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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.

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

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

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

$$\frac{\partial C_f(r,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD_f\frac{\partial C_f(r,t)}{\partial r}\right), \quad 0 \le r \le R_f, \tag{1}$$

with boundary conditions

$$\nabla C_f(R,t) = 0 \tag{2}$$

at the fiber radius R and

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

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 ($C^* \le C_s$). 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