g. a different positioning of the levels and consequently the overlap zone, and what changes if we use the actual concentration instead of the volume average in the overlapping zone equations.

2. One-dimensional overlap zone

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

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

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 (1)(b):

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

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

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:

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

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_f, D_y and D are the respective diffusion coefficients, which are assumed to be constant, v_{fy} and v_{yr} are the evaporation speeds from fiber to yarn and from yarn to room level resp. α_{yr} is a constant of proportion for the evaporation from yarn to room level. The constant τ is the tortuosity of the textile used. The term Γ_{in} in (1)(b) is the volume averaged condensation/evaporation rate and is calculated as $\alpha_{fy}v_{fy}(C_f(\rho_{\max}) - C_y(r))$ with α_{fy} the surface/volume ratio of the fiber.

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

As described in [5] we will extend the domain of the yarn model with an overlap zone Ω_o, i.e. a part of the domain of the yarn will coincide with the domain of room model. There the PDE above is adapted with an extra sink-term $\Gamma_{out}(t,\Omega_o)$ which stands for the amount of AI that is removed from the meso-level due to diffusion to the macro-level. Also the BC at the right boundary is changed to a homogeneous Neumann BC.

We are interested in the exchange of AI in this overlap zone, particularly the relation between the AI at the left boundary of Ω_o and that at its outer right boundary:

$$\begin{pmatrix} \mathcal{L}C_1 \\ \mathcal{L}F_1 \end{pmatrix}_{R_{1\ell}} = \underbrace{\begin{pmatrix} a & b \\ c & d \end{pmatrix}}_{\mathsf{A}} \begin{pmatrix} \mathcal{L}C_2 \\ \mathcal{L}F_2 \end{pmatrix}_{R_{2r}},$$

where we used the Laplace transforms of the concentration of the AI in level 1 and 2, C_1 and C_2, and the Laplace transformed flux of these concentrations, F_1 and F_2. We denote the left and right boundary of the overlap zone in the domain of level i by $R_{i\ell}$ and R_{ir}. We will work with the Laplace transformation of the quantities to be able to calculate the characteristic times of the model as explained in [9,8].

For illustrative purpose we will explain the method used in the following sections with the one-dimensional diffusion in one level from $R = 0$ to $R = L$. The relation between the left and right concentration and flux is then given by

$$\begin{pmatrix} \mathcal{L}C \\ \mathcal{L}F \end{pmatrix}_{R=0} = \begin{pmatrix} \cosh\left(\sqrt{\dfrac{L^2s}{D}}\right) & \dfrac{1}{\sqrt{sD}}\sinh\left(\sqrt{\dfrac{L^2s}{D}}\right) \\ \sqrt{sD}\sinh\left(\sqrt{\dfrac{L^2s}{D}}\right) & \cosh\left(\sqrt{\dfrac{L^2s}{D}}\right) \end{pmatrix} \begin{pmatrix} \mathcal{L}C \\ \mathcal{L}F \end{pmatrix}_{R=L},$$

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according to the PDE

$$\frac{\partial C}{\partial t}(x,t) = D\frac{\partial^2 C}{\partial x^2}(x,t), \quad x \in [0,L].$$

To get to this matrix the equation is Laplace transformed

$$s\mathcal{L}C(x,s) = D\frac{\partial^2 \mathcal{L}C(x,s)}{\partial x^2},$$

and solved

$$\mathcal{L}C(x,s) = A\cosh\left(\sqrt{\frac{sx^2}{D}}\right) + B\sinh\left(\sqrt{\frac{sx^2}{D}}\right).$$

Substituting $x = 0$ and $x = L$ in this solution and $(-D$ times) it's derivative with respect to x for the flux gives 4 equations, and 6 unknowns. Solving this system to $\mathcal{L}C(0,s)$ and $\mathcal{L}F(0,s)$ in function of $\mathcal{L}C(L,s)$ and $\mathcal{L}F(L,s)$ gives the above matrix. For the more complex systems of equations this exchange matrix A will need further simplification using both Maple and calculations by hand.

We will now introduce the overlap zone equations for two overlapping levels in one dimension as

$$\begin{cases} \dfrac{\partial C_1}{\partial t} = D\dfrac{\partial^2 C_1}{\partial x^2} + k\left(\bar{C_2} - C_1\right), \\ \dfrac{\partial C_2}{\partial t} = D\dfrac{\partial^2 C_2}{\partial x^2} + k\left(\bar{C_1} - C_2\right), \end{cases}$$

where $\bar{C_1}$ and $\bar{C_2}$ stand for the mean concentration of AI in domain 1 and 2, resp., k is a constant of proportionality corresponding to the rate of exchange between both levels.

The boundary conditions are

$$F_1|_{R_{1r}} = 0, \qquad F_2|_{R_{2l}} = 0.$$

Taking the Laplace transform of these equations and solving for $\mathcal{L}C_1$ and $\mathcal{L}C_2$ gives

$$\begin{cases} \mathcal{L}C_1 = A\cosh\left(x\sqrt{\dfrac{(s+k)}{D}}\right) + B\sinh\left(x\sqrt{\dfrac{(s+k)}{D}}\right) + \dfrac{k}{s+k}\mathcal{L}\bar{C_2}, \\ \mathcal{L}C_2 = \tilde{A}\cosh\left(x\sqrt{\dfrac{(s+k)}{D}}\right) + \tilde{B}\sinh\left(x\sqrt{\dfrac{(s+k)}{D}}\right) + \dfrac{k}{s+k}\mathcal{L}\bar{C_1}, \end{cases}$$

and makes it possible to look at the left and right boundaries of both domains. We will denote $\mathcal{L}C_i$ and $\mathcal{L}F_i$ at the left boundary of domain i as $\mathcal{L}C_{i\ell}$ and $\mathcal{L}F_{i\ell}$. This leads to ten equations each giving an expression for the ten unknowns $\mathcal{L}C_{1\ell}$, $\mathcal{L}F_{1\ell}$, $\mathcal{L}C_{2\ell}$, $\mathcal{L}F_{2\ell}$, $\mathcal{L}C_{1r}$, $\mathcal{L}F_{1r}$, $\mathcal{L}C_{2r}$, $\mathcal{L}F_{2r}$, $\mathcal{L}\bar{C_1}$ and $\mathcal{L}\bar{C_2}$. However according to the BC's we put $\mathcal{L}F_{1r} = \mathcal{L}F_{2\ell} = 0$. Furthermore we have the unknowns A, B, $\tilde{A}$ and $\tilde{B}$. In total we end up with 10 equations for 12 unknowns, which leads to a solution with two degrees of freedom. Solving this system for all unknowns except for $\mathcal{L}C_{2r}$ and $\mathcal{L}F_{2r}$ leads to a solution in function of the latter two. In particular we are interested in the solutions for $\mathcal{L}C_{1\ell}$ and $\mathcal{L}F_{1\ell}$, in order to be able to calculate the matrix of interest A,

$$\mathsf{A} = \begin{pmatrix} \dfrac{(2k+s)s}{k(k+s)}T + \dfrac{k}{k+s} & \dfrac{(2k+s)s}{Lk(k+s)^2}T^2 + \dfrac{2k}{L(k+s)^2}T - \dfrac{k}{L(k+s)^2} \\ \dfrac{(2k+s)sL}{k} & \dfrac{(2k+s)s}{k(k+s)}T + \dfrac{k}{k+s} \end{pmatrix},$$

where $T = \coth\left(\frac{\sqrt{k+s}\,L}{\sqrt{D}}\right)\frac{\sqrt{k+s}\,L}{\sqrt{D}}$. The diagonal entries are equal which means both concentration and flux of the AI at the left boundary of domain 1 have the same dependence on concentration and flux respectively at the right boundary of domain 2. If there was a perfect exchange between the two overlap zones this matrix becomes ($\lim_{k\to\infty}$)

$$\mathsf{A} = \begin{pmatrix} 1 & 0 \\ 2Ls & 1 \end{pmatrix},$$

where we see that the Laplace transformed concentration in both levels is the same at both boundaries and the flux changes linearly with this concentration. The system thus acts as if there was only one level with double length. If we should want to calculate the first moment of the system i.e. the mean position in time when a particle passes a certain position in space, we are interested in the above matrix with s equal to zero

$$\mathsf{A} = \begin{pmatrix} 1 & \dfrac{2T(0)-1}{kL} \\ 0 & 1 \end{pmatrix},$$

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where we notice that the first moment and consequently also the residence time of the first level is the same as that of the second system.

In a more general setting the diffusion coefficients of the two levels are not equal, and the exchange rate decreases with the length of the overlap zone, which also doesn't need to be equal in a more general case,

$$\begin{cases} \dfrac{\partial C_1}{\partial t} = D_1 \dfrac{\partial^2 C_1}{\partial x^2} + \dfrac{k}{L_1}\left(\bar{C}_2 - C_1\right), \\ \dfrac{\partial C_2}{\partial t} = D_2 \dfrac{\partial^2 C_2}{\partial x^2} + \dfrac{k}{L_2}\left(\bar{C}_1 - C_2\right). \end{cases}$$

Following the same technique as above the needed matrix then becomes

$$\mathsf{A} = \begin{pmatrix} \dfrac{(L_1(k+L_2 s)+L_2 k)\,s}{(k+L_1 s)k} T_1 + \dfrac{k}{k+L_1 s} & \dfrac{(L_1(k+L_2 s)+L_2 k)\,s}{(k+L_1 s)(k+L_2 s)k} T_1 T_2 \\ & + \dfrac{k}{(k+L_1 s)(k+L_2 s)}(T_1+T_2-1) \\ \dfrac{(L_1(k+L_2 s)+L_2 k)\,s}{k} & \dfrac{(L_1(k+L_2 s)+L_2 k)\,s}{(k+L_2 s)k} T_2 + \dfrac{k}{k+L_2 s} \end{pmatrix}.$$

Here D_i and L_i are the diffusion coefficient and length of the overlap zone in the domain of level i and $T_i = \coth\left(\frac{\sqrt{L_i s+k}}{\sqrt{D_i}}\sqrt{L_i}\right)\frac{\sqrt{L_i s+k}}{\sqrt{D_i}}\sqrt{L_i}$.

3. Two-dimensional cylindrical and one-dimensional Cartesian diffusion

The application in mind is described using three levels of diffusion, Eq. (1). The overlap zone is situated between the last two levels, i.e. the yarn level which is described by a two-dimensional cylindrical equation and the room level which is described by a one-dimensional Cartesian equation. In this overlap zone the governing equations of Eq. (1) are adapted to

$$\begin{cases} \dfrac{\partial C_1}{\partial t} = \dfrac{D_1}{r}\dfrac{\partial}{\partial r}\left(r\dfrac{\partial C_1}{\partial r}\right) + \dfrac{q}{\pi\left(R_2^2 - R_1^2\right)h}\left(\bar{C}_2 - C_1\right), \\ \dfrac{\partial C_2}{\partial t} = D_2 \dfrac{\partial^2 C_2}{\partial x^2} + \dfrac{q}{AL}\left(\bar{C}_1 - C_2\right), \end{cases}$$

where R_1 and R_2 are the outer left and outer right boundary of the overlap zone of the yarn cylinder, h is the height of a yarn cylinder, A is the area of the room's wall perpendicular to the dimension, L is the length of the overlap zone of the room in the direction of the dimension, D_1 and the D_2 are the respective diffusion coefficients. The proportionality constant q stands for the discharge of the concentration in $\frac{\mathrm{m}^3}{\mathrm{s}}$. The Laplace transformed system reads

$$\begin{cases} -\left(s + \dfrac{q}{\pi\left(R_2^2 - R_1^2\right)h}\right)\mathcal{L}C_1 + \dfrac{D_1}{r}\dfrac{\partial}{\partial r}\left(r\dfrac{\partial \mathcal{L}C_1}{\partial r}\right) = -\dfrac{q}{\pi\left(R_2^2 - R_1^2\right)h}\mathcal{L}\bar{C}_2, \\ -\left(s + \dfrac{q}{AL}\right)\mathcal{L}C_2 + D_2\dfrac{\partial^2}{\partial x^2}\left(\mathcal{L}C_2\right) = -\dfrac{q}{AL}\mathcal{L}\bar{C}_1, \end{cases}$$

with its solution

$$\begin{cases} \mathcal{L}_1(r) = A_1\, \mathcal{I}_0\left(\sqrt{\dfrac{V_1 s+q}{V_1 D_1}}r\right) + B_1\, \mathcal{K}_0\left(\sqrt{\dfrac{V_1 s+q}{V_1 D_1}}r\right) + \dfrac{q}{V_1 s+q}\mathcal{L}_{2m}, \\ \mathcal{L}_2(x) = A_2 \cosh\left(\sqrt{\dfrac{ALs+q}{ALD_2}}x\right) + B_2 \sinh\left(\sqrt{\dfrac{ALs+q}{ALD_2}}x\right) + \dfrac{q}{ALs+q}\mathcal{L}_{1m}, \end{cases}$$

where $V_1 = \pi\left(R_2^2 - R_1^2\right)h$, $\mathcal{L}_i$ denotes $\mathcal{L}C_i$ and $\mathcal{L}_{im}$ stands for $\mathcal{L}\bar{C}_i$, $i = 1, 2$, $\mathcal{I}_0$ and $\mathcal{K}_0$ are the modified Bessel functions of the first and second kind of order zero.

Using the boundary conditions for the flux $-D_1\left.\frac{\partial \mathcal{L}_1}{\partial r}\right|_{r=R2} = 0$ and $-D_2\left.\frac{\partial \mathcal{L}_2}{\partial x}\right|_{x=0} = 0$ we are able to rewrite these solutions and eliminate two unknowns:

$$\begin{cases} \mathcal{L}_1(r) = \tilde{A}_1 \mathcal{B}_{0,1}\left(r, R_2, \dfrac{V_1 s+q}{V_1 D_1}\right) + \dfrac{q}{V_1 s+q}\mathcal{L}_{2m}, \\ \mathcal{L}_2(x) = A_2 \cosh\left(\sqrt{\dfrac{ALs+q}{ALD_2}}x\right) + \dfrac{q}{ALs+q}\mathcal{L}_{1m}, \end{cases}$$

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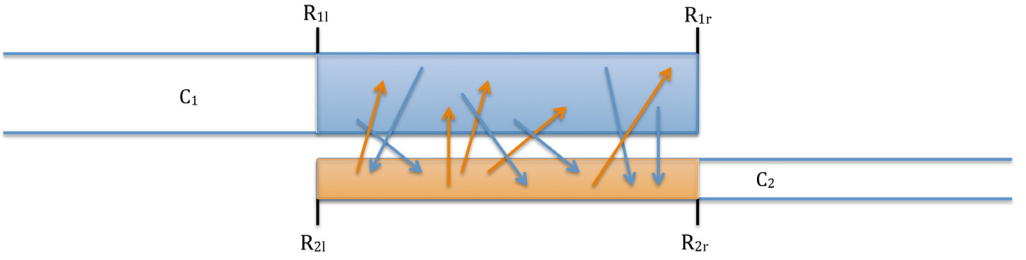

Fig. 1. Overlap zone of two levels in the model.

with

$$\mathcal{B}_{n,m}(r_1, r_2, C) = (-1)^{|n-m|+1} \frac{\mathcal{I}_n\left(\sqrt{C}r_1\right)}{\mathcal{I}_m\left(\sqrt{C}r_2\right)} + \frac{\mathcal{K}_n\left(\sqrt{C}r_1\right)}{\mathcal{K}_m\left(\sqrt{C}r_2\right)},$$

a combination of $\mathcal{I}_n$ and $\mathcal{K}_n$, i.e. the modified Bessel functions of first and second kind of order n.

Then for $s = 0$ the aimed matrix is

$$\mathsf{A} = \begin{pmatrix} 1 & \dfrac{\sqrt{AL}}{\sqrt{D_2 q}} \dfrac{1}{\tanh\left(\sqrt{\frac{qL}{AD_2}}\right)} - \dfrac{A}{q} + \dfrac{A\sqrt{V_1}}{\sqrt{qD_1}R_1 h} \dfrac{\mathcal{B}_{0,1}\left(R_1, R_2, \frac{q}{V_1 D_1}\right)}{\mathcal{B}_{1,1}\left(R_1, R_2, \frac{q}{V_1 D_1}\right)} \\ \left.\dfrac{s\,(ALV_1 s + ALq + V_1 q)}{hR_1 q}\right|_{s=0} = 0 & \dfrac{A}{hR_1} \end{pmatrix}.$$

It is clear that the law of conservation of mass is satisfied since we get that $hR_1 \mathcal{L}F_{1\ell} = A\mathcal{L}F_{2r}$.

For the limit q to infinity, i.e. the perfect exchange of material as if there were no two separate levels, the matrix is

$$\mathsf{A} = \begin{pmatrix} 1 & 0 \\ \dfrac{s\,(AL + V_1)}{hR_1} & \dfrac{A}{hR_1} \end{pmatrix}.$$

4. Multidimensional diffusion in both levels

We now will investigate the most general setting possible, where both the yarn and room level have different given dimensions d_1 and d_2 and different diffusion coefficients D_1 and D_2. We suppose that both overlap zones are oriented as in Fig. 1.

The governing equations for the two overlapping levels are

$$\begin{cases} \dfrac{\partial C_1}{\partial t} = \dfrac{D_1}{r^{d_1-1}} \dfrac{\partial}{\partial r}\left(r^{d_1-1} \dfrac{\partial C_1}{\partial r}\right) + \dfrac{q}{V_{d_1} W_{d_1} (\Delta r^{d_1})} \left(\bar{C}_2 - C_1\right), \\ \dfrac{\partial C_2}{\partial t} = \dfrac{D_2}{r^{d_2-1}} \dfrac{\partial}{\partial r}\left(r^{d_2-1} \dfrac{\partial C_2}{\partial r}\right) + \dfrac{q}{V_{d_2} W_{d_2} (\Delta r^{d_2})} \left(\bar{C}_1 - C_2\right), \end{cases}$$

where V_{d_i} is the volume of the overlap zone, W_{d_i} is the codimension such that the total volume is that of the unit ball, q is the exchange rate of AI from one level to another. In this setting the volume averages are calculated as

$$\bar{C}_i = \frac{d_i}{\Delta r^{d_i}} \int_{R_{\min}}^{R_{\max}} C_i r^{d_i - 1}\, \mathrm{d}\, r, \quad i = 1,\ 2,\ 3.$$

This system of equations is Laplace transformed and solved as

$$\begin{cases} \mathcal{L}_1(r, s) = \dfrac{A_1}{r^{\frac{d_1}{2}-1}}\, \mathcal{I}_{\frac{d_1}{2}-1}\left(\sqrt{\dfrac{s+q_1}{D_1}} r\right) + \dfrac{B_1}{r^{\frac{d_1}{2}-1}}\, \mathcal{K}_{\frac{d_1}{2}-1}\left(\sqrt{\dfrac{s+q_1}{D_1}} r\right) + \dfrac{q_1}{s+q_1} \mathcal{L}_{2m}(s), \\ \mathcal{L}_2(r, s) = \dfrac{A_2}{r^{\frac{d_2}{2}-1}}\, \mathcal{I}_{\frac{d_2}{2}-1}\left(\sqrt{\dfrac{s+q_2}{D_2}} r\right) + \dfrac{B_2}{r^{\frac{d_2}{2}-1}}\, \mathcal{K}_{\frac{d_2}{2}-1}\left(\sqrt{\dfrac{s+q_2}{D_2}} r\right) + \dfrac{q_2}{s+q_2} \mathcal{L}_{1m}(s), \end{cases}$$

where $q_i = \frac{q}{V_{d_i} W_{d_i} (\Delta r^{d_i})}$, $\mathcal{L}_i$ denotes $\mathcal{L}C_i$ and $\mathcal{L}_{im}$ stands for $\mathcal{L}\bar{C}_i$, $R_{i\ell} < r < R_{ir}$, the functions $\mathcal{I}_{\frac{d_i}{2}-1}$ and $\mathcal{K}_{\frac{d_i}{2}-1}$ are the Bessel functions of first and second kind of order $\frac{d_i}{2} - 1$, $i = 1, 2$. The matrix A again uses the combination of Bessel functions

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$\mathcal{B}_{n,m}$ for $s = 0$,

$$\mathsf{A} = \begin{pmatrix} 1 & \dfrac{R_{2r}^{d_2-1}}{R_{1\ell}^{d_1-1}} \dfrac{d_2}{d_1 q_2} \dfrac{\sqrt{q_1}}{\sqrt{D_1}} \dfrac{\left(\Delta r^{d_1}\right)}{\left(\Delta r^{d2}\right)} \dfrac{\mathcal{B}_{\frac{d_1}{2}+1,\frac{d_1}{2}}\left(R_{1\ell}, R_{1r}, \frac{q_1}{D_1}\right)}{\mathcal{B}_{\frac{d_1}{2},\frac{d_1}{2}}\left(R_{1\ell}, R_{1r}, \frac{q_1}{D_1}\right)} \\ & + \dfrac{d_2}{q_2 R_{2r}} \left(1 + \left(\dfrac{R_{1r}}{R_{1\ell}}\right)^{d_1} \dfrac{R_{2r}^{d_2}}{\left(\Delta r^{d_2}\right)}\right) - \dfrac{1}{\sqrt{q_2 D_2}} \dfrac{\mathcal{B}_{\frac{d_2}{2}+1,\frac{d_2}{2}}\left(R_{2r}, R_{2\ell}, \frac{q_2}{D_2}\right)}{\mathcal{B}_{\frac{d_2}{2},\frac{d_2}{2}}\left(R_{2r}, R_{2\ell}, \frac{q_2}{D_2}\right)} \\ 0 & \dfrac{V_{d_2} W_{d_2} d_2 R_{2r}^{d_2-1}}{V_{d_1} W_{d_1} d_1 R_{1\ell}^{d_1-1}} \end{pmatrix}.$$

The limit situation for perfect exchange of the active ingredient corresponds to the matrix

$$\mathsf{A} = \begin{pmatrix} 1 & 0 \\ \dfrac{sR_{1\ell}}{d_1}\left(\dfrac{\left(\Delta r^{d_2}\right) V_{d_2} W_{d_2}}{R_{1\ell} V_{d_1} W_{d_1}} + \left(\dfrac{R_{1r}}{R_{1l}}\right)^{d_1} - 1\right) & \dfrac{V_{d_2} W_{d_2} d_2 R_{2r}^{d_2-1}}{V_{d_1} W_{d_1} d_1 R_{1\ell}^{d_1-1}} \end{pmatrix}.$$

Both mentioned matrices for general dimensions are according with the above results for more specific dimensions.

5. Application

With the above matrices it is possible to calculate the exchange of concentration of the active ingredient for specific fluxes and functions at the left boundary of the overlap zone of one of the domains. For example if we take the Dirac-function for the concentration or the flux at one of the boundaries, respectively we can easily calculate the unknown concentration and/or flux at the other boundary, see Table 1. Each of these values can be helpful in the determination of the characteristic times of the system. We are particularly interested in the Area Under Curve (AUC), i.e. the concentration at $s = 0$, the first moment, i.e. the mean flux and the first cumulant, i.e. the residence time. For the first setting $s = 0$ in $\frac{1}{\mathsf{A}_{11}}$ gives the Laplace transform of the concentration at the right boundary of the second domain, i.e. the AUC for this domain, which is the Dirac-function itself. Since at the left boundary of the first domain there is a peak of concentration and the system is isolated at the right boundary of the second domain, a concentration build up happens until everything stabilizes to the equilibrium concentration at the right boundary, equaling the initial concentration $C_{1\ell}$. The second case lets us calculate the mean flux and the residence time if the concentration of AI is taken away immediately at the right boundary of the second domain. The mean flux, i.e. the first moment, equals $\frac{V_{d_1} W_{d_1} d_1 R_{1\ell}^{d_1-1}}{V_{d_2} W_{d_2} d_2 R_{2r}^{d_2-1}}$, the residence time is

$$\frac{q_1+q_2}{q_1 q_2}\left(\left(\frac{R_{2\ell}}{R_{2r}}\right)^{d_2} - \frac{R_{2r}}{d_2}\sqrt{\frac{q_2}{D_2}} \frac{\mathcal{B}_{\frac{d_2}{2}+1,\frac{d_2}{2}}\left(R_{2r}, R_{2\ell}, \frac{q_2}{D_2}\right)}{\mathcal{B}_{\frac{d_2}{2},\frac{d_2}{2}}\left(R_{2r}, R_{2\ell}, \frac{q_2}{D_2}\right)}\left[\left(\frac{R_{2\ell}}{R_{2r}}\right)^{d_2} - 1\right]\right) - \frac{1}{q_1}.$$

The third case gives the AUC for the first domain. This again is equal to the Dirac-function. The fourth case also can be used to calculate the first moment and cumulant of the system with a similar result as above but with indices 1 and 2 interchanged. Once the dimensions and other parameters of the system are known, we can numerically calculate the characteristic times using these formulas.

6. Adaptation of C-code and mass balance in time domain

The system of Eqs. (1) was programmed in C code and solved using `lsoda` and `fortran77`. Using the input of Table 2 for the variables the plot in Fig. 2 was generated.

To solve this system numerically the ρ-domain was divided into n_f intervals, the r-domain into n_y intervals and the x-domain into n_r intervals. The time domain was divided in varying intervals using δ_t as default value, but these intervals are adjusted during calculations by the `lsoda`-solver according to the given relative and absolute tolerances. The variable $h_{\max}$ is the maximal stepsize for this solver. The mass balance was calculated as an extra control system on the solution and is displayed as the constant orange line. Also the average fiber, yarn and room concentration are displayed. First the fiber and yarn concentration coincide to an equilibrium concentration at approximately 10^2 s, afterwards at approximately 10^6 s that concentration reaches the equilibrium concentration. In this case no overlap zone is used, but volume averaging is used as an upscaling method assuming perfectly smooth exchange between the different levels.

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Table 1
Dirac-concentration or Dirac-flux at one of the boundaries.

Case	Setting	Result	
1	$C_{1\ell} = \delta, F_{2r} = 0$	$\mathcal{L}C_{2r} = \frac{1}{A_{11}}$	$\mathcal{L}F_{1\ell} = \frac{A_{21}}{A_{11}}$
2	$F_{1\ell} = \delta, C_{2r} = 0$	$\mathcal{L}F_{2r} = \frac{1}{A_{22}}$	$\mathcal{L}C_{1\ell} = \frac{A_{12}}{A_{22}}$
3	$C_{2r} = \delta, F_{1\ell} = 0$	$\mathcal{L}C_{1\ell} = \frac{1}{A_{11}^{-1}}$	$\mathcal{L}F_{2r} = -\frac{A_{21}}{A_{22}}$
4	$F_{2r} = \delta, C_{1\ell} = 0$	$\mathcal{L}F_{1\ell} = \frac{1}{A_{22}^{-1}}$	$\mathcal{L}C_{2r} = -\frac{A_{12}}{A_{11}}$

Table 2
Input variables.

t_0	1×10^{-8}	α_{fy}	1000
Δt	1.01	α_{yr}	100 or 0.0131111
$t_{\max}$	1.0×10^{10}	v_{fy}	1
n_f	20	v_{yr}	1
n_y	60	D_f	1×10^{-10}
n_r	40	D_y	1×10^{-6}
n_{y_o}	2	D_r	1×10^{-5}
n_{r_o}	2	rel tol	1×10^{-6}
$\rho_{\min}$	0	abs tol	1×10^{-13}
$\rho_{\max}$	0.0001	$h_{\max}$	10 000
R_y	0.001	h	2.0
L	5	A	10.0
$C_f(\rho, r, 0)$	1		
k	1 or 10 000		

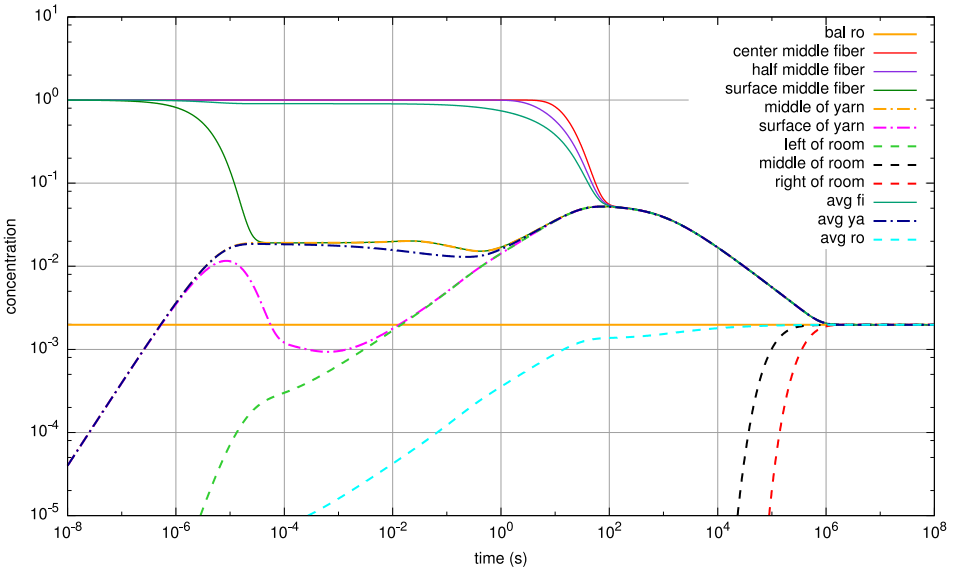

Fig. 2. Solution without overlapping domain decomposition, but with volume averaging as upscaling between the three levels.

The complete model with overlapping domain decomposition is the adjusted version of (1) in the overlap zone:

$$\begin{cases} \dfrac{\partial C_f(\rho,r,t)}{\partial t} = \dfrac{1}{\rho}\dfrac{\partial}{\partial \rho}\left(\rho D_f \dfrac{\partial C_f(\rho,r,t)}{\partial \rho}\right), & \rho \in [\rho_{\min}, \rho_{\max}] \quad \text{(a)} \\ \dfrac{\partial C_y(r,t)}{\partial t} = \dfrac{1}{r}\dfrac{\partial}{\partial r}\left(r\dfrac{D_y}{\tau_y}\dfrac{\partial C_y(r,t)}{\partial r}\right) + \alpha_{fy} v_{fy}\left(C_f(\rho_{\max},r,t) - C_y(r,t)\right) \\ \qquad + k\left(\overline{C_r} - C_y(r,t)\right), & r \in [R_{y_o}, R_y] \quad \text{(b)} \\ \dfrac{\partial C_r(x,t)}{\partial x} = \dfrac{\partial}{\partial x}\left(D\dfrac{\partial C_r(x,t)}{\partial x}\right) + k\alpha_{yr}\left(\overline{C_y} - C_r(x,t)\right), & x \in [0, L_o] \quad \text{(c)} \end{cases} \tag{5}$$

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and (1) in the rest of the domain. The boundary conditions of (1) are changed to

$$\frac{\partial C_f}{\partial \rho}(0,r,t)=0, \qquad -D_f\frac{\partial C_f}{\partial \rho}(\rho_{\max},r,t)=v_{fy}(C_f(\rho_{\max},t)-C_y(r,t)),$$
$$\frac{\partial C_y}{\partial r}(0,t)=0, \qquad \frac{\partial C_y}{\partial r}(R_y,t)=0,$$
$$\frac{\partial C_r}{\partial x}(0,t)=0, \qquad \frac{\partial C_r}{\partial x}(L,t)=0,$$

where $\overline{C_y}$ and $\overline{C_r}$ denote the average concentrations in the overlap zone of the yarn and room level and R_{y_o} is the radius in the yarn corresponding to the beginning of the overlap zone. The factor k is the factor $\frac{q}{\pi(R_y^2-{R_y}_o^2)h}$ we used previously for mass balance purposes. Since it is easier for programming and notation we also used this k in the room model, adjusted with the constant of proportion α_{yr} which as a result slightly changes in physical meaning and thus in size. That is also the reason why there is a second number for α_{yr} in Table 2. With the second number the same mass balance concentration is reached and the physical behavior is mimicked. There is also a second number in Table 2 for the constant k where it becomes relatively big. With this large k it is possible to mimic the kinetical behavior of the problem as seen in the case of only volume averaging as an upscaling method. In the above derivation of the exchange matrix A it became clear that for big k or q a perfect smooth exchange is seen and the exchange matrix can be simplified as if there was no overlap zone. This is also visible in Fig. 4.

The original code was adjusted with using a part of the r-domain as the overlap zone of the yarn, and a part of the x-domain for the room overlap zone, each divided in smaller intervals, n_{y_o} and n_{r_o} resp., for numerical calculation purposes. The fluxes were adapted and the extra source and sink terms were added to the concentration array in each space interval. The adjusted number of equations was calculated in order to be able to allocate the memory needed by the band matrix produced by the solver. The solution is visible in Fig. 3. Here the equilibrium concentration where the fiber and yarn level solution coincide also seems to be reached at approximately 10^2 s which is according with what one would expect, since the upscaling method between the fiber and yarn level has not been adapted. The concentration is, however, getting in to the room at a later time but at a higher pace. Before the fiber and yarn concentration are getting to there equilibrium concentration there is a build-up in the yarn concentration which is still behaving separately from the room concentration. This can be explained by the used proportionality constant α_{yr} which regulates how quick the concentration of AI is getting into the room, and is obviously acting as an inhibitor in this system.

Again the mass balance is calculated and displayed as the constant yellow line.

For this mass conservation the three averages of each level, which are each displayed in the solution plot, are calculated as

$$\overline{\overline{C_f}}=\frac{\int_0^{R_y} r\,\mathrm{d}\,r\int_{\rho_{\min}}^{\rho_{\max}} C_f\rho\,\mathrm{d}\,\rho}{\int_0^{R_y} r\,\mathrm{d}\,r\int_{\rho_{\min}}^{\rho_{\max}}\rho\,\mathrm{d}\,\rho},$$
$$\overline{\overline{C_y}}=\frac{\int_0^{R_y} C_y r\,\mathrm{d}\,r}{\int_0^{R_y} r\,\mathrm{d}\,r}, \qquad \overline{\overline{C_r}}=\frac{\int_0^{L} C_r\,\mathrm{d}\,x}{\int_0^{L}\mathrm{d}\,x}.$$

Taking the correct integrals of Eqs. (5) gives the change in time of the averages over the complete domain $\overline{\overline{C_i}}$, $i=f,y,r$, which should sum up to zero for mass conservation. Using the BC's and carrying out some basic calculations leads to the mass balance equation:

$$\overline{\overline{C_r}}+\frac{L_o}{L}\frac{1}{1-\left(\frac{R_{y_o}}{R_y}\right)^2}\alpha_{yr}\left(\overline{\overline{C_y}}+\frac{\alpha_{fy}}{\rho_{\max}}\frac{\rho_{\max}^2-\rho_{\min}^2}{2}\overline{\overline{C_f}}\right)=\mathcal{C},$$

where $\mathcal{C}$ is the mass balance constant visible in Figs. 3 and 4.

7. Conclusion and future work

A three-scale diffusion model for textiles consisting of a fiber, yarn and room model was further analyzed. Its characteristic times, the first moment and cumulant, were calculated symbolically in an overlap zone. Between the different levels this overlap zone is considered in an overlapping domain decomposition technique for upscaling the exchanged concentration of AI. The original C-code was adjusted, results were interpreted and the mass balance was calculated. Later on we will investigate what will happen if the setting is changing, e.g. a different positioning of the levels and consequently the overlap zone, and what changes if we use the actual concentration instead of the volume average in the overlapping zone equations.

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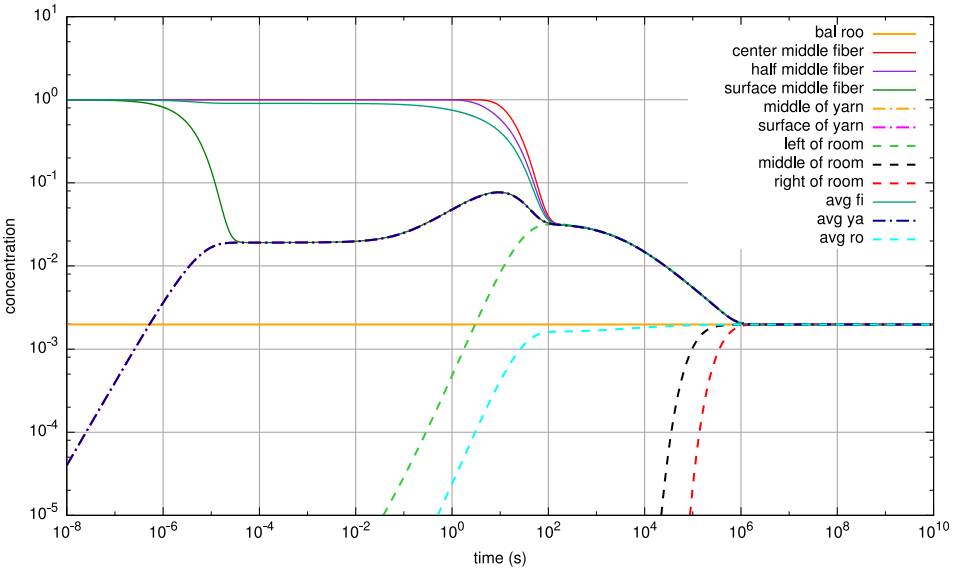

Fig. 3. Solution with overlapping domain decomposition as upscaling between the yarn and room level.

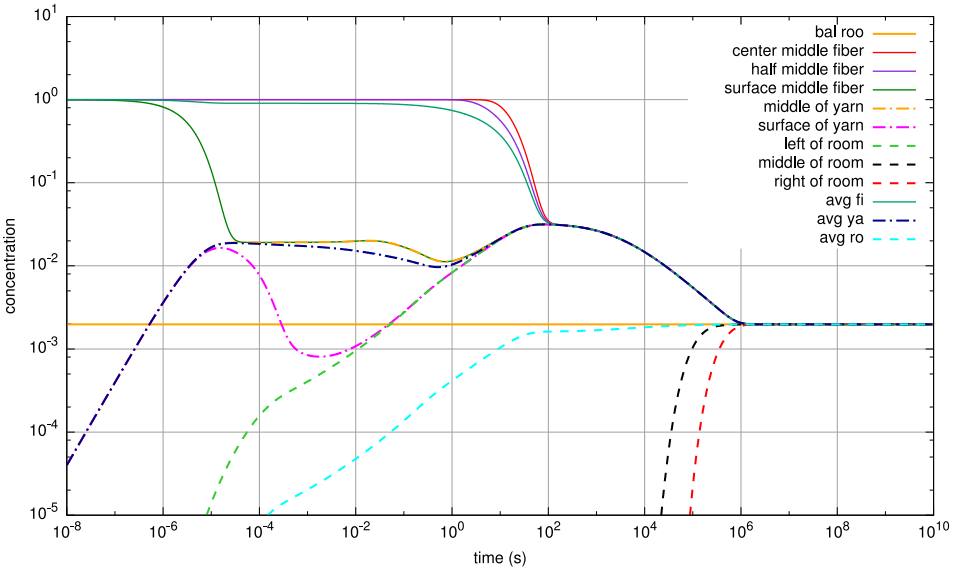

Fig. 4. Solution with overlapping domain decomposition as upscaling between the yarn and room level, with big k, mimicking the kinetical behavior as seen in Fig. 2.

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