SHAPE OPTIMIZATION IN MASS DIFFUSION WITHIN COMPOSITE DRESSINGS

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Abstract
Dressings are the composite structures made of different layers of textile materials, semi-permeable membrane and microcapsules with the active therapeutic substance. The activating agent is the exudate from the wound which initiate the chemical reaction within the microcapsules. The mass transport to the surrounding is reduced mechanically because the semi-permeable membrane stops the diffusion of the particles of the prescribed diameter, i.e. the particles of therapeutic substance. The exudate diffuses normally to the surrounding. State variables are the exudate concentration and the concentration of therapeutic substance. The state equations, the boundary and the initial conditions describe the problem. The sensitivity of an arbitrary functional is analyzed and implemented into the problem of shape optimization. The objective functionals and the optimality conditions are formulated. Numerical example of shape optimization is presented.
Key words: mass diffusion, shape optimization, composite dressing

1. Problem definition

The important composite is the multilayer textile dressing made of the textile materials, the semi-permeable membrane and the microcapsules with the therapeutic substance. The shape optimization of composite dressings is very important because the optimal structures can introduce the therapeutic substance more effectively into the skin and improve the recovery process.The diffusion of exudate and therapeutic substance is defined by the state equations and a set of boundary and initial conditions, which have the different forms for the particular structures. The general reference here is Crank [1]. The diffusion can be determined in the macro-scale and in the micro-scale. The so-called Knudsen diffusion introduced in this case exists within the typical porous material of the pores diameter less than the mean value of the free path of the diffusing molecules. The problem can be described physically by the diffusion coefficient and the diffusive potentials. The standard reference here is Gilron, Soffer [2].
We optimize the shape of multilayer textile dressing subjected to the coupled diffusion. There is necessary to introduce the first-order sensitivity of an arbitrary behavioral functional as well as the sensitivities of state fields and the sensitivity expressions within the structure. The material derivative concept and the direct approach to sensitivity analysis is considered, see for example Dems, Korycki, Rousselet [3]; Korycki [4].

2. Physical model

The oppositely directed diffusion is typical for some composite structures. The activating agent is the exudate from the wound which initiate the chemical reaction within the layer with microcapsules. The mass transport to the surrounding is reduced mechanically because the semi-permeable membrane stops the diffusion of the particles of the prescribed diameter. Thus, the exudate diffuses normally because the mean diameter of particles is different. The microcapsulated substance is the complexing agent located inside the dressing. The prescribed fluid concentration initiates the chemical reaction within microcapsules and releases the therapeutic substance. Consequently, the process begins after the dead time and the gradient of diffusion velocity increases rapidly. Therpeutic agent is transferred to the skin, because the semi-permeable membrane secures the direction. The exudate flux density from the wound is reduced after some time and the gradient of the diffusion velocity decreases progressively. The dressing is removed for the saturated conditions of exudate within structure.

The textiles used for the dressing can have different morphology. The most common are made of the simple non-woven subjected to the finishing process on the external surface. The material is cheap, easy to connect by the stitching, finish the surface and introduce the microcapsules. The typical structure has (i) the one or more internal layers which drain the exudate from the wound; (ii) the layer with the microcapsulated therapeutic substance; (iii) the semi-permeable membrane and (iv) the external protective layer which is subjected to finishing procedure. The microcapsules are introduced into the central layer (iii) during the stitching process but its internal distribution is irregular which is very difficult to describe.

3. Mathematical model. Primary structure. First-order sensitivity analysis

The state variables are the concentrations of the activating agent C_1 and the therapeutic agent C_2. Design variables are the coordinates **b** of the selected points within the structure. The diffusion depends on the configuration of the dressing and the wound parameters. Let us next assume the same cross-section of the dressing and the same boundary conditions. The analysis can be simplified from 3D space to 2D plane problem. Let us next assume that the wound is located on the middle of structure, i.e. only a half of dressing is considered.

The oppositely directed diffusion is characterized by two connected processes. Each is described by the state equation (the second-order correlation with respect to design variables and the first-order with respect to time) as well as the set of boundary and initial conditions. The exudate diffuses from the wound through the textile dressing and finally is transported by convection from the external surface to the surrounding. This agent is not subjected to the chemical reaction and the equation is expressed for the i-th layer of structure, cf. Korycki [4]

$$\mathrm{div}\mathbf{q}_1^{(i)} = \dot{C}_1^{(i)} \;;\; \dot{C}_1^{(i)} = \frac{dC_1^{(i)}}{dt} \;;\; \mathbf{q}_1^{(i)} = D_1^{(i)} \nabla C_1^{(i)} + \mathbf{q}_1^{*(i)}; \quad \text{within } \Omega; \tag{1}$$

where $\dot{C}_1$ is the time derivative of activating agent concentration for primary problem, D_1 is the diffusion coefficient of the activating agent, $\mathbf{q}_1$ is the vector of diffusion flux density of the activating agent, $\mathbf{q}_1^*$ is the vector of initial diffusion flux density of the activating agent.

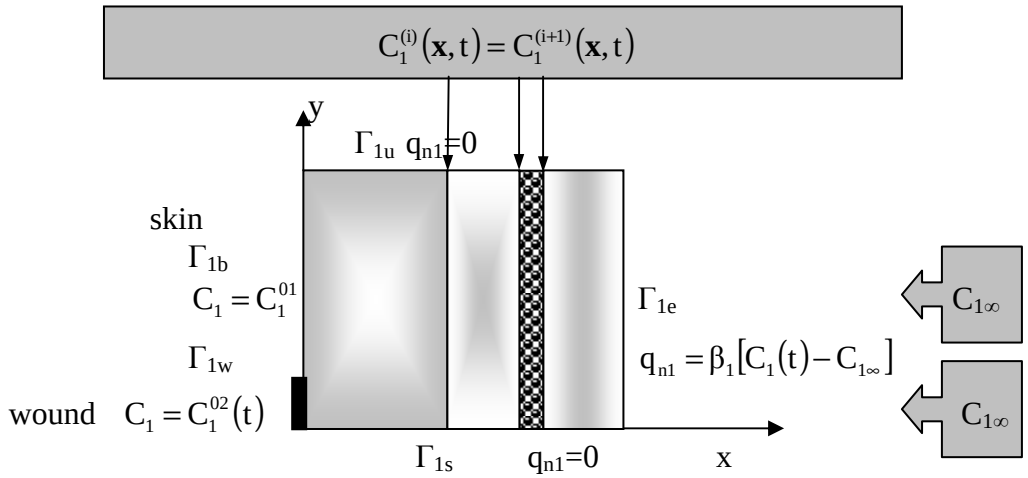

Figure 1. Boundary conditions for exudate diffusion within dressing structure

The boundary conditions are shown in Fig.1. The boundary contacting the skin $\Gamma_1=\Gamma_{1b}\cup\Gamma_{1w}$ is subjected to the first-kind conditions: (i) the time-dependent exudate concentration of the wound $C_1 = C_1^{02}(t)$; (ii) the exudate concentration for the skin less than for the wound $C_1^{01} << C_1^{02}$. Practically speaking, we can assume the constant value $C_1 = C_1^{01}$ for the skin. The

symmetrical boundary of dressing Γ_{1s} is characterized by the second-kind condition, i.e. the diffusion flux density normal to this portion is $q_{n1}=0$. The part of boundary Γ_{1u} is diffusive isolated, the diffusion flux density normal to this boundary is $q_{n1}=0$. The external part of dressing Γ_{1e} is subjected to the transient diffusive convection, i.e. the third-kind condition exists. Summarizing, the boundary conditions are the following

$$\begin{gathered}\Gamma_{1b}: C_1 = C_1^{01};\ \Gamma_{1w}: C_1 = C_1^{02}(t);\ \Gamma_{1u}: q_{n1}=0;\ \Gamma_{1s}: q_{n1}=0; \\ \Gamma_{1e}: q_{n1}(t) = \beta_1\left[C_1(t) - C_{1\infty}\right];\end{gathered} \tag{2}$$

Substance from microcapsules diffuses to the skin and the wound, is activated by the chemical reaction. The state equation has the form (cf. Korycki [4]) for the i-th layer of composite

$$\mathrm{div}\mathbf{q}_2^{(i)} + \dot{R}_2^{(i)} = \dot{C}_2^{(i)};\ \dot{C}_2^{(i)} = \frac{dC_2^{(i)}}{dt};\ \dot{R}_2^{(i)} = \frac{dR_2^{(i)}}{dt};\ \mathbf{q}_2^{(i)} = D_2^{(i)}\nabla C_2^{(i)} + \mathbf{q}_2^{*(i)};\ \text{within } \Omega. \tag{3}$$

where the symbols are the same as the in Eqs.(1), $\dot{R}_2$ is the chemical reaction velocity of the microcapsulated substance. The reaction velocity is $\dot{R}_2 > 0$ within the layer with microcapsules whereas within other layers can be neglected $\dot{R}_2 = 0$.

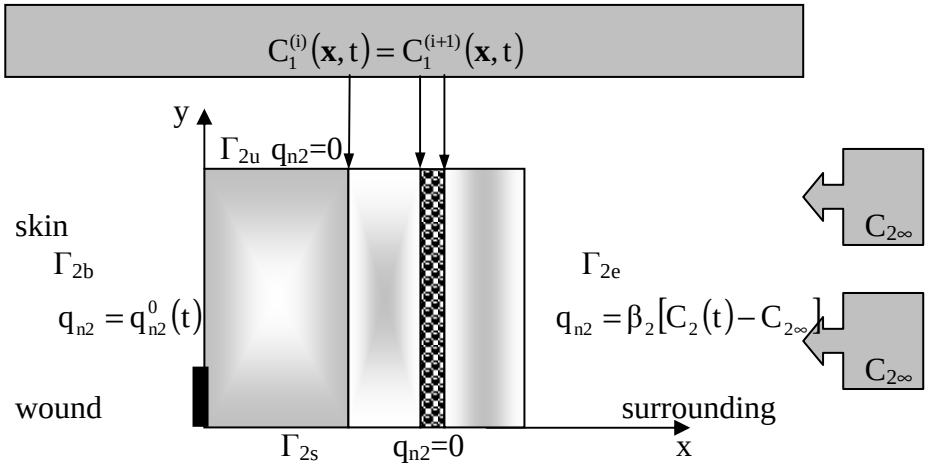

Figure 2. Boundary conditions for therapeutic agent diffusion within dressing structure

Therapeutic effect is secured by the prescribed diffusion flux density normal to the skin (the boundary Γ_{2b}) $q_{n2} = q_{n2}^0(t)$, cf. Fig.2. The initial value is $q_{n2}=0$ because the chemical reaction is negligible at the beginning of the process. After the dead time the mass flux density increases rapidly to maximum, next decreases asymptotically. Thus, the second-kind condition $q_{n2}=0$ exists on the symmetrical boundary of dressing Γ_{2s} and the upper part of structure Γ_{2u}. The membrane reduces the transport of agent to the surrounding but the external boundary Γ_{2e} is subjected to the diffusive convection. The boundary conditions are the following

$$\Gamma_{2b}:\ q_{n2} = q_{n2}^0(t);\quad \Gamma_{2u}: q_{n2}=0;\quad \Gamma_{2s}: q_{n2}=0;\quad \Gamma_{2e}:\ q_{n2}(t) = \beta_2\left[C_2(t) - C_{2\infty}\right];\ \tag{4}$$

The fourth-kind conditions on the internal boundaries Γ_N as well as the initial conditions at the beginning of the process have the form

$$\begin{gathered}C_1^{(i)}(\mathbf{x},t) = C_1^{(i+1)}(\mathbf{x},t);\ C_2^{(i)}(\mathbf{x},t) = C_2^{(i+1)}(\mathbf{x},t);\quad \mathbf{x}\in\Gamma_N \\ C_1(\mathbf{x},0) = C_{10};\ C_2(\mathbf{x},0) = C_{20};\ \mathbf{x}\in(\Omega\cup\Gamma)\end{gathered} \tag{5}$$

Let us introduce an arbitrary behavioral functional associated with the diffusion problem

$$F=\int_0^{t_f}\left[\int_\Omega \Psi_1(C_1,\nabla C_1,\mathbf{q}_1,\dot{C}_1)\,d\Omega+\int_\Gamma \gamma_1(C_1,q_{n1},C_{1\infty})\,d\Gamma\right]dt+$$
$$\int_0^{t_f}\left[\int_\Omega \Psi_2(C_2,\nabla C_2,\mathbf{q}_2,\dot{R}_2,\dot{C}_2)\,d\Omega+\int_\Gamma \gamma_2(C_2,q_{n2},C_{2\infty})\,d\Gamma\right]dt; \tag{6}$$

where Ψ_1; Ψ_2; γ_1; γ_2 are the integrands which are the continuous and differentiable functions of the listed arguments. The first-order sensitivity is the material derivative of the functional (6) with respect to design parameters $F_p=DF/Db_p$. The correlation can be transformed to the basic equation of the first-order sensitivity, cf. Korycki [4]

$$F_p=\int_0^{t_f}\left\{\int_\Omega\left[\Psi_{1,C_1}(C_1)_p+\nabla_{C_1}\Psi_1(\nabla C_1)_p+\Psi_{1,q_1}(\mathbf{q}_1)_p+\Psi_{1,\dot{C}_1}(\dot{C}_1)_p+\Psi_1 v^p{}_{,x}\right]d\Omega+\right.$$
$$\int_\Omega\left[\Psi_{2,C_2}(C_2)_p+\nabla_{C_2}\Psi_2(\nabla C_2)_p+\Psi_{2,q_2}(\mathbf{q}_2)_p+\Psi_{2,\dot{R}_2}(\dot{R}_2)_p+\Psi_{2,\dot{C}_2}(\dot{C}_2)_p+\Psi_2 v^p{}_{,x}\right]d\Omega+$$
$$\int_\Gamma\left[\gamma_{1,C_1}(C_1)_p+\gamma_{1,q_{n1}}(q_{n1})_p+\gamma_{1,C_{1\infty}}(C_{1\infty})_p+\gamma_1\left(\mathrm{div}_\Gamma\mathbf{v}^p-2H\gamma_1 v_n^p\right)\right]d\Gamma+ \tag{7}$$
$$\left.\int_\Gamma\left[\gamma_{2,C_2}(C_2)_p+\gamma_{2,q_{n2}}(q_{n2})_p+\gamma_{2,C_{2\infty}}(C_{2\infty})_p+\gamma_2\left(\mathrm{div}_\Gamma\mathbf{v}^p-2H\gamma_2 v_n^p\right)\right]d\Gamma\right\}dt;$$

where $\Psi_{1,C_1}=\dfrac{\partial\Psi_1}{\partial C_1}$; $\nabla_{C_1}\Psi_1=\left|\dfrac{\partial\Psi_1}{\partial C_{1,x}};\dfrac{\partial\Psi_1}{\partial C_{1,y}}\right|$; $\Psi_{1,\mathbf{q}_1}=\dfrac{\partial\Psi_1}{\partial\mathbf{q}_1}$; $\Psi_{1,\dot{C}_1}=\dfrac{\partial\Psi_1}{\partial\dot{C}_1}$; $\Psi_{1,\dot{R}_2}=\dfrac{\partial\Psi_1}{\partial\dot{R}_2}$; etc.

The sensitivity is analyzed by using the direct approach convenient for a few design variables **b**, cf. Dems, Korycki, Rousselet [3], Korycki [4]. We determine the set of additional problems associated with variation of each design parameter. The additional structure has the same shape and the diffusion properties as the primary body. The state equation, boundary and initial conditions for the additional body are determined by the differentiation of the equations for the primary structure with respect to the variable b_p; p=1..P. The state variables are the concentrations $C_1^p=\partial C_1/\partial b_p$; $C_2^p=\partial C_2/\partial b_p$. The solutions of the problem associated with each design parameter are the additional state fields on the boundary and within the structure. The state equation for the exudate diffusion in the i-th layer are obtained from Eq.(1)

$$\mathrm{div}\mathbf{q}_1^{p(i)}=\dot{C}_1^{p(i)}\;;\;\dot{C}_1^{p(i)}=\frac{dC_1^{p(i)}}{dt}\;;\;\mathbf{q}_1^{p(i)}=D_1^{(i)}\nabla C_1^{p(i)}+\mathbf{q}_1^{*p(i)};\quad \text{within }\Omega. \tag{8}$$

The boundary conditions for the additional structure are defined on the portions shown in Fig.1, by introducing the material derivative correlations (cf. Dems, Korycki, Rousselet [3], Korycki [4]) and the convection coefficients which are design variables independent

$$\Gamma_{1b}\text{: } C_1^p=\left(C_1^{01}\right)^p=\left(C_1^{01}\right)_p-\nabla C_1^{01}\cdot\mathbf{v}^p\;;\quad \Gamma_{1w}\text{: } C_1^p=\left(C_1^{02}\right)^p=\left(C_1^{02}\right)_p-\nabla C_1^{02}\cdot\mathbf{v}^p\;;$$
$$\Gamma_{1u}\text{: } q_{n1}^p=\mathbf{n}\cdot\mathbf{q}_1^p=\left(q_{n1}^0\right)_p+\mathbf{q}_{1\Gamma}^0\cdot\nabla_\Gamma v_n^p-\nabla_\Gamma q_{n1}^0\cdot\mathbf{v}_\Gamma^p-q_{n1,n}^0 v_n^p=0\;;$$
$$\Gamma_{1s}\text{: } q_{n1}^p=\mathbf{n}\cdot\mathbf{q}_1^p=\left(q_{n1}^0\right)_p+\mathbf{q}_{1\Gamma}^0\cdot\nabla_\Gamma v_n^p-\nabla_\Gamma q_{n1}^0\cdot\mathbf{v}_\Gamma^p-q_{n1,n}^0 v_n^p=0\;; \tag{9}$$
$$\Gamma_{1e}\text{: } q_{n1}^p=q_{n1}^p(t)=\beta_1\left[C_1^p(t)-C_{1\infty}^p\right]+\mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p.$$

The state equation for the microcasulated therapeutic agent is defined by the differentiation of the state correlation for the particular layer of composite material Eq.(3)

$$\begin{aligned} &\mathrm{div}\mathbf{q}_2^{p(i)} + \dot{R}_2^{p(i)} = \dot{C}_2^{p(i)} \;\; ; \;\; \dot{C}_2^{p(i)} = \frac{dC_2^{p(i)}}{dt} \;\; ; \;\; \dot{R}_2^{p(i)} = \frac{dR_2^{p(i)}}{dt}; \\ &\mathbf{q}_2^{p(i)} = D_2^{(i)} \nabla C_2^{p(i)} + \mathbf{q}_2^{*p(i)} \;\; ; \;\; \text{within } \Omega. \end{aligned} \tag{10}$$

The conditions on the external boundaries can be obtained by differentiation of Eqs.(5)

$$\begin{aligned} &\Gamma_{2b}: \;\; q_{n2}^p = q_{n2}^{0p} = \left(q_{n2}^0\right)_p - \nabla q_n^0 \cdot \mathbf{v}^p; \\ &\Gamma_{2u}: \; q_{n2}^p = \mathbf{n}\cdot\mathbf{q}_2^p = \left(q_{n2}^0\right)_p + \mathbf{q}_{2\Gamma}^0 \cdot \nabla_\Gamma v_n^p - \nabla_\Gamma q_{n2}^0 \cdot \mathbf{v}_\Gamma^p - q_{n2,n}^0 v_n^p = 0; \\ &\Gamma_{2s}: \; q_{n2}^p = \mathbf{n}\cdot\mathbf{q}_2^p = \left(q_{n2}^0\right)_p + \mathbf{q}_{2\Gamma}^0 \cdot \nabla_\Gamma v_n^p - \nabla_\Gamma q_{n2}^0 \cdot \mathbf{v}_\Gamma^p - q_{n2,n}^0 v_n^p = 0; \\ &\Gamma_{1e}: \;\; q_{n2}^p = q_{n2}^p(t) = \beta_2\left[C_2^p(t) - C_{2\infty}^p\right] + \mathbf{q}_{2\Gamma}\cdot\nabla_\Gamma v_n^p. \end{aligned} \tag{11}$$

The fourth-kind boundary conditions on the internal boundaries and the initial conditions of both concentrations are obtained by the same method in the form

$$\begin{aligned} &C_1^{p(i)}(\mathbf{x},t) = C_1^{p(i+1)}(\mathbf{x},t); \qquad C_2^{p(i)}(\mathbf{x},t) = C_2^{p(i+1)}(\mathbf{x},t); \quad x \in \Gamma_T \\ &C_1^p(x,0) = C_{10}^p = \left(C_{10}\right)_p - \nabla C_1 \cdot \mathbf{v}^p; \quad x \in (\Omega \cup \Gamma); \\ &C_2(x,0) = C_{20}^p = \left(C_{20}\right)_p - \nabla C_2 \cdot \mathbf{v}^p; \quad x \in (\Omega \cup \Gamma). \end{aligned} \tag{12}$$

To determine the first-order sensitivity expression we integrate by parts and in time the corresponding terms of Eq.(7) and introduce Eqs.(9) and Eqs.(11). For more details I refer the reader to [3] for the steady problem as well as [4] for the transient problem. The external boundary Γ is composed for the exudate diffusion of: (i) the part contacting the skin $\Gamma_{11}=\Gamma_{1b}\cup\Gamma_{1w}$; (ii) the diffusive isolated part $\Gamma_{12}=\Gamma_{1u}\cup\Gamma_{1s}$; (iii) the part $\Gamma_{13}=\Gamma_{1e}$ subjected to the diffusive convection. The external boundary for the diffusion of therapeutic agent has: (i) the part $\Gamma_{22}=\Gamma_{2b}\cup\Gamma_{2u}\cup\Gamma_{2s}$ of the assumed diffusive flux density; (ii) the part $\Gamma_{23}=\Gamma_{2e}$ subjected to the diffusive convection. We formulate also the following first-order sensitivity correlation

$$\begin{aligned} F_P = &\left[\int_\Omega \Psi_{1,\dot{C}_1} C_1^p d\Omega\right]_0^{t_f} + \left[\int_\Omega \Psi_{1,\dot{C}_2} C_2^p d\Omega\right]_0^{t_f} + \\ &\int_0^{t_f}\left\{\int_\Omega\left[\left(\Psi_{1,C_1} - \frac{d}{dt}\left(\Psi_{,\dot{C}_1}\right)\right)C_1^p + \nabla_{\nabla C_1}\Psi_1 \cdot \nabla C_1^p + \nabla_{\mathbf{q}_1}\Psi_1 \cdot \mathbf{q}_1^p\right]d\Omega + \right. \\ &\int_\Omega\left[\left(\Psi_{2,C_2} - \frac{d}{dt}\left(\Psi_{,\dot{C}_2}\right)\right)C_2^p + \nabla_{\nabla C_2}\Psi_2 \cdot \nabla C_2^p + \nabla_{\mathbf{q}_2}\Psi_2 \cdot \mathbf{q}_2^p + \Psi_{,\dot{R}_2}\dot{R}_2^p\right]d\Omega + \\ &\int_{\Gamma_{11}}\left[\gamma_{1,C_1}\left(C_{1p}^0 - \nabla_\Gamma C_1^0 \cdot \mathbf{v}_\Gamma^p - C_{1,n}^0 v_n^p\right) + \gamma_{1,q_{n1}}\left(q_{n1}^p - \mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p\right)\right]d\Gamma_{11} + \\ &\int_{\Gamma_{12}}\left[\gamma_{1,C_1} C_1^p + \gamma_{1,q_{n1}}\left(q_{n1p}^0 - \nabla_\Gamma q_{n1}^0 \cdot \mathbf{v}_\Gamma^p - q_{n1,n}^0 \cdot v_n^p\right)\right]d\Gamma_{12} + \\ &\int_{\Gamma_{22}}\left[\gamma_{1,C_2} C_2^p + \gamma_{2,q_{n2}}\left(q_{n2p}^0 - \nabla_\Gamma q_{n2}^0 \cdot \mathbf{v}_\Gamma^p - q_{n2,n}^0 \cdot v_n^p\right)\right]d\Gamma_{22} + \\ &\int_{\Gamma_{13}}\left[\gamma_{1,C_1} C_1^p + \gamma_{1,q_{n1}}\beta_1\left(C_1^p - C_{1\infty}^p\right)\right]d\Gamma_{13} + \int_{\Gamma_{23}}\left[\gamma_{2,C_2} C_2^p + \gamma_{2,q_{n2}}\beta_2\left(C_2^p - C_{2\infty}^p\right)\right]d\Gamma_{23} + \\ &\int_\Gamma\left[\left(\Psi_1 + \gamma_{1,n} - 2H\gamma_1\right)v_n^p + \left(\Psi_2 + \gamma_{2,n} - 2H\gamma_2\right)v_n^p\right]d\Gamma \\ &\left. + \int_\Gamma\left(\gamma_{1,C_{1\infty}} C_{1\infty}^p + \gamma_{2,C_{2\infty}} C_{2\infty}^p\right)d\Gamma + \int_\Sigma\left]\gamma_1\mathbf{v}^p\cdot\boldsymbol{\upsilon}\right[+ \int_\Sigma\left]\gamma_2\mathbf{v}^p\cdot\boldsymbol{\upsilon}\right[\right\}dt; \qquad p = 1, 2, \ldots P. \end{aligned} \tag{13}$$

The expression is a sum of the integrals defined in time, within the domain Ω, on the whole external boundary Γ, the particular parts of the external boundary, and along the discontinuity line Σ, cf. Dems, Mróz [5]. The first two terms are the time integrals for the time values $t_{initial}=0$; $t_{final}=t_f$. To determine the direct approach to sensitivity analysis we have to solve the primary problem and P additional problems. The number of problems is the same as the number of design variables P, we solve also (P+1) problems. Each additional problem for the exudate diffusion is described by the state equation Eq.(8) as well as the set of conditions, cf. Eqs.(9), (12). The additional problem for therapeutic agent is given by Eqs.(10)–(12).

4. Shape optimization problem

The shape of the dressing structure can be obtained with respect to minimum or maximum of the functional of the diffusion flux density on the whole or the part of external boundary. The composite dressings are characterized by the diffusion flux densities of both agents $q_{n1}>0$ and $q_{n2}>0$ and the objective functional has the form

$$F=\int_0^{t_f}\left[\int_\Gamma (q_{n1}+q_{n2})\,d\Gamma\right]dt\ ;\ \Gamma\in\Gamma_{ext} \tag{14}$$

Minimization of the above functional corresponds to the optimal diffusive isolator whereas the model of diffusive radiator requires the maximization of the functional.

Shape optimization is the minimization or maximization of the objective functional with the imposed constraint on the structural cost K. Let us assume the homogenized structure of the cost which is linear function of the domain Ω. The factor of proportionality is the unit cost of structure u, and the problem can be defined in the form

$$F\to\min\ \text{ or }(-F)\to\min \qquad \text{for} \qquad K-K_0=\int_\Omega u\,d\Omega-K_0\le 0. \tag{15}$$

Considering the stationarity of the Lagrange functional and introducing the slack variable ξ for the inequality problems, we formulate the general form of optimality conditions

$$\frac{DF}{Db_p}=-\chi\frac{DK}{Db_p}=-\chi\int_\Omega uv_n^p d\Omega \quad \text{and} \quad \int_\Omega u\,d\Omega-K_0+\xi^2=0. \tag{16}$$

The left-hand side of the first equation contains the first-order sensitivity DF/Db_p. It is clear, that the form of the optimality conditions depends on the form of the objective functional.

5. Numerical example

Let us optimize the shape of the composite dressing made of three material layers. There is no free space between the composite and the dressing to improve the therapeutic effect. The dressing layers are connected like the composite and the structure contacts directly the skin. The most used material is the non-woven fabric, because the draining of exudate to the surrounding and the transport of therapeutic agent to the skin are optimal. The internal layer contacting the skin is made of the non-woven fabrics, the central layer contains the microcapsules, and the external layer is made of the non-wovens subjected to the finishing procedure. Design variables are 15 coordinates of the points within the structure, cf. Fig.3.

The non-woven fabrics is a typical porous material of the pores diameter less than the mean value of the free path of the diffusing molecules. The diffusion is so-called Knudsen diffusion of the coefficient described by the formula, cf. Gilron, Soffer [2] $D_j=\frac{2}{3}d_p\sqrt{2RT/\Pi M_j}$.

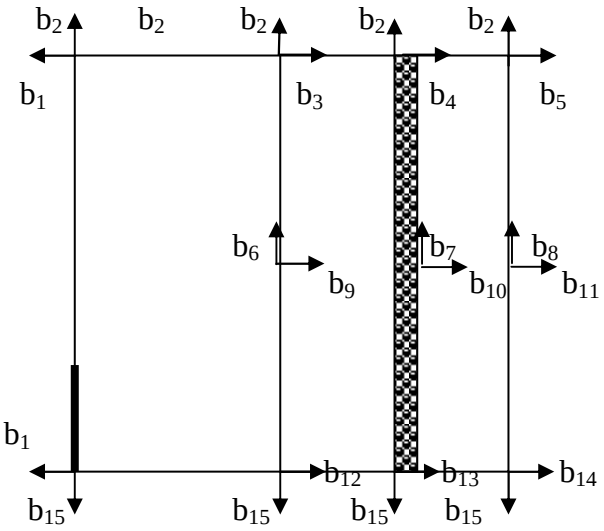

Figure 3. Design parameters of textile composite dressing

The diameter of pores within the non-woven for the dressing is equal to $d_p=5\cdot10^{-4}$ m, whereas for the layers with microcapsules and after the finishing $d_p=3.5\cdot10^{-4}$ m. The temperature is assumed T=310K. The molar mass depends on the agent. Thus, the molecules of exudate are composed from the body fluid of a low concentration of the elements and the molar mass can be assumed the same as for the water vapor M_1=18kg/kmol. The therapeutic agent is the liquid substance which can have the different molar masses. Let us introduce the water solution of NaCl (50% of water and 50% of NaCl) of the molar mass 38 kg/kmol.

The time changes from $t_0=0$ to $t_k=600$s in 5 steps with the increase $\Delta t=120$s. The diffusive convection on the external boundary is described by coefficients $\beta_1=10^{-3}$m/s; $\beta_2=0{,}25\cdot10^{-3}$m/s. Let us assume the distribution of the agent concentrations in the surrounding $C_{1\infty}=0{,}1C_1$ on Γ_{1e}; $C_{2\infty}=0{,}1C_2$ on Γ_{2e}. The flux density of the therapeutic agent on the skin is arbitrary assumed as the parabolic function of time. The boundary and initial conditions have the form

$$D_1^{\text{simple non-woven}}=1.01\cdot10^{-7}\ \text{m}^2/\text{s};\quad D_1^{\text{micr+finishing}}=0.70\cdot10^{-7}\ \text{m}^2/\text{s};$$
$$D_2^{\text{simple non-woven}}=0.69\cdot10^{-7}\ \text{m}^2/\text{s};\quad D_2^{\text{micr+finishing}}=0.48\cdot10^{-7}\ \text{m}^2/\text{s}.$$
$$\Gamma_{1b}:\ C_1=C_1^{01}=0{,}01\ \text{kmol/m}^3=\text{const};$$
$$\Gamma_{1w}:\ C_1=C_1^{02}(t)=0{,}05\left[1-0{,}2t/3600\right]\text{kmol/m}^3;$$
$$\Gamma_{1u}:\ q_n=0;\qquad \Gamma_{1s}:\ q_n=0;\qquad \Gamma_{1e}:\ q_n=q_{c1}(t)=\beta_1(C_1-C_{1\infty}).$$
$$\Gamma_{2b}:\ q_n=q_n^0(t)=1{,}5\cdot10^{-4}\left[1-10^{-4}\ t/3600-10^{-3}(t/3600)^2\right]\text{kmol}/(\text{m}^2\text{s}); \qquad (17)$$
$$\Gamma_{2u}:\ q_n=0;\qquad \Gamma_{2s}:\ q_n=0;\qquad \Gamma_{2e}:\ q_n=q_{c2}(t)=\beta_2(C_2-C_{2\infty}).$$
$$C_1(\mathbf{x},0)=C_{10}=\left[0{,}05\,x^2/b^2-0{,}1\,x/b+0{,}05\right]\text{kmol/m}^3;\quad \mathbf{x}\in(\Omega\cup\Gamma)$$
$$C_2(\mathbf{x},0)=C_{20}=\begin{cases}0{,}5\cdot10^{-4}x/x_M+1{,}5\cdot10^{-4} & \text{kmol/m}^3\\ -0{,}85\cdot10^{-4}(x-x_M)/(b-x_M)+2\cdot10^{-4} & \text{kmol/m}^3\end{cases};\quad \mathbf{x}\in(\Omega\cup\Gamma)$$

Let us optimize the shape of the diffusive radiator with imposed equality constraint on the cost

$$\begin{cases}F=\int_0^{t_f}\left[\int_{\Gamma_{1e}}q_{n1}\,d\Gamma_{1e}+\int_{\Gamma_{2e}}q_{n2}\,d\Gamma_{2e}\right]dt\to\max\ \Rightarrow\ F=-\int_0^{t_f}\left[\int_{\Gamma_{1e}}q_{n1}\,d\Gamma_{1e}+\int_{\Gamma_{2e}}q_{n2}\,d\Gamma_{2e}\right]dt\to\min;\\ \text{subject to}\ C-C_0=0.\end{cases} \qquad (18)$$

Let us compose the external boundary from a few piecewise linear portions, the curvatures of the boundary are H→0. Assuming the material derivatives $\left(C_1^{01}\right)_p$ on Γ_{1b}; $\left(C_1^{02}\right)_p$ on Γ_{1w}; $\left(C_{10}\right)_p$ within $(\Omega \cup \Gamma)$; $\left(q_{n2}^0\right)_p$ on Γ_{2b}; and $\left(C_{20}\right)_p$ on $(\Omega \cup \Gamma)$ known in advance, we obtain the optimal shape shown in Fig.4.

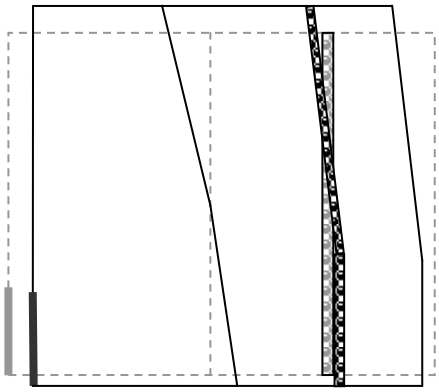

Figure 4. Initial (broken line) and optimal (continuous line) shapes of optimized structure

6. Conclusions

The aim of the paper is to apply the sensitivity analysis in the shape optimization for the oppositely directed coupled diffusion within textile dressings. The first-order sensitivity vector is formulated by means of the material derivative concept and the direct approach. The advantage is the relatively simple form of both state equations and boundary conditions.
The optimal solution was improved with 18,5% in comparison to the initial value of the objective functional. The dressing is equipped with the semi-permeable membrane and the diffusive flux density caused by the exudate diffusion is greater than that for therapeutic agent. It follows that the functional reduction is consequently caused by maximization of the exudate diffusion. We introduce also an effective tool for generating the optimal shapes for a wide class of design and redesign problems within the composite textile dressings.

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