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A volume averaging and overlapping domain decomposition technique to model mass transfer in textiles

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ABSTRACT

A new three scale approach for textile models is suggested: a one-dimensional fiber model and a fabric model, with a meso-level in between, i.e. the yarn scale, Goessens et al. (2012). For loose textile substrates this seems appropriate as the yarn level plays an important role. This is because the saturation vapor pressure will influence the release rate from the fibers, and its value will vary over the yarn cross section. Therefore, in this work we present two upscaling techniques for the three step multiscale model. The active component is tracked in the fiber, the yarn, and finally at the fabric level. At the fiber level a one-dimensional reduction to a non-linear diffusion equation is performed, and solved on an as needed basis. The outcome is upscaled via the volume averaging method and used as an input for the yarn level. At this level a one-dimensional model can be applied to calculate the concentration, which on its turn is upscaled using the overlapping domain decomposition as an input for the fabric level model.

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1. Introduction

Health-workers, soldiers, and other people who are frequently exposed to vector-borne diseases during missions in hot and tropical conditions, are recommended to use a combination of repellent-based creme on exposed body parts and treated garments to protect themselves against mosquitoes infected with malaria and other life threatening diseases. Current solutions have some deficits because they are not used in a proper way, application is too complex or people do not want to use them because of a certain degree of toxicity mentioned in the press. Next to product failure, the limited lifetime of effectiveness is a matter of concern. Therefore the NO BUG project, in the framework of the European Commission program FP7, focuses on the improvement of treated garments, and the future construction of garments with natural and bio-repellents.

We focus on the mathematical modeling of these garments, in particular the emphasis is on the diffusion of a substance to the outer boundary of textiles that are coated with a polymer solution of an active ingredient (AI), e.g. a perfume or a healing substance. This substance can easily be replaced by other volatiles which have a repellent effect or other substances under consideration. Based on the results of this study an inverse problem is encountered and once solved it can answer the question of how much of the AI has to be present on the textile fiber, so the concentration at the outer boundary of the textile stays high enough for as long as possible to be effective (e.g. repel or even kill mosquitoes, have a noticeable odor for humans, a healing effect ...).

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Existing models for mass transfer in textiles only consist of two levels, a fiber and fabric level, with no level in between, [1–7]. Most of them are concentrating on the transfer of water through textiles, whereas the use of an AI has not been studied yet. These models and algorithms for standard multilayer systems were extended to the needs that have arisen during the research on the polymer finishes. The application in mind has the purpose to track the diffusion of an active component released by the fibers of a scrim, e.g. a gauze bandage. For textile substrates with an open structure like these scrims a meso-level model that describes the release of the active component in the yarn cross section is needed. Because of this extra level in the model, we need a method to upscale the results from one level to another.

The models have been developed and solved using the programming language Python in a toolbox called STICK (Sophisticated Textile Information Computation Kit). It uses the finite volume method which has been implemented with the FiPy package [8]. A full coupling between the three scales is present and the effect of different micro and meso-level layouts can be determined. The mathematical model under consideration is a complete multilayer model for volatiles with three levels, the fiber, yarn and net level, where upscaling is done by volume averaging and the overlapping domain decomposition method, respectively.

2. Multiscale model

2.1. Setting

In this study treated scrims are considered. To model this application we make a distinction on three levels of the scrim. First, we model the fiber with a coating containing an active ingredient (AI). To this end the fiber will be seen as a cylindrical object. The boundary conditions depend on the chosen textile and the void space characteristics. Second, we model the yarn, a porous structure built out of fibers, upscaling the outcome of the fiber model using a volume averaging technique. The third model represents the scrim or fabric itself, with its environment, now using the overlapping domain decomposition as an upscaling method to calculate the overall properties of the fabric using the yarn properties.

2.2. The micro-level

If we consider the fiber as a long cylinder we can choose to work with a cylindrical coordinate system in which diffusion is everywhere radial. Diffusion of the AI in the fiber is then generally described by

$$\frac{\partial C_f}{\partial t} = \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r D_f \frac{\partial C_f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\frac{D_f}{r} \frac{\partial C_f}{\partial \theta} \right) + \frac{\partial}{\partial z} \left(r D_f \frac{\partial C_f}{\partial z} \right) \right\},$$

where C_f is the concentration of the AI in the fiber and D_f is the diffusion coefficient of the AI in the fiber. According to a radial symmetric diffusion in a long cylinder [9] concentration is a function of the radial position r and time t only, so azimuth θ and height z can be ignored and the diffusion equation becomes

$$\frac{\partial C_f(r, t)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r D_f \frac{\partial C_f(r, t)}{\partial r} \right), \quad 0 \leq r \leq R_f, \quad (1)$$

with boundary conditions

$$\nabla C_f(R, t) = 0 \quad (2)$$

at the fiber radius R and

$$\nabla C_f = \alpha (C_f(R_f, t) - C_s(t)) \cdot \mathcal{H}(C_f(R_f, t) - C_b, C^*(T) - C_s(t)) \quad (3)$$

at the coated fiber radius R_f . Here, α is a proportionality constant, $C^*(T)$ is the equilibrium concentration at temperature T , C_s is the concentration of the volatile at the outside-surface of the fiber which will be determined from the meso-level or yarn model, C_b is the concentration bound to the fiber that cannot be released and $\mathcal{H}(x, y)$ is defined as the Heaviside function $H(x)$ if $y > 0$, otherwise it is the identity, extending the BC in [10,11]. This models evaporation of AI ($C^* > C_s$) and condensation ($C^* \leq C_s$). Because we study diffusion through a polymer the diffusion coefficient D_f is taken to be concentration dependent. It also depends on the polymer used in the coating, the diffusing species, temperature and the water vapor concentration. Here we have opted for a diffusion coefficient of the form $D_f(C_f) = D_{f0} \exp(-c C_f)$, with D_{f0} and c known constants. We consider these constants at a known humidity and temperature, as would be the case in a climate room. For the more general case, these constants should be considered as a function of humidity and temperature. Furthermore, several other models can be found in the literature all describing a particular form of the diffusion coefficient [12].

This model has been solved using both a finite differences approach and the method of lines (MOL) based on a finite volume approach (FVM), [13].

2.3. The meso-level with volume averaging and overlapping domain decomposition technique

Based on the model prescribed in [2], we choose to work with cylindrical coordinates (r, θ, z) . By assuming we can neglect diffusion in the θ and z directions and diffusion is everywhere radial and symmetrical we can work in only one

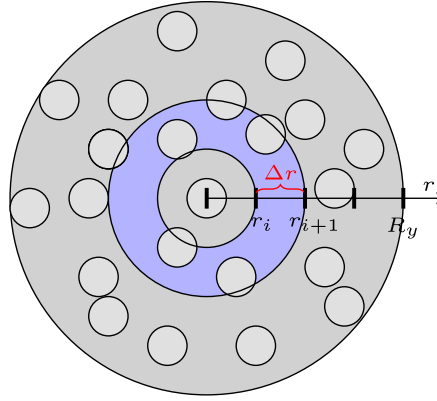


Fig. 1. Yarn discretization in cylindrical coordinates.

dimension. The governing model for the concentration of the AI on the yarn level then is, according to the radial diffusion equation in a cylinder,

$$\epsilon \frac{\partial C_y(r, t)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(\epsilon r \frac{D_y}{\tau_y} \frac{\partial C_y(r, t)}{\partial r} \right) + \Gamma_{in}(r, t), \quad (4)$$

with as a BC a diffusive flux to the outside

$$\frac{\partial C_y}{\partial r}(R_y, t) = -\frac{D_y}{d_{out}} (C_{out}(t) - C_y(R_y, t)),$$

where D_y is the diffusion coefficient of the AI in the yarn air gaps, ϵ is the porosity depending on the position and τ_y is the tortuosity of the yarn. In the BC $C_{out}(t)$ is the concentration of AI in the air surrounding the yarn at a prescribed distance d_{out} to the yarn.

The term $\Gamma_{in}(r, t)$ in the equation above is a source term that describes the amount of AI coming out of a cross section of the fibers into the yarn air space. It is calculated by upscaling the boundary condition at the fiber level (3), representing the flux of AI over the boundary, using the volume averaging technique [14].

In order to solve this model we divide the radial space $[0, R_y]$ in N intervals $\Omega_i = [r_i, r_i + \Delta r] = [r_i, r_{i+1}]$ with length $\Delta r = \frac{R_y}{N}$, where R_y is the yarn radius. If afterwards we also consider the θ -coordinate we get concentric circles for each space interval, Fig. 1. In each of these shells we consider n fibers. N is chosen so in each interval we can describe one fiber model, with the same initial conditions and boundary conditions. The number of fibers in a shell $[r_i, r_{i+1}]$ can be calculated as

$$n = \frac{m(r_{i+1}^2 - r_i^2)}{R_y^2},$$

where m is the number of fibers in a yarn cross section.

In every time step t_j and space interval $[r_i, r_{i+1}]$ we solve one fiber model, assuming all n fibers in the same shell satisfy the same evaporation boundary condition

$$D_f \frac{\partial C_f^{ij}}{\partial r}(R_f) = -S_f h_{b \rightarrow f} \left(C_f^{i,j-1}(R_f) - C_y^{i+j-1} \right) \cdot \mathcal{H} \left(C_f^{i,j-1}(R_f) - C_b, C^*(T) - C_y^{i+j-1} \right),$$

where $C_y^{i+j-1} = C_y(r_i^+, t_{j-1})$ is the concentration in the middle of the space interval Ω_i , i.e. $r_i^+ = r_i + \frac{\Delta r}{2}$, of the previous time step, and $C_f^{i,j-1}(R_f) = C_f(R_f, r_i, t_{j-1})$ is the concentration on the fiber surface of a fiber in Ω_i of the previous time step. S_f is the effective area of evaporation $\epsilon \frac{2}{R_f}$, $h_{b \rightarrow f}$ is the mass transfer coefficient for the AI from bounded to free material and \mathcal{H} is the adjusted Heaviside function as defined earlier, [10,15]. We then take the volume average of the difference between the resulting fiber mass

$$M_f^{ij} = \frac{2\pi}{V_f} \int_0^{R_f} C_f^{ij}(r) r dr,$$

for fibers at $[r_i, r_{i+1}]$ at time t_j , and the mass at the previous time step $M_f^{i,j-1}$. This difference gives us the amount removed from fibers at that position over a time step. Doing so we find the source term Γ_{in} representing the amount coming from all n fibers in the shell.

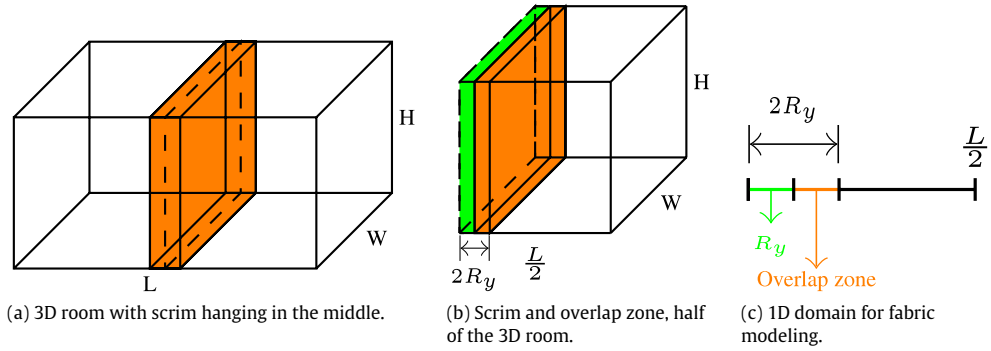


Fig. 2. Simplification from a 3D room to a 1D domain for fabric modeling via ODD.

For this we need the intrinsic average concentration, [14], using the *averaging* volume V of a shell,

$$\Gamma_{in}(r_i^+, t_j) = \frac{2\pi n}{\epsilon V} \int_{r_i}^{r_{i+1}} (M_f^{i,j-1} - M_f^{i,j}) r dr \quad (5)$$

$$= n \frac{M_f^{i,j-1} - M_f^{i,j}}{\epsilon}. \quad (6)$$

Using MOL in Ω_i we then need to implement the partial derivative of $u_i^+ = u(r_i^+, t) = r_i^+ C_y(t)$

$$\frac{\partial u_i^+}{\partial t} = \frac{1}{\Delta r_i^+} \left(\frac{D_y}{\tau_y} [\text{flux}_{\text{edge}_{i+1}} - \text{flux}_{\text{edge}_i}] + n \frac{\Delta M_f(r_i, t)}{\epsilon^2} \right),$$

with

$$\text{flux}_{\text{edge}_i} = \frac{\epsilon D_y}{\tau_y} \left(r \frac{\partial}{\partial r} \left(\frac{u}{r} \right) \right) \Big|_{r_i} = \frac{\epsilon D_y}{\tau} 2r_i \frac{\frac{u_i^+}{r_i^+} - \frac{u_i^-}{r_i^-}}{(\Delta r)_i^+ + (\Delta r)_i^-}.$$

To upscale to the macro-level model of the total fabric we will use the overlapping domain decomposition technique. Therefore the original domain $[0, R_y]$ is extended with an overlapping domain Ω_o at the interval $[R_y, 2R_y]$ where the PDE (4) is slightly adapted to

$$\epsilon \frac{\partial C_y(r, t)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(\epsilon r \frac{D_y}{\tau_y} \frac{\partial C_y(r, t)}{\partial r} \right) + \Gamma_{in}(r, t) - \Gamma_{out}(t, \Omega_o), \quad (7)$$

with a homogeneous Neumann BC

$$\frac{\partial C_y}{\partial r}(2R_y) = 0.$$

The sink term $\Gamma_{out}(t, \Omega_o)$ is the amount of AI that is removed from the meso-scale due to diffusion to the macro-level, see Section 2.4.

2.4. The macro-level and domain decomposition method

In a previous approach an analytical solution was given for the macro-level model based on solving a Cauchy problem. Implementing these analytical solutions though was unstable due to the need to cut-off the infinite series arising in them. So a numerical analysis was asserted. This numerical method is the overlapping domain decomposition method. As indicated in Section 2.3, we use an overlap zone to upscale from the meso-level to the fabric level.

Here a room with dimensions $L \times W \times H$ is modeled with a net hanging in the middle of the room, so at $\frac{L}{2}$, see Fig. 2. This can be reduced to a 1D model. The domain under consideration is the interval $[0, \frac{L}{2}]$. The yarn in the net is modeled as a 1D cylindrical object over an extended domain $[0, 2R_y]$ with two *no flux*-BC's $\partial_r C_y(0, t) = 0$ and $\partial_r C_y(2R_y, t) = 0$, the way mentioned in Section 2.3. The mass coming from the yarn is going to the surrounding air of the yarn into the overlap zone $[R_y, 2R_y]$. The room model on its turn runs over $[R_y, \frac{L}{2}]$, again with a *no flux*-BC's $\partial_x C(R_y, t) = 0$ and $\partial_x C(\frac{L}{2}, t) = 0$, because no AI is leaving the room. The calculations made only serve for one side of the net, but due to symmetry the other site behaves in the same way, so we can predict the outcome for the whole room domain $[0, L]$.

The room 1D diffusion equation is

$$\partial_t C = \partial_x (D \partial_x C) + \Gamma_s(x, t),$$

with D the diffusion of the AI in air and $\Gamma_s(x, t)$ the concentration per time unit added/removed at x . To solve this differential equation the domain $[0, \frac{L}{2}]$ is divided into smaller intervals of length Δx and integrating over one cell gives

$$\partial_t C_i = \frac{\text{flux}_{\text{edge}_{i+1}} - \text{flux}_{\text{edge}_i}}{\Delta x_i} + \Gamma_s(\Delta x_i),$$

where $\Gamma_s(\Delta x_i)$ is the concentration per time unit added to or removed from the interval $[x_i, x_{i+1}]$ and the fluxes are obtained via MOL.

We situate the overlap zone in the first cell for integration so there the source term is corresponding to the amount of AI coming out of the yarns.

Now the yarn and fabric models will be solved alternately per time step, using the outcome of one model as the source term for the other model.

Per time step t_j the overlapping domain decomposition method exists of three steps:

1. we solve the 1D yarn model, calculate the mass coming out of one yarn using the above meso-level model with the sink term $\Gamma_{\text{out}}(t_{j-1}, \Omega_o)$ of the previous time step and calculate the corresponding concentration by dividing by the volume of a yarn cross section πR_y^2 ;
2. we solve the room model to obtain a new concentration value near a yarn. For this model we use the mass released by one yarn to the overlap zone in the first step which needs to be upscaled to a concentration source per second per mm^3 for all yarns in the scrim. To upscale we need to calculate how many yarns are present in the scrim. Because we model only half the room eventually everything should be multiplied by 2;
3. for the next time step, due to the domain overlap, the BC is now homogeneous Neumann always. Then, we need to set a correct $\Gamma_{\text{out}}(t_j, \Omega_o)$ on the yarn level, so we need to downscale the mass calculated from the room model in this time step to keep mass balance. The sink term $\Gamma_{\text{out}}(t_j, \Omega_o)$ for the yarn model is what was present in the overlap zone, so being the mass removed from the yarns, approximated from the concentration given by the solved room model, downscaled to one yarn and again using a factor 2 as we model only half the room.

2.5. The total three step model and discussion

On each time step one complete three step model is solved. Beginning with the fiber level with all initial conditions and boundary concentrations set to zero. Afterwards a yarn model is solved over a domain $[0, 2R_y]$, including an overlap zone, with an upscaled source term Γ_{in} calculated via volume averaging of the fiber results, a sink term $\Gamma_{\text{out}}(t, \Omega_o) = 0$ and with a homogeneous Neumann BC. Next a fabric model is solved over a domain $[R_y, \frac{L}{2}]$ using a source term Γ_s calculated from the upscaled yarn results in the overlap zone. In the next time step we again begin by solving a fiber model, but now with adjusted initial conditions on boundary concentrations, afterwards a yarn level model and a fabric level model, and so on.

For the numerical scheme of the algorithm we make the distinction between the r -coordinate of the fiber level, r_i , $1 \leq i \leq I$ and the r -coordinate of the yarn level, r'_k , $1 \leq k \leq K$.

In time step t_1 we use the initial conditions and first solve the fiber system:

$$\begin{cases} \partial_t C_f(r, r', t)|_{r=r_i, r'=r'_k, t=t_1} = \frac{1}{r_i} \partial_r (r D_f \partial_r C_f(r, r', t))|_{r=r_i, r'=r'_k, t=t_1} \\ C_f(r_i, r'_k, t_0) = C_{\text{init}}(r'_k) \\ D_f \partial_r C_f(R, r'_k, t_1) = 0 \\ D_f \partial_r C_f(R_f, r'_k, t_1) = -S_f h_{b \rightarrow f} C_f(R_f, r'_k, t_0), \end{cases}$$

where per r'_k index i runs from 1 to I , to get $C_f(r_i, r'_k, t_1)$, $1 \leq i \leq I$, and $1 \leq k \leq K$. C_{init} is the initial concentration of AI applied in the fiber coating during fabrication.

Then we solve the yarn system:

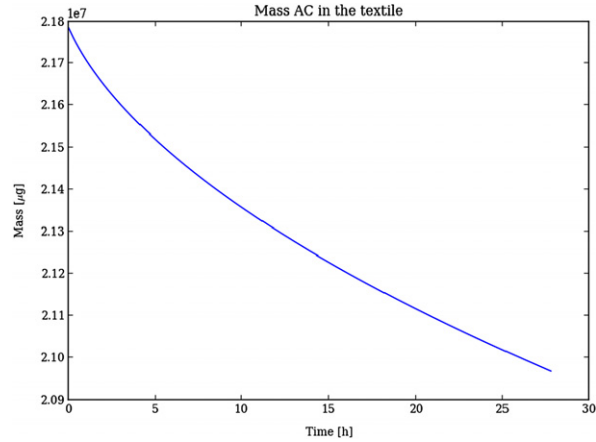
$$\begin{cases} \epsilon \partial_t C_y(r', t)|_{r'=r'_k, t=t_1} = \frac{1}{r'_k} \partial_{r'} \left(\epsilon r' \frac{D_y}{\tau_y} \partial_{r'} C_y(r', t) \right) \Big|_{r'=r'_k, t=t_1} + \Gamma_{\text{in}}(r'_k, t_1) \\ C_y(r'_k, t_0) = 0 \\ \partial_r C_y(0, t_1) = 0 \\ \partial_r C_y(R_y, t_1) = 0, \end{cases}$$

to get $C_y(r'_k, t_1)$, for $1 \leq k \leq K$.

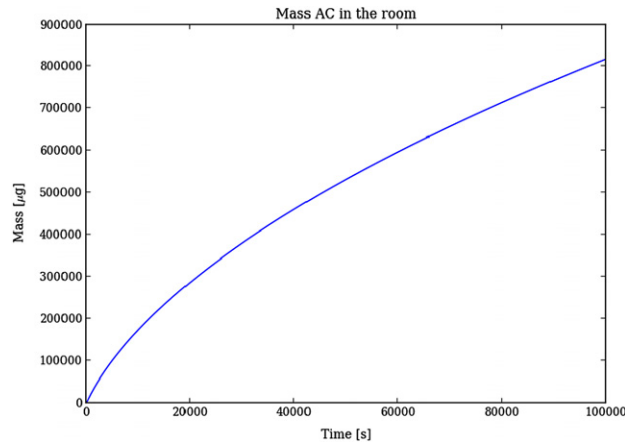
Then we solve the fabric system:

$$\begin{cases} \partial_t C(x, t)|_{x=x_l, t=t_1} = \partial_x (D \partial_x C(x, t))|_{x=x_l, t=t_1} + \Gamma_s(\Delta x_l, t_1) \\ C(x_l, t_0) = 0 \\ \partial_x C(R_y, t_1) = 0 \\ \partial_x C\left(\frac{L}{2}, t_1\right) = 0 \\ \Gamma_s(\Delta x_l, t_1) = \text{upscaled change in } C_y(t_1, \Omega_o), \end{cases}$$

to get $C(x_l, t_1)$ for $1 \leq l \leq L$.



(a) Mass of the AI in the bed net.



(b) Mass of the AI in the room.

Fig. 3. Mass of DEET diffusing to the outside from a polymer coating on a fiber in a room with standard dimensions.

For the next time steps t_j , $2 \leq j \leq J$ the three systems are per time step:

$$\begin{cases} \partial_t C_f(r, r', t)|_{r=r_i, r'=r'_k, t=t_j} = \frac{1}{r_i} \partial_r (r D_f \partial_r C_f(r, r', t))|_{r=r_i, r'=r'_k, t=t_j} \\ D_f \partial_r C_f(R, r'_k, t_j) = 0 \\ D_f \partial_r C_f(R_f, r'_k, t_j) = -S_f h_{b \rightarrow f} (C_f(R_f, r'_k, t_{j-1}) - C_y(r'_k, t_{j-1})) \cdot \mathcal{H}(C_f(R_f, r'_k, t_{j-1}) - C_b, C^*(T) - C_y(r'_k, t_{j-1})), \end{cases}$$

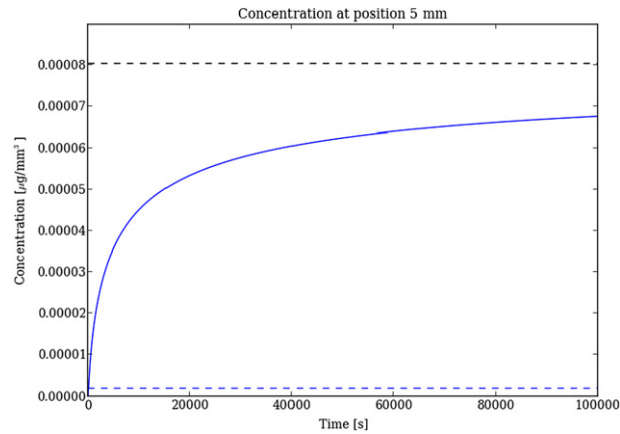
where per r'_k index i runs from 1 to l , to get $C_f(r_i, r'_k, t_j)$, $1 \leq i \leq l$, and $1 \leq k \leq K$.

$$\begin{cases} \epsilon \partial_t C_y(r', t)|_{r'=r'_k, t=t_j} = \frac{1}{r'_k} \partial_{r'} \left(\epsilon r' \frac{D_y}{\tau_y} \partial_{r'} C_y(r', t) \right) \Big|_{r'=r'_k, t=t_j} + \Gamma_{in}(r'_k, t_j) - \Gamma_{out}(t_{j-1}), \\ \partial_r C_y(0, t_j) = 0 \\ \partial_r C_y(2R_y, t_j) = 0 \\ \Gamma_{out}(t_{j-1}) = \text{downscaled change in } C(t_{j-1}, \Omega_o), \end{cases}$$

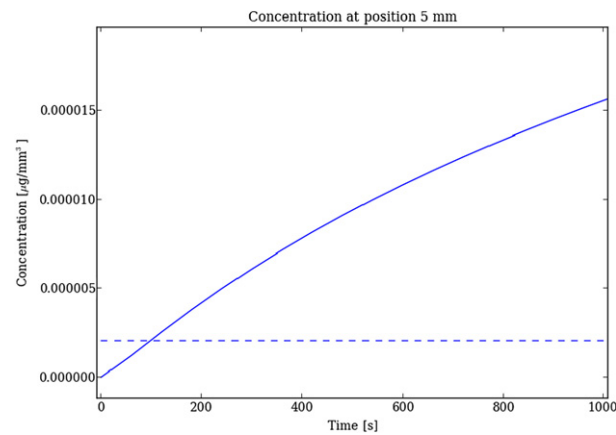
to get $C_y(r'_k, t_j)$, for $1 \leq k \leq K$.

$$\begin{cases} \partial_t C(x, t)|_{x=x_l, t=t_j} = \partial_x (D \partial_x C(x, t))|_{x=x_l, t=t_j} + \Gamma_s(\Delta x_l, t_j) \\ \partial_x C(R_y, t_j) = 0 \\ \partial_x C\left(\frac{L}{2}, t_j\right) = 0 \\ \Gamma_s(\Delta x_l, t_j) = \text{upscaled change in } C_y(t_j, \Omega_o), \end{cases}$$

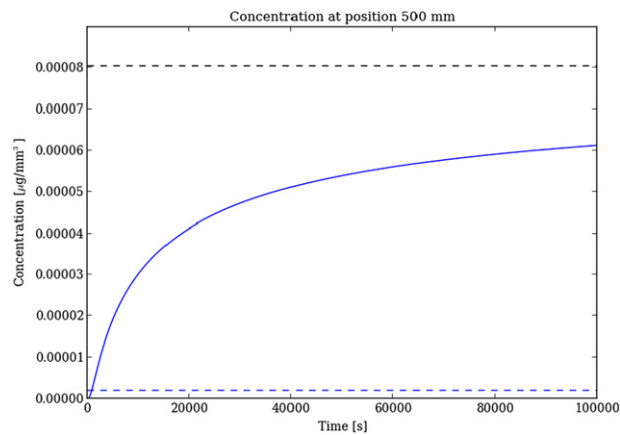
to get $C(x_l, t_j)$ for $1 \leq l \leq L$.



(a) Concentration of AI at 5 mm from the scrim.



(b) Concentration of AI at 5 mm from the scrim in the first 1000 s.

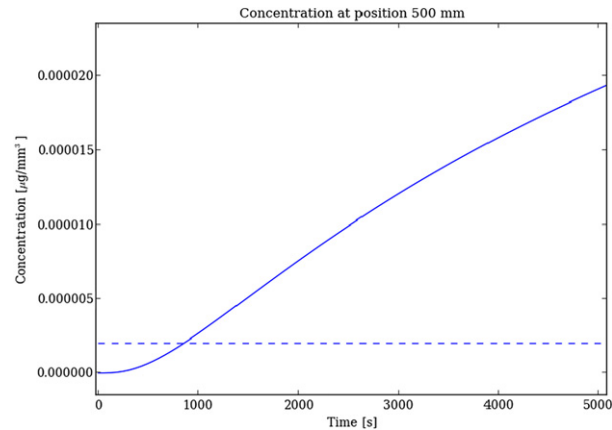


(c) Concentration of AI at 500 mm from the scrim.

Fig. 4. Concentration of DEET diffusing to the outside from a polymer coating on a fiber in a room with standard dimensions at 5 and 500 mm from the scrim.

If we know $C(x_l, t_j)$ for all $0 \leq l \leq L$ and $0 \leq j \leq J$ we can study the concentration of AI in the air at a certain distance from the scrim.

When simulating a closed room of length 5 m, width 3 m and height 2.1 m for 100 000 s and starting from an initial concentration of $0.9 \cdot 10^3 \frac{\mu\text{g}}{\text{mm}^3}$ for the AI DEET captured in one polymer coating on a cotton scrim placed in the middle of the room we get the following results, presented in Figs. 3 and 4. The mass of the AI in the bed net is dropping down, in the room



(d) Concentration of Al at 500 mm from the scrim in the first 5000 s.

Fig. 4. (continued)

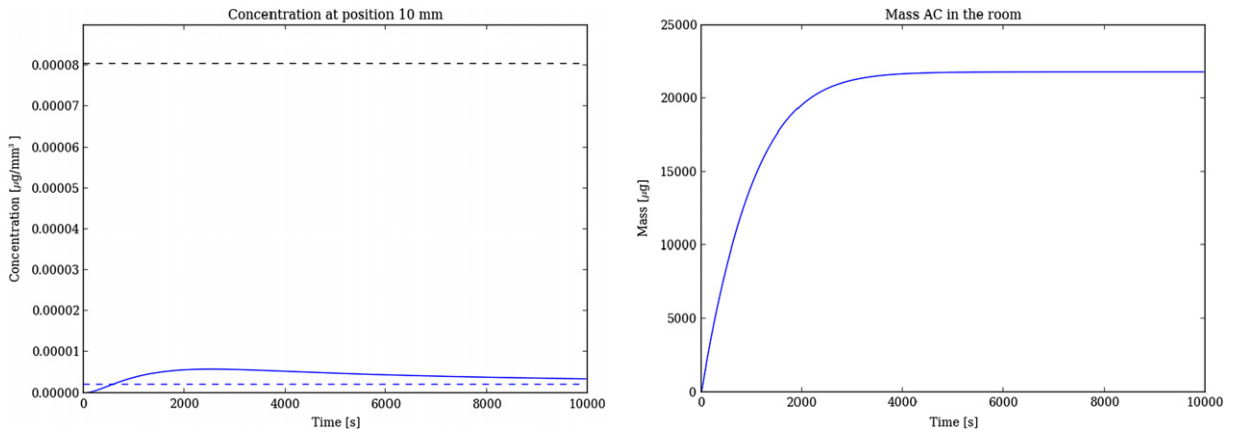


Fig. 5. The concentration and mass in the room stays constant after the Al in the fiber coating is depleted.

it is increasing. First the Al is diffusing to the surface of the polymer coating around the fibers. Once the concentration in this coating is depleted the Al is diffusing to the surrounding air until no mass is coming from the fibers any longer. Since no ventilation is allowed concentration should go to a constant value or the saturation concentration should be reached after a certain time. For the application in mind the concentration is not yet depleted after 100 000 s. For illustrative purposes we have used a much smaller initial concentration and a higher evaporation coefficient (which is not in accordance with the application) to visualize this effect in Fig. 5.

By construction of our algorithm, the total mass remains constant during simulation. The concentration at the given different positions (5, 500 mm) in the room increases and exceeds the threshold concentration for repellency represented by the lower dashed line quickly enough to satisfy required standards. The higher dashed line represents the saturation concentration for the Al used in the simulation.

3. Conclusion and future work

A three-scale model consisting of a micro-, meso- and macrolevel was constructed, implemented in Python and solved. An upscaling was done by volume averaging for the concentration calculated from the micro-level to serve as a source term and BC for the meso-level. An overlapping domain decomposition was carried out to establish a source term for the macro model. The outcome of the implemented three-step model is in accordance with the expected outcome. Further validation should be done with obtained experimental data and ventilation of the room should be taken into account. An inverse problem can be solved to establish the right form of the diffusion coefficients in the model, including the dependence on temperature and water vapor concentration.

There are several potential engineering applications of this study of the diffusion of substances in and through polymer coatings. These can be found in settings where controlled release plays an important role such as drug delivery and their encapsulation in the medical context, polymer melts and the inflation of elastic membranes for the construction

of plastic materials, and even in architecture and building and many others. In the textile context polymer coating and encapsulation of substances for application on fibers creates functional materials such as dyes, fragrances, phase change materials, smart polymers and nano-materials found in sports, defense, health care, environmental pollution control, space, and even everyday use products like rain coats, mattresses and floor mats.

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References

- [1] Q. Zhang, W. Sun, A numerical study of air–vapor–heat transport through textile materials with a moving interface, *J. Comput. Appl. Math.* 236 (5) (2011) 819–833.
- [2] C. Ye, H. Huang, J. Fan, W. Sun, Numerical study of heat and moisture transfer in textile materials by a finite volume method, *Commun. Comput. Phys.* 4 (4) (2008) 929–948.
- [3] R. Korycki, Method of thickness optimization of textile structures during coupled heat and mass transport, in: *FIBRES & TEXTILES in Eastern Europe*, Vol. 17, 2009, pp. 33–38. 1(72).
- [4] J. Fan, Z. Luo, Y. Li, Heat and moisture transfer with sorption and condensation in porous clothing assemblies and numerical simulation, *Int. J. Heat Mass Transfer* 43 (16) (2000) 2989–3000.
- [5] P. Nordon, H.G. David, Coupled diffusion of moisture and heat in hygroscopic textile materials, *Int. J. Heat Mass Transfer* 10 (7) (1967) 853–866.
- [6] P.S.H. Henry, The diffusion of moisture and heat through textiles, *Discuss. Faraday Soc.* 3 (1948) 243–257.
- [7] H. Huang, C. Ye, W. Sun, Moisture transport in fibrous clothing assemblies, *J. Engrg. Math.* 61 (1) (2008) 35–54.
- [8] J.E. Guyer, D. Wheeler, J.A. Warren, FiPy: partial differential equations with python, *Comput. Sci. Eng.* 11 (3) (2009) 6–15.
- [9] J. Crank, *The Mathematics of Diffusion*, Clarendon Press, Oxford, 1979.
- [10] Y. Li, Q. Zhu, Simultaneous heat and moisture transfer with moisture sorption, condensation, and capillary liquid diffusion in porous textiles, *Text. Res. J.* 73 (6) (2003) 515–524.
- [11] Q.Y. Zhu, Y. Li, Numerical simulation of the transient heat and liquid moisture transfer through porous textiles with consideration of electric double layer, *Int. J. Heat Mass Transfer* 53 (7–8) (2010) 1417–1425.
- [12] L. Masaro, X.X. Zhu, Physical models of diffusion for polymer solutions, gels and solids, *Prog. Polym. Sci.* 24 (5) (1999) 731–775.
- [13] T. Goessens, B. Malengier, P. Li, R.H. De Staelen, Diffusion of active ingredients in textiles, *J. Math. Model. Algorithms* (2012) 1–12.
- [14] S. Whitaker, *The Method of Volume Averaging*, in: *Theory and Applications of Transport in Porous Media*, Kluwer Academic, 1999.
- [15] Z. Wang, Heat and moisture transfer and clothing thermal comfort, Ph.D. Thesis, Hong Kong Polytechnic University, 2002.