ARTICLE IN PRESS

Journal of Computational and Applied Mathematics ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

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

ARTICLE INFO

Article history:
Received 19 July 2015
Received in revised form 19 January 2016

Keywords:
Diffusion
Textile modeling
Multiscale modeling
Controlled release
Characteristic time

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).

http://dx.doi.org/10.1016/j.cam.2016.01.031
0377-0427/

Please cite this article in press as: T. Goessens, D. Constales, Characteristic times in a three scale model with overlapping domain decomposition, Journal of Computational and Applied Mathematics (2016), http://dx.doi.org/10.1016/j.cam.2016.01.031

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

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

Please cite this article in press as: T. Goessens, D. Constales, Characteristic times in a three scale model with overlapping domain decomposition, Journal of Computational and Applied Mathematics (2016), http://dx.doi.org/10.1016/j.cam.2016.01.031