Sensitivity oriented shape optimization and identification during opposite coupled diffusion within composites

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Abstract

The special structures of textile dressings contain the therapeutic substance in microcapsules. The diffusion of the activating agent (the exudate from the wound) through the material initiates the chemical reaction within microcapsules and releases the therapeutic agent. The semi-permeable membrane on the surface reduces the diffusion of therapeutic agent to surrounding, whereas the exudate diffuses normally. The oppositely directed coupled diffusion is analyzed within 2D cross-section of dressing. State variables are both activating agent concentration and therapeutic substance concentration. State equations, boundary and initial conditions are determined. The sensitivity of an arbitrary functional is analyzed by means of direct and adjoint approaches and implemented into the problem of shape optimization. Numerical example of 2D shape optimization is presented.

Keywords: shape optimization, sensitivity analysis, oppositely directed diffusion, composites

1. Oppositely directed diffusion within dressings

The opposite coupled diffusion is typical for the multilayer textile dressings and characterized by two connected processes, cf. Korycki [7,8]. The activating agent diffuses through the structure and initiates the diffusion of the complexing agent in the opposite direction. The transport of complexing agent to the surrounding is mechanically reduced by the semi-permeable membrane within the composite structure. The activating agent is the exudate from the wound, the complexing agent is the therapeutic substance from microcapsules within the dressing. The microcapsules are introduced during the stitching process but its internal distribution is irregular and difficult to describe.

The typical dressing is the simple non-woven subjected to the finishing process. The typical structure has: (i) the internal layers which drain the exudates from the wound; (ii) the layer with the therapeutic substance in microcapsules; (iii) the semi-permeable membrane and (iv) the external protective layer subjected to finishing procedure. The exudate diffuses from the wound through the composite structure to the surrounding. The prescribed fluid concentration initiates the chemical reaction within microcapsules. The process begins after the dead time and the gradient of diffusion velocity of therapeutic agent increases rapidly. This agent is transferred from microcapsules to the skin, because the semi-permeable membrane secures the one direction. The exudate flux from the wound is reduced after the duration time, the gradient of the exudate diffusion velocity decreases progressively.

The state variables are the activating agent concentration C_1 and the complexing agent concentration C_2. Design variables are the coordinates of the selected points in the composite **b**.

Let us assume the same cross-section of the structure and the boundary conditions, which simplify the analysis from 3D to 2D problem. The dressing structure is complicated because the textile parts have the special shape to secure the transport of: (i) the exudate from the skin to the surrounding; (ii) the therapeutic agent from the microcapsules to the skin.

The structure are made of the textile materials and some parts are covered by the microcapsules. The principle of the oppositely directed diffusion is shown in Fig.1. The basic mathematical correlations for the simple diffusion cf. Crank [1].

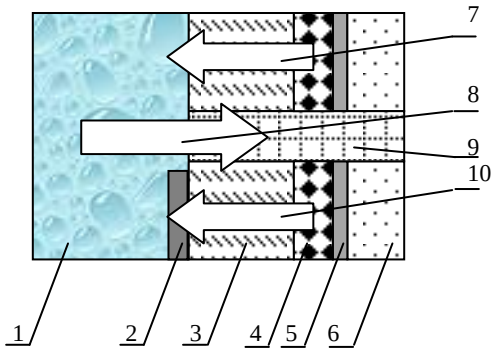

Figure 1: Oppositely directed diffusion in composite dressings
1: skin, 2: wound, 3: internal textile layer; 4: pcm-layer, microcapsules, 5: membrane, 6: external textile layer, 7 and 10: diffusion of therapeutic agent, 8: exudate diffusion, 9: textile layer securing the exudate transport

2. Primary opposite coupled diffusion

The diffusion problem is complicated and depends on the structure of textile dressing. The basic principle is easy and described by two processes of elementary diffusion, cf [1]. Let us first define the physical model of the problem.

The exudate is transported from the source (i.e. the wound), through the dressing and by diffusive convection from the external surface to the surrounding. This agent is not subjected to the chemical reaction. The state equation can be expressed for the i-th layer of the dressing as follows

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

where C_1 is the activating agent concentration, D_1 is the diffusion coefficient, $\mathbf{q}_1$ is the vector of diffusion flux density, $\mathbf{q}_1^*$ is the vector of initial diffusion flux density.

Physically speaking, the dressing contacts the skin and the wound. The boundary sections Γ_{1b} Γ_{1w} are subjected to the first-kind conditions of the prescribed concentrations of the exudate. The exudate is transported in the one direction and the upper Γ_{1u}

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as well as the symmetry part Γ_{1s} are subjected to the second-kind condition. The external boundary Γ_{1e} has the defined diffusive convection, i.e. the third-kind conditions. The internal boundaries Γ_{1n} are subjected to fourth-kind conditions. The problem is accompanied by the initial condition. The set of conditions has the form

$$\Gamma_{1b}\colon C_1 = C_1^{01};\quad \Gamma_{1w}\colon C_1 = C_1^{02}(t);\quad \Gamma_{1u}\colon q_{n1}=0;\quad \Gamma_{1s}\colon q_{n1}=0;$$

$$\Gamma_{1e}\colon q_{n1}(t)=\beta_1\left[C_1(t)-C_{1\infty}\right]\ ;\ \Gamma_{1N}\colon C_1^{(i)}(\mathbf{x},t)=C_1^{(i+1)}(\mathbf{x},t).$$
$$C_1(\mathbf{x},0)=C_{10};\quad \mathbf{x}\in(\Omega\cup\Gamma) \tag{2}$$

where $q_{n1}=\mathbf{n}\cdot\mathbf{q}_1$ is the diffusion flux density normal to the external boundary, β_1 is the convection coefficient, $C_{1\infty}$ is the agent concentration in the surrounding. The conditions are shown in Fig.2.

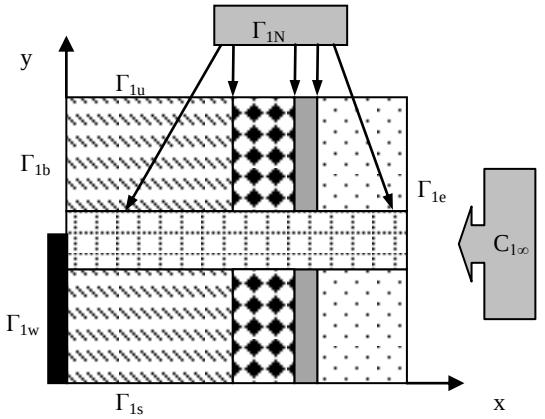

Figure 2: Boundary conditions for the exudate diffusion

The therapeutic agent is transported from the microcapsules, through the dressing to the skin. This agent is subjected to the chemical reaction for the layers containing the microcapsules and not subjected for the other layers. The state equation for the i-th layer of the dressing has the form [7]

$$\mathrm{div}\mathbf{q}_2^{(i)}+\dot{R}_2^{(i)}=\dot{C}_2^{(i)}\ ;\ \dot{C}_2^{(i)}=\frac{dC_2^{(i)}}{dt}\ ;$$
$$\dot{R}_2^{(i)}=\begin{cases}\dfrac{dR_2^{(i)}}{dt} & \text{pcm-layer}\\ 0 & \text{non-pcmlayer}\end{cases};\ \mathbf{q}_2^{(i)}=D_2^{(i)}\nabla C_2^{(i)}+\mathbf{q}_2^{*(i)};\ \text{within}\Omega. \tag{3}$$

where $\dot{R}_2$ is the chemical reaction velocity of the agent.

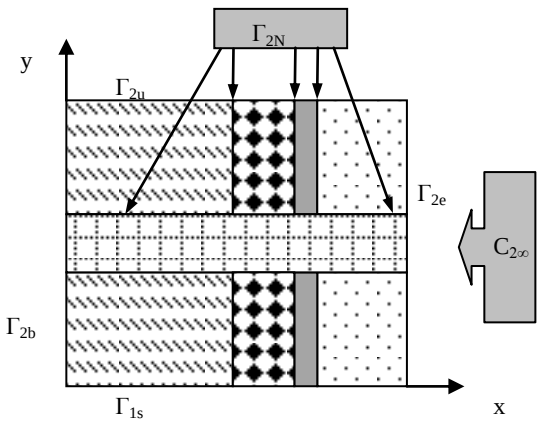

Figure 3: Boundary conditions for therapeutic agent diffusion

Therapeutic agent is transported to the skin. It follows that the heat flux density of the substance is defined on this portion Γ_{2b}. The upper Γ_{2u} and the symmetry Γ_{2s} boundary portions are subjected to the second-kind conditions. The external part Γ_{2e} of the boundary is subjected to diffusive convection. The internal portions Γ_{2n} are subjected to the fourth-kind conditions. The boundary and the initial conditions are the following, cf. Fig.3

$$\Gamma_{2b}\colon q_{n2}=q_{n2}^0(t);\quad \Gamma_{2u}\colon q_{n2}=0;\quad \Gamma_{2s}\colon q_{n2}=0;$$

$$\Gamma_{2e}\colon q_{n2}(t)=\beta_2\left[C_2(t)-C_{2\infty}\right]\ ;\ \Gamma_{2N}\colon C_2^{(i)}(\mathbf{x},t)=C_2^{(i+1)}(\mathbf{x},t).$$
$$C_2(\mathbf{x},0)=C_{20};\quad \mathbf{x}\in(\Omega\cup\Gamma) \tag{4}$$

3. First-order sensitivity analysis

The shape optimization and identification need to introduce the sensitivity concept of the analysis. First-order sensitivity is defined as the material derivative of the objective functional F with respect to design parameters b_p, i.e. $F_p=DF/Db_p$. We introduce an arbitrary behavioral functional associated with the above diffusion problems in the following form

$$F=\int_0^{t_f}\left[\int_\Omega \Psi_1(C_1,\nabla C_1,\mathbf{q}_1,\dot{C}_1)\,d\Omega+\int_\Gamma \gamma_1(C_1,q_{n1},C_{1\infty})\,d\Gamma\right]dt+$$
$$\int_0^{t_f}\left[\int_\Omega \Psi_2(C_2,\nabla C_2,\mathbf{q}_2,\dot{R}_2,\dot{C}_2)\,d\Omega+\int_\Gamma \gamma_2(C_2,q_{n2},C_{2\infty})\,d\Gamma\right]dt; \tag{5}$$

We can analyze the problem by means of both direct and adjoint approaches. The direct approach is more convenient for calculating the sensitivities of entire response field with respect to a few design variables **b**, cf. [2]. We introduce the set of additional diffusion problems associated with variation of each design parameter. The state equations and the boundary conditions are defined by differentiation of the primary equations with respect to the variable b_p; p=1..P. The state variables are the concentrations for the additional approach $C_1^p=\partial C_1/\partial b_p$; $C_2^p=\partial C_2/\partial b_p$.

Thus, the state equation within the i-th layer can be given with respect to Eq.(1) in the form

$$\mathrm{div}\mathbf{q}_1^{p(i)}=\dot{C}_1^{p(i)}\ ;\ \dot{C}_1^{p(i)}=\frac{dC_1^{p(i)}}{dt}\ ;$$
$$\mathbf{q}_1^{p(i)}=D_1^{(i)}\nabla C_1^{p(i)}+\mathbf{q}_1^{*p(i)};\ \text{within}\Omega. \tag{6}$$

The conditions for the exudate diffusion can be formulated with respect to Eqs.(2) as follows

$$\Gamma_{1b}\colon C_1^p=\left(C_1^{01}\right)^p=\left(C_1^{01}\right)_p-\nabla C_1^{01}\cdot\mathbf{v}^p;$$
$$\Gamma_{1w}\colon C_1^p=\left(C_1^{02}\right)^p=\left(C_1^{02}\right)_p-\nabla C_1^{02}\cdot\mathbf{v}^p;$$
$$\Gamma_{1u}\colon q_{n1}^p=\mathbf{n}\cdot\mathbf{q}_1^p=\left(q_{n1}^0\right)_p+\mathbf{q}_{1\Gamma}^0\cdot\nabla_\Gamma v_n^p-\nabla_\Gamma q_{n1}^0\cdot\mathbf{v}_\Gamma^p-q_{n1,n}^0 v_n^p=0;$$
$$\Gamma_{1s}\colon q_{n1}^p=\mathbf{n}\cdot\mathbf{q}_1^p=\left(q_{n1}^0\right)_p+\mathbf{q}_{1\Gamma}^0\cdot\nabla_\Gamma v_n^p-\nabla_\Gamma q_{n1}^0\cdot\mathbf{v}_\Gamma^p-q_{n1,n}^0 v_n^p=0;$$
$$\Gamma_{1e}\colon q_{n1}^p=q_{n1}^p(t)=\beta_1\left[C_1^p(t)-C_{1\infty}^p\right]+\mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p.$$
$$\Gamma_{1N}\colon C_1^{p(i)}(\mathbf{x},t)=C_1^{p(i+1)}(\mathbf{x},t).$$
$$C_1^p(x,0)=C_{10}^p=\left(C_{10}\right)_p-\nabla C_1\cdot\mathbf{v}^p;\quad x\in(\Omega\cup\Gamma) \tag{7}$$

The boundary conditions can be still introduced along the boundaries shown in Fig.2.

The necessary equations for the diffusion of the therapeutic agent are obtained by the differentiation of the primary problem equations. The state equation has the form with respect to Eqs.(3)

$$\mathrm{div}\mathbf{q}_2^{p(i)} + \dot{R}_2^{p(i)} = \dot{C}_2^{p(i)};\ \dot{C}_2^{p(i)} = \frac{dC_2^{p(i)}}{dt};$$

$$\dot{R}_2^{p(i)} = \begin{cases} \dfrac{dR_2^{p(i)}}{dt} & \text{for pcm-layer} \\ 0 & \text{for non-pcm layer} \end{cases};$$

$$\mathbf{q}_2^{p(i)} = D_2^{(i)} \nabla C_2^{p(i)} + \mathbf{q}_2^{*p(i)};\ \text{within}\Omega. \tag{8}$$

Next, we formulate the boundary conditions. Let us differentiate the Eqs.(4) with respect to design variable b_p

$$\Gamma_{2b}:\ q_{n2}^p = \mathbf{n}\cdot\mathbf{q}_2^p = \left(q_{n2}^0\right)_p + \mathbf{q}_{2\Gamma}^0 \cdot \nabla_\Gamma v_n^p - \nabla_\Gamma q_{n2}^0 \cdot \mathbf{v}_\Gamma^p - q_{n2n}^0 v_n^p;$$

$$\Gamma_{2u}:\ q_{n2}^p = \mathbf{n}\cdot\mathbf{q}_2^p = \left(q_{n2}^0\right)_p + \mathbf{q}_{2\Gamma}^0 \cdot \nabla_\Gamma v_n^p - \nabla_\Gamma q_{n2}^0 \cdot \mathbf{v}_\Gamma^p - q_{n2n}^0 v_n^p = 0;$$

$$\Gamma_{2s}:\ q_{n2}^p = \mathbf{n}\cdot\mathbf{q}_2^p = \left(q_{n2}^0\right)_p + \mathbf{q}_{2\Gamma}^0 \cdot \nabla_\Gamma v_n^p - \nabla_\Gamma q_{n2}^0 \cdot \mathbf{v}_\Gamma^p - q_{n2n}^0 v_n^p = 0;$$

$$\Gamma_{2e}:\ q_{n2}^p = q_{n2}^p(t) = \beta_2\left[C_2^p(t) - C_{2\infty}^p\right] + \mathbf{q}_{2\Gamma}\cdot\nabla_\Gamma v_n^p.$$

$$\Gamma_{2N}:\ C_2^{p(i)}(\mathbf{x},t) = C_2^{p(i+1)}(\mathbf{x},t).$$

$$C_2(\mathbf{x},0) = C_{20}^p = \left(C_{20}\right)_p - \nabla C_2\cdot\mathbf{v}^p;\ \ \mathbf{x}\in(\Omega\cup\Gamma) \tag{9}$$

The problem should be accompanied by the sensitivity correlation. We can formulate these equation after some transformations by introducing the general form according [7]

$$F_p = \left[\int_\Omega \Psi_1, _{\dot{C}_1} C_1^p d\Omega\right]_0^{t_f} + \left[\int_\Omega \Psi_1, _{\dot{C}_2} C_2^p d\Omega\right]_0^{t_f} +$$

$$\int_0^{t_f}\left\{\int_\Omega\left[\left(\Psi_1, _{C_1} - \frac{d}{dt}\left(\Psi, _{\dot{C}_1}\right)\right)C_1^p + \nabla_{\nabla C_1}\Psi_1\cdot\nabla C_1^p + \nabla_{\mathbf{q}_1}\Psi_1\cdot\mathbf{q}_1^p\right]d\Omega +\right.$$

$$\left.\int_\Omega\left[\left(\Psi_2, _{C_2} - \frac{d}{dt}\left(\Psi, _{\dot{C}_2}\right)\right)C_2^p + \nabla_{\nabla C_2}\Psi_2\cdot\nabla C_2^p + \nabla_{\mathbf{q}_2}\Psi_2\cdot\mathbf{q}_2^p + \Psi, _{\dot{R}_2}\dot{R}_2^p\right]d\Omega +\right.$$

$$\int_{\Gamma_{1b}}\left[\gamma_1, _{C_1}\left(C_{1p}^{01} - \nabla_\Gamma C_1^{01}\cdot\mathbf{v}_\Gamma^p - C_1^{01}, _n v_n^p\right) + \gamma_1, _{q_{n1}}\left(q_{n1}^p - \mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p\right)\right]d\Gamma_{1b} +$$

$$\int_{\Gamma_{1w}}\left[\gamma_1, _{C_1}\left(C_{1p}^{02} - \nabla_\Gamma C_1^{02}\cdot\mathbf{v}_\Gamma^p - C_1^{02}, _n v_n^p\right) + \gamma_1, _{q_{n1}}\left(q_{n1}^p - \mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p\right)\right]d\Gamma_{1w} +$$

$$\int_{\Gamma_{1u}}\gamma_1, _{C_1} C_1^p\, d\Gamma_{1u} + \int_{\Gamma_{1s}}\gamma_1, _{C_1} C_1^p\, d\Gamma_{1s} +$$

$$\int_{\Gamma_{2b}}\left[\gamma_1, _{C_2} C_2^p + \gamma_2, _{q_{n2}}\left(q_{n2p}^0 - \nabla_\Gamma q_{n2}^0\cdot\mathbf{v}_\Gamma^p - q_{n2}^0, _n\cdot v_n^p\right)\right]d\Gamma_{2b} +$$

$$\int_{\Gamma_{2u}}\gamma_1, _{C_2} C_2^p\, d\Gamma_{2u} + \int_{\Gamma_{2s}}\gamma_1, _{C_2} C_2^p\, d\Gamma_{2s} +$$

$$\int_{\Gamma_{1e}}\left[\gamma_1, _{C_1} C_1^p + \gamma_1, _{q_{n1}}\beta_1\left(C_1^p - C_{1\infty}^p\right)\right]d\Gamma_{1e} +$$

$$\int_{\Gamma_{2e}}\left[\gamma_2, _{C_2} C_2^p + \gamma_2, _{q_{n2}}\beta_2\left(C_2^p - C_{2\infty}^p\right)\right]d\Gamma_{2e} +$$

$$\int_\Gamma\left[\left(\Psi_1 + \gamma_1, _n - 2H\gamma_1\right)v_n^p + \left(\Psi_2 + \gamma_2, _n - 2H\gamma_2\right)v_n^p\right]d\Gamma$$

$$\left.+\int_\Gamma\left(\gamma_1, _{C_{1\infty}} C_{1\infty}^p + \gamma_2, _{C_{2\infty}} C_{2\infty}^p\right)d\Gamma + \int_\Sigma\right]\gamma_1\mathbf{v}^p\cdot\boldsymbol{\upsilon}\left[+\int_\Sigma\right]\gamma_2\mathbf{v}^p\cdot\boldsymbol{\upsilon}\left.\right\}dt;$$

$$p = 1, 2, \ldots P. \tag{10}$$

The above expression is a sum of the integrals defined:

- for the characteristic values of time $t_{initial}=0$; $t_{final}=t_f$,
- in time for the whole structure,
- within the domain Ω,
- on the whole external boundary Γ,
- on the particular parts of the external boundary,
- along the discontinuity line Σ (cf. Dems, Mróz [3]).

We should solve the primary problem and a set of additional problems associated with each design parameter. The number of problems is the same as the number of design variables P, we solve summarizing (P+1) problems. Each additional problem is described by the state equation Eq.(6) and the set of boundary and initial conditions, cf. Eqs.(7). The additional problem for therapeutic agent is given by the state equation Eqs.(8) and boundary conditons Eqs.(9).

The alternative solution is the adjoint approach which is convenient for calculating the sensitivities with respect to a few optimization functionals, cf. [2]. The adjoint problem is defined by the state equation, boundary and initial conditions of the similar form as the primary equations. The state variables are the concentrations of both activating and therapeutic agents for the adjoint structure C_1^a; C_2^a. The state equation of exudate diffusion has the form

$$\mathrm{div}\mathbf{q}_1^{a(i)} = \dot{C}_1^{a(i)};\ \dot{C}_1^{a(i)} = \frac{dC_1^{a(i)}}{d\tau};$$
$$\mathbf{q}_1^{a(i)} = D_1^{(i)}\nabla C_1^{a(i)} + \mathbf{q}_1^{*a(i)};\ \text{within}\Omega \tag{11}$$

The boundary and initial conditions have the general form analogical to the correlations for the primary problem

$$\Gamma_{1b}:\ C_1^a = C_1^{01a};\ \ \Gamma_{1w}:\ C_1^a = C_1^{02a}(t);\ \ \Gamma_{1u}:\ q_{n1}^a = 0;\ \Gamma_{1s}:\ q_{n1}^a = 0;$$

$$\Gamma_{1e}:\ q_{n1}^a(t) = \beta_1\left[C_1^a - C_{1\infty}^a\right];\ \Gamma_{1N}:\ C_1^{a(i)}(\mathbf{x},t) = C_1^{a(i+1)}(\mathbf{x},t).$$

$$C_1^{a(i)}(\mathbf{x},t) = C_1^{a(i+1)}(\mathbf{x},t);\ \ \mathbf{x}\in(\Omega\cup\Gamma) \tag{12}$$

The adjoint problem of therapeutic agent is defined by means of the state equations in the form

$$\mathrm{div}\mathbf{q}_2^{a(i)} + \dot{R}_2^{a(i)} = \dot{C}_2^{a(i)};\ \dot{C}_2^{a(i)} = \frac{dC_2^{a(i)}}{d\tau};$$

$$\dot{R}_2^{a(i)} = \begin{cases} \dfrac{dR_2^{(i)}}{d\tau} & \text{for pcm-layer} \\ 0 & \text{for non-pcm layer} \end{cases}; \tag{13}$$

$$\mathbf{q}_2^{a(i)} = D_2^{(i)}\nabla C_2^{a(i)} + \mathbf{q}_2^{*a(i)};\ \text{within}\Omega.$$

The boundary conditions are formulated by the form analogical to Eqs.(4) defined for the primary problem

$$\Gamma_{2b}:\ q_{n2}^a = q_{n2}^{0a}(t);\ \ \Gamma_{2u}:\ q_{n2}^a = 0;\ \ \Gamma_{2s}:\ q_{n2}^a = 0;$$

$$\Gamma_{2e}:\ q_{n2}^a(t) = \beta_2\left[C_2^a - C_{2\infty}^a\right];\ \Gamma_{2N}:\ C_2^{a(i)}(\mathbf{x},t) = C_2^{a(i+1)}(\mathbf{x},t) \tag{14}$$

The necessary state fields are defined by means of the identities for the adjoint structure. Introducing the correlations according [7,8], we have the following state fields

$$C_1^a(\mathbf{x},\tau=0) = \Psi, _{\dot{C}_1}(\mathbf{x},t=t_f)\ \text{within}(\Omega\cup\Gamma);$$

$$C_2^a(\mathbf{x},\tau=0) = \Psi, _{\dot{C}_2}(\mathbf{x},t=t_f)\ \text{within}(\Omega\cup\Gamma);$$

$$\dot{R}_2^a(\mathbf{x},\tau) = \Psi_2, _{C_2}(\mathbf{x},t) - \frac{d}{dt}\Psi_2, _{\dot{C}_2}(\mathbf{x},t)\ \text{within}\Omega;$$

$$\mathbf{q}_1^{*a}(\mathbf{x},\tau) = \nabla_{\nabla C_1}\Psi_1(\mathbf{x},t) + \nabla_{\mathbf{q}_1}\Psi_1(\mathbf{x},t)\cdot D_1\ \text{within}\Omega;$$

$$\mathbf{q}_2^{*a}(\mathbf{x},\tau) = \nabla_{\nabla C_2}\Psi_2(\mathbf{x},t) + \nabla_{\mathbf{q}_2}\Psi_2(\mathbf{x},t)\cdot D_2\ \text{within}\Omega;$$

$$C_1^{0a}(\mathbf{x},\tau) = \gamma_1, _{q_{n1}}(\mathbf{x},t)\ \text{on}\ \Gamma_{1b}\ \text{and}\ \Gamma_{1w};$$

$$q_{n1}^{0a}(\mathbf{x},\tau) = -\gamma_1, _{C_1}(\mathbf{x},t)\ \text{on}\ \Gamma_{1u}\ \text{and}\ \Gamma_{1s};$$

$$q_{n2}^{0a}(\mathbf{x},\tau) = -\gamma_2, _{C_2}(\mathbf{x},t)\ \text{on}\ \Gamma_{2b}\ \text{and}\ \Gamma_{2u}\ \text{and}\ \Gamma_{2s};$$

$$C_{1\infty}^a(\mathbf{x},\tau) = \frac{1}{\beta_1}\gamma_1, _{C_1}(\mathbf{x},t) + \gamma_1, _{q_{n1}}(\mathbf{x},t)\ \text{on}\ \Gamma_{1e};$$

$$C_{2\infty}^a(\mathbf{x},\tau) = \frac{1}{\beta_2}\gamma_2, _{C_2}(\mathbf{x},t) + \gamma_2, _{q_{n2}}(\mathbf{x},t)\ \text{on}\ \Gamma_{2e} \tag{15}$$

The problem should be accompanied by the sensitivity correlations. Thus, we introduce now the Eq.(10) as well as the Eqs.(11) – (15) and finally describe

$$
\begin{aligned}
&F_p = -\left[\int_\Omega \left(\Psi_{1,\dot{C}_1} - C_1^a\right)\left(C_{1p} - \nabla C_1 \cdot \mathbf{v}^p\right) d\Omega\right]_{t=0} \\
&-\left[\int_\Omega \left(\Psi_{2,\dot{C}_2} - C_2^a\right)\left(C_{2p} - \nabla C_2 \cdot \mathbf{v}^p\right) d\Omega\right]_{t=0} + \\
&\int_0^{t_f}\left\{\int_\Omega \left(\nabla_{q_1}\Psi_1 + \nabla C_1^a\right)\cdot \mathbf{q}_1^{*p} d\Omega + \right. \\
&\int_\Omega \left[\left(\nabla_{q_2}\Psi_2 + \nabla C_2^a\right)\cdot \mathbf{q}_2^{*p} + \left(\Psi_{2,\dot{R}_2} + C_2^a\right)\dot{R}_2^p\right] d\Omega + \\
&\int_{\Gamma_{1b}} \left[\left(\gamma_{1,C_1} + q_{n1}^a\right)\left(C_{1p}^{01} - \nabla_\Gamma C_1^{01}\cdot \mathbf{v}_\Gamma^p - C_{1,n}^{01} v_n^p\right) - \gamma_{1,q_{n1}}\mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p\right] d\Gamma_{1b} + \\
&\int_{\Gamma_{1w}} \left[\left(\gamma_{1,C_1} + q_{n1}^a\right)\left(C_{1p}^{02} - \nabla_\Gamma C_1^{02}\cdot \mathbf{v}_\Gamma^p - C_{1,n}^{02} v_n^p\right) - \gamma_{1,q_{n1}}\mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p\right] d\Gamma_{1w} + \\
&\int_{\Gamma_{1u}} \left[-C_1^a \mathbf{q}_{1\Gamma}^0\cdot\nabla_\Gamma v_n^p\right] d\Gamma_{1u} + \int_{\Gamma_{1s}} \left[-C_1^a \mathbf{q}_{1\Gamma}^0\cdot\nabla_\Gamma v_n^p\right] d\Gamma_{1s} + \\
&\int_{\Gamma_{2b}} \left[\left(\gamma_{2,q_{n2}} - C_2^a\right)\left(q_{n2p}^0 - \nabla_\Gamma q_{n2}^0\cdot\mathbf{v}_\Gamma^p - q_{n2,n}^0 v_n^p\right) - C_2^a \mathbf{q}_{2\Gamma}^0\cdot\nabla_\Gamma v_n^p\right] d\Gamma_{2b} + \\
&\int_{\Gamma_{2u}} \left[-C_2^a \mathbf{q}_{2\Gamma}^0\cdot\nabla_\Gamma v_n^p\right] d\Gamma_{2u} + \int_{\Gamma_{2s}} \left[-C_2^a \mathbf{q}_{2\Gamma}^0\cdot\nabla_\Gamma v_n^p\right] d\Gamma_{2s} + \\
&\int_{\Gamma_{1e}} \left[C_1^a \beta_1 C_{1\infty}^p - C_1^a \mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p - \gamma_{1,q_{n1}}\beta_1 C_{1\infty}^p\right] d\Gamma_{1e} + \\
&\int_{\Gamma_{2e}} \left[C_2^a \beta_2 C_{2\infty}^p - C_2^a \mathbf{q}_{2\Gamma}\cdot\nabla_\Gamma v_n^p - \gamma_{2,q_{n2}}\beta_2 C_{2\infty}^p\right] d\Gamma_{2e} + \\
&\int_\Gamma \left[\Psi_1 + \Psi_2 + \gamma_{1,n} + \gamma_{2,n} - 2H\left(\gamma_1 + \gamma_2\right)\right] v_n^p \, 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 (16)
\end{aligned}
$$

The above expression is a sum of the integrals defined:

- for the initial time $t_{initial}=0$,
- in time for the whole structure,
- within the domain Ω,
- on the whole external boundary Γ,
- on the particular parts of the external boundary,
- along the discontinuity line Σ (cf. Dems, Mróz [3]).

We solve the primary problem and a set of adjoint problems associated with each optimization functional. The number of problems is the same as the number of functionals N, we solve summarizing (N+1) problems. For the most simple problem of the one objective functional we have to solve 1 primary and 1 adjoint problem, i.e. two problems. Each adjoint problem is described by the state equation Eqs(11) and the set of boundary and initial conditions, cf. Eqs.(12) and Eqs.(15). The additional problem for therapeutic agent is given by the state equations Eqs.(13) and the conditions Eqs.(14) and (15).

4. Problems of shape optimization and identification

Mathematically speaking, the shape optimization problem is the minimization or maximization of the objective functional with the imposed constraint on the structural cost J. 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. The optimality conditions are determined by means of the discussed first-order sensitivities. Generally speaking the optimization problem has the basic form

$$
\begin{cases}
F \to \min \;\; \text{or} \left(-F\right) \to \min; \\
J - J_0 = \int_\Omega u \, d\Omega - J_0 \le 0.
\end{cases} \qquad (17)
$$

To obtain the minimum of the objective functional we have to introduce the stationarity of the Lagrange functional given for inequality problems by means of the slack variable ξ as follows

$$
F' = F + \chi\left(J - J_0 + \xi^2\right); \qquad (18)
$$

where J is the structural cost and J_0 is the assumed value of the cost. Consequently we obtain the optimality conditions in the well-known form for the inequality problems

$$
\begin{cases}
\dfrac{DF}{Db_p} = -\chi \dfrac{DK}{Db_p} = -\chi \int_\Omega u v_n^p d\Omega \\
\int_\Omega u \, d\Omega - J_0 + \xi^2 = 0.
\end{cases} \qquad (19)
$$

The particular form of the optimality conditions in Eqs.(19) depends on the form of the objective functional. Let us define a few typical optimization functionals.

We can optimize the structure by minimizing or maximizing the diffusion flux density on the whole or the part of external boundary. Thus, the measure is the following sum

$$
F = \int_0^{t_f}\left[\int_\Gamma \left(q_{n1} + q_{n2}\right) d\Gamma\right] dt \; ; \; \Gamma \in \Gamma_{ext} \qquad (20)
$$

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

The functional can be the global measure of local maximum concentrations. Minimization of this functional secures the minimization of concentration distribution in the optimal shape

$$
F = \int_0^{t_f}\left[\int_\Omega \left[\left(\frac{C_1}{C_{10}}\right)^n + \left(\frac{C_2}{C_{20}}\right)^n\right] d\Omega\right]^{\frac{1}{n}} dt \; ; \; n \to \infty \qquad (21)
$$

For $n \to \infty$ the objective functional is the global measure of maximal local concentrations within the optimal domain Ω.

Shape identification is the search of the real shape of the textile products by introducing the current values of state variables and the state variables for the real shape. We introduce the model of the textile product because the identification needs the change of the structural shape. The state variables are measured along the whole or the part of the external boundary.

Mathematically speaking, the shape identification is the minimization of the objective functional without constraints. The stationarity conditions are formulated by means of the sensitivity correlations and have the form

$$
F \to \min \Rightarrow F_p = \frac{DF}{Db_p} = 0 \qquad (22)
$$

where DF/Db_p is the first-order sensitivity of the objective functional with respect to the design variables.

The most popular identification functional is the distance between the concentrations C_1 C_2 of the model and the real structure C_{1m} C_{2m} on the part Γ_m of the external boundary

$$
F = \frac{1}{2}\int_0^{t_f}\left[\int_{\Gamma_m}\left[\left(C_1 - C_{1m}\right)^2 + \left(C_2 - C_{2m}\right)^2\right] d\Gamma_m\right] dt \; ; \; \Gamma_m \in \Gamma_{ext} \qquad (23)
$$

The objective functional can be the measure of the concentrations calculated and measured. The functional defined is homogeneous and reduces the distance between the concentrations of the model and the real body.

$$
F = \frac{1}{2}\int_0^{t_f}\left[\int_{\Gamma_m}\left[\left(\frac{C_1}{C_{1m}}\right)^n + \left(\frac{C_2}{C_{2m}}\right)^n\right] d\Gamma_m\right] dt \; ; \; n \to \infty; \; \Gamma_m \in \Gamma_{ext} \qquad (24)
$$

Minimization of the above functional for n →∞ causes the minimization of the distance between the concentrations as well as the minimization of the maximal local values.
The objective functional can be the global measure of the local state variables, defined in time and along the boundary. Thus, the form is similar to the most popular functional Eq.(23). The basic form was introduced by Mota Soares [10] to describe the mechanical properties of the composite materials. The same functional can be applied to describe the vibration problems. The simple adaptation allows to describe

$$G = \frac{1}{2}\int_0^{t_f}\left[\int_{\Gamma_m}\frac{\left[(C_1)^2-(C_{1m})^2\right]^2}{(C_{1m})^4}d\Gamma_m+\int_{\Gamma_m}\frac{\left[(C_2)^2-(C_{2m})^2\right]^2}{(C_{2m})^4}d\Gamma_m\right]dt \quad (25)$$

The one functional introduced has the specified form which simplify the problem, particularly the form of the first-order sensitivity correlation.

5. Numerical example of shape optimization

Let us optimize the textile dressing made of the different material layers, Fig.4. The main goal is to secure the transport of the exudate from the skin to the surrounding and the therapeutic agent from the microcapsules to the wound. We can apply the special textile layer transporting the exudate directly to the surrounding. A part of the moisture contacts the microcapsules and dissolves the therapeutic agent. The diffusion is oppositely directed and the heat flux of the therapeutic substance reach the skin.

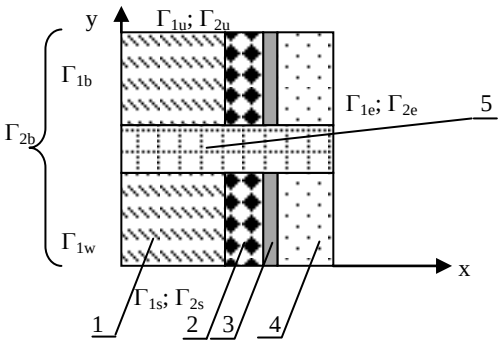

Figure 4: Structure of composite dressings
1: internal layer, 2: pcm-layer (microcapsules), 3: membrane, 4: external textile layer, 5: layer securing the exudate transport

The composite dressing contacts directly the skin to force and secure the therapeutic effect. Thus, the air layers within the structure are minimized. We assume the negligible thickness of the air layer between the dressing and the skin.

The most common material is the non-woven fabric because the exudate diffuses within the material very easy. The external layer is made of the non-woven fabric subjected to the finishing procedure, which changes the physical properties. The different properties are also within the layer with microcapsules. The semi-permeable membrane is a thin layer made of polyamide, polyester or polypropylene.

The diffusion process is defined by the diffusion coefficient within the material. We describe the diffusion coefficient by the Knudsen diffusion within the pores of the diameter less than the mean value of the free path of the diffusing molecules. The typical formula is according Gilron, Soffer [4]

$$D_j = \frac{2}{3}d_p\sqrt{\frac{2RT}{\Pi M_j}} \quad (26)$$

Alternatively we determine the diffusion coefficient within the fabric material and homogenize the material to describe the coefficient for the whole fabrics. Li and Luo [9] introduce the diffusion coefficients as time-dependent. At the first-stage the coefficient depends on the moisture concentration within the material and is the quadratic function. The second-stage begins after the equilibrium time t_{eq}=540s and the diffusion process is slow. Assuming now that the non-woven fabric is made of basic cotton material, we describe the following diffusion coefficients for the j-th agent according Haghi [6]

$$D_j = \left[0{,}8481+50{,}6\frac{C_j}{\rho}-1100\left(\frac{C_j}{\rho}\right)^2\right]\cdot 10^{-14};\ t<540s; \quad (27)$$

$$D_j = 2{,}5\left\{1-\exp\left[-3{,}5385\exp\left(-45\frac{C_j}{\rho}\right)\right]\right\}\cdot 10^{-14};\ t\geq 540s$$

where ρ is the density of the fibers.

The finishing procedure changes the physical properties. The diffusion coefficient is assumed arbitrarily as follows

$$D_j = \left[0{,}9+45\frac{C_j}{\rho}-1000\left(\frac{C_j}{\rho}\right)^2\right]\cdot 10^{-14};\ t<540s; \quad (28)$$

$$D_j = 2{,}5\left\{1-\exp\left[-3{,}5385\exp\left(-40\frac{C_j}{\rho}\right)\right]\right\}\cdot 10^{-14};\ t\geq 540s$$

The diffusion coefficient within the air is time-independent as well as material-independent and equal to

$$D_j = 2{,}5e^{-5} \quad (29)$$

The structure should be homogenized by means of "rule of mixture", cf. Golanski, Terada, Kikuchi [5] as the analogy to the mixture and its components. This method gives the good results to the composites. The substitute diffusion coefficient is now equal to

$$D_j = D_{j\,mat}\,\xi_{mat} + D_{j\,fil}\,\xi_{fil};$$
$$\xi_{mat} = \frac{V_{mat}}{V_{mat}+V_{fil}};\ \xi_{fil} = \frac{V_{fil}}{V_{mat}+V_{fil}}, \quad (30)$$

where ξ_{mat} and ξ_{fil} are the volume coefficients of the textile material of the volume V_{mat} and the free spaces between material of the volume V_{fil}. The substitute diffusion coefficients within the non-woven fabric, layer with microcapsules and layer after the finishing procedure are equal to

$$D_1^{\text{simple non-woven}} = 1.05\cdot 10^{-11}\frac{m^2}{s};\ D_1^{\text{micr+finishing}} = 0.70\cdot 10^{-11}\frac{m^2}{s};$$
$$D_2^{\text{simple non-woven}} = 0.62\cdot 10^{-11}\frac{m^2}{s};\ D_2^{\text{micr+finishing}} = 0.42\cdot 10^{-11}\frac{m^2}{s}. \quad (31)$$

The diffusion coefficient for the polypropylene fibers is time-independent and equal to

$$D_j = 1{,}3e^{-13} \quad (32)$$

Let us first introduce the transient problem of the initial t_0=0 and final time t_f=600s divided into 5 steps of the time Δt=120s.

The state equation for the exudate diffusion within each layer is determined by Eq.(1). The exudate is not subjected to the chemical reaction. The boundary Γ_{1b} is characterized by the constant exudate concentration. The exudate concentration from the wound Γ_{1w} changes linearly as the arbitrary, time-dependent function. The external boundary is described by the convection of the coefficient $\beta_1=10^{-3}$m/s. The surrounding concentrations

for the exudate is equal to $C_{1\infty}=0{,}1C_1$. The boundary conditions for the activating agent are according to Eqs.(2) equal to

$$\Gamma_{1b}:\ C_1=C_1^{01}=0{,}01\ \text{kmol/m}^3=\text{const};$$

$$\Gamma_{1w}:\ C_1=C_1^{02}(t)=0{,}05\left[1-\frac{1{,}5t}{36000}\right]\text{kmol/m}^3;$$

$$\Gamma_{1u}{:}q_{n1}=0;\quad \Gamma_{1s}{:}q_{n1}=0;\quad \Gamma_{1e}{:}\ q_{n1}(t)=\beta_1\left[C_1(t)-C_{1\infty}\right];$$

$$\Gamma_{1N}:\ C_1^{(i)}(\mathbf{x},t)=C_1^{(i+1)}(\mathbf{x},t). \tag{33}$$

The state equation for the diffusion of therapeutic agent within each layer of dressing is determined by Eq.(3). Let us assume the chemical reaction velocity $\dot{R}_2=2\cdot10^{-4}$kmol/(m^{3}s) within microcapsules and $\dot{R}_2=0$ for other layers. The diffusive flux density of the therapeutic agent on Γ_{2b} is assumed as the parabolic function of time. The external boundary is described by the diffusive convection of the coefficient $\beta_2=0{,}25\cdot10^{-3}$m/s. The surrounding concentration for the therapeutic agent is respectively equal to $C_{2\infty}=0{,}1C_2$. The boundary conditions for the activating agent are according to Eqs.(4) equal to

$$\Gamma_{2b}:\ q_n=1{,}5\cdot10^{-4}\left[1-10^{-4}\frac{1{,}5t}{3600}-10^{-3}\left(\frac{1{,}5t}{3600}\right)^2\right]\text{kmol}/(\text{m}^2\text{s});$$

$$\Gamma_{2u}{:}q_{n2}=0;\quad \Gamma_{2s}{:}q_{n2}=0;$$

$$\Gamma_{2e}:\ q_{n2}(t)=\beta_2\left[C_2(t)-C_{2\infty}\right];\ \Gamma_{2N}:\ C_2^{(i)}(\mathbf{x},t)=C_2^{(i+1)}(\mathbf{x},t). \tag{34}$$

The initial condition for the exudate is assumed as the parabolic function of coordinate x along the cross-section of dressing cf. Fig.4, and for the therapeutic agent as the linear functions of x. We can denote

$$C_1(\mathbf{x},0)=\left[0{,}05\frac{x^2}{b^2}-0{,}1\frac{x}{b}+0{,}05\right]\text{kmol/m}^3;$$

$$C_2(\mathbf{x},0)=\begin{cases}\dfrac{0.5\cdot10^{-4}}{x_M}x+1.5\cdot10^{-4}\quad \text{kmol/m}^3\\ -\dfrac{0.85\cdot10^{-4}}{b-x_M}(x-x_M)+2\cdot10^{-4}\quad \text{kmol/m}^3\end{cases}. \tag{35}$$

where b is the width of the textile structure assumed as $b=1.5\cdot10^{-2}$m; $x_M=0.75b$ is the initial coordinate of the membrane location. The exudate is removed from the wound by the draining of the textile material and through the diffusive convection to the surrounding. The less the exudate within the material the better the pharmacological effect. Thus, the shape optimization is to create the diffusive radiator with imposed equality constraint on the cost in the form

$$\begin{cases}F=F=\int\limits_0^{t_f}\left[\int\limits_{\Gamma_{1e}}q_{n1}d\Gamma_{1e}+\int\limits_{\Gamma_{2e}}q_{n1}d\Gamma_{2e}\right]dt\to\max;\\ \text{subject to}\ C-C_0=0.\end{cases} \tag{36}$$

which is equivalent to the following minimization

$$\begin{cases}F=F=-\int\limits_0^{t_f}\left[\int\limits_{\Gamma_{1e}}q_{n1}d\Gamma_{1e}+\int\limits_{\Gamma_{2e}}q_{n1}d\Gamma_{2e}\right]dt\to\min;\\ \text{subject to}\ C-C_0=0.\end{cases} \tag{37}$$

The problem can be simplified for the piecewise linear portions, because the main curvatures of the boundary are now negligible $H\to0$.

Let us define the direct approach to sensitivity analysis. The state equations for the exudate diffusion are formulated by means of Eqs.(6), whereas the boundary conditions by Eqs.(7). Assuming the material derivatives $\left(C_1^{01}\right)_p$ on the portion Γ_{1b}; $\left(C_1^{02}\right)_p$ on the part Γ_{1w}; and $\left(C_{10}\right)_p$ within $(\Omega\cup\Gamma)$ as known in advance, we define the additional structure for exudate diffusion in the form

$$\Gamma_{1b}:\ C_1^p=\left(C_1^{01}\right)^p=-\nabla C_1^{01}\cdot\mathbf{v}^p;\qquad \Gamma_{1w}:\ C_1^p=\left(C_1^{02}\right)^p=-\nabla C_1^{02}\cdot\mathbf{v}^p;$$

$$\Gamma_{1u}:\ q_{n1}^p=\mathbf{n}\cdot\mathbf{q}_1^p=0;\qquad \Gamma_{1s}:\ q_{n1}^p=\mathbf{n}\cdot\mathbf{q}_1^p=0;$$

$$\Gamma_{1e}:\ q_{n1}^p=q_{n1}^p(t)=\beta_1\left[C_1^p(t)-C_{1\infty}^p\right]+\mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p.$$

$$\Gamma_{1N}:\ C_1^{p(i)}(\mathbf{x},t)=C_1^{p(i+1)}(\mathbf{x},t).$$

$$C_1^p(x,0)=C_{10}^p=-\nabla C_1\cdot\mathbf{v}^p;\quad x\in(\Omega\cup\Gamma) \tag{38}$$

The state equation for the diffusion of the therapeutic agent are formulated by the Eqs.(8). Introducing next the material derivatives $\left(q_{n2}^0\right)_p$ on Γ_{2b}; and $\left(C_{20}\right)_p$ on $(\Omega\cup\Gamma)$ as known in advance, we formulate the following conditions

$$\Gamma_{2b}:\ q_{n2}^p=\mathbf{n}\cdot\mathbf{q}_2^p=\mathbf{q}_{2\Gamma}^0\cdot\nabla_\Gamma v_n^p-\nabla_\Gamma q_{n2}^0\cdot\mathbf{v}_\Gamma^p-q_{n2n}^0v_n^p=0;$$

$$\Gamma_{2u}:\ q_{n2}^p=\mathbf{n}\cdot\mathbf{q}_2^p=0;\qquad \Gamma_{2s}:\ q_{n2}^p=\mathbf{n}\cdot\mathbf{q}_2^p=0;$$

$$\Gamma_{2e}:\ q_{n2}^p=q_{n2}^p(t)=\beta_2\left[C_2^p(t)-C_{2\infty}^p\right]+\mathbf{q}_{2\Gamma}\cdot\nabla_\Gamma v_n^p.$$

$$\Gamma_{2N}:\ C_2^{p(i)}(\mathbf{x},t)=C_2^{p(i+1)}(\mathbf{x},t).$$

$$C_2^p(x,0)=C_{20}^p=-\nabla C_2\cdot\mathbf{v}^p;\quad x\in(\Omega\cup\Gamma) \tag{39}$$

The first-order sensitivity vector can be determined by the simple adaptation of Eq.(10). Defining the objective functional by Eq.(37), we have the following first-order sensitivity vector

$$F_p=-\int_0^{t_f}\left\{\int_{\Gamma_{1e}}\beta_1\left(C_1^p-C_{1\infty}^p\right)d\Gamma_{1e}+\int_{\Gamma_{2e}}\beta_2\left(C_2^p-C_{2\infty}^p\right)d\Gamma_{2e}+\right.$$

$$\left.\int_{\Gamma_{1e}}q_{n1,n}v_n^p\,d\Gamma_{1e}+\int_{\Gamma_{2e}}q_{n2,n}v_n^p\,d\Gamma_{2e}+\int_\Sigma\right]q_{n1}\mathbf{v}^p\cdot\boldsymbol{\upsilon}\left[+\int_\Sigma\right]q_{n2}\mathbf{v}^p\cdot\boldsymbol{\upsilon}\left[\right\}dt;$$

$$p = 1, 2, \ldots P. \tag{40}$$

Let us next determine the state equations for the adjoint structure of dressing. The state equation of the exudate diffusion is defined by Eq.(11) and the set of conditions in general form by Eqs.(12). The adjoint problem of therapeutic agent is defined by means of Eqs.(13), the boundary and initial conditions by Eqs.(14). Let us define the integrands according Eqs.(37). Thus, the state fields introduced by Eqs.(15) have now the form

$$C_1^a(\mathbf{x},\tau=0)=0\ \text{within}(\Omega\cup\Gamma);\quad C_2^a(\mathbf{x},\tau=0)=0\ \text{within}(\Omega\cup\Gamma);$$

$$\dot{R}_2^a(\mathbf{x},\tau)=0\ \text{ within}\Omega;\qquad \mathbf{q}_1^{*a}(\mathbf{x},\tau)=0\ \text{within}\Omega;$$

$$\mathbf{q}_2^{*a}(\mathbf{x},\tau)=0\ \text{within}\Omega;\qquad C_1^{0a}(\mathbf{x},\tau)=0\ \text{on}\Gamma_{1b}\ \text{and}\Gamma_{1w};$$

$$q_{n1}^{0a}(\mathbf{x},\tau)=0\ \text{on}\Gamma_{1u}\ \text{and}\Gamma_{1s};$$

$$q_{n2}^{0a}(\mathbf{x},\tau)=0\ \text{on}\Gamma_{2b}\ \text{and}\Gamma_{2u}\ \text{and}\Gamma_{2s};$$

$$C_{1\infty}^a(\mathbf{x},\tau)=\gamma_{1,q_{n1}}(\mathbf{x},t)=-1\ \text{on}\Gamma_{1e};$$

$$C_{2\infty}^a(\mathbf{x},\tau)=\gamma_{2,q_{n2}}(\mathbf{x},t)=-1\ \text{on}\Gamma_{2e} \tag{41}$$

The first-order sensitivity vector by means of Eq.(16). Introducing the integrands according to Eqs.(37) we obtain

$$F_p=-\left[\int_\Omega C_1^a\left(\nabla C_1\cdot\mathbf{v}^p\right)d\Omega\right]_{t=0}-\left[\int_\Omega C_2^a\left(\nabla C_2\cdot\mathbf{v}^p\right)d\Omega\right]_{t=0}+$$

$$\int_0^{t_f}\left\{\int_\Omega\nabla C_1^a\cdot\mathbf{q}_1^{*p}d\Omega+\int_\Omega\left[\nabla C_2^a\cdot\mathbf{q}_2^{*p}\right]d\Omega+\right.$$

$$- \int_{\Gamma_{1b}} \left[q^{a}_{n1} \left(\nabla_{\Gamma} C_1^{01} \cdot \mathbf{v}^{p}_{\Gamma} + C_{1,n}^{01} v^{p}_{n} \right) \right] d\Gamma_{1b} +$$

$$- \int_{\Gamma_{1w}} \left[q^{a}_{n1} \left(\nabla_{\Gamma} C_1^{02} \cdot \mathbf{v}^{p}_{\Gamma} + C_{1,n}^{02} v^{p}_{n} \right) \right] d\Gamma_{1w} +$$

$$- \int_{\Gamma_{2b}} \left[C^{a}_{2} \left(\nabla_{\Gamma} q^{0}_{n2} \cdot \mathbf{v}^{p}_{\Gamma} + q^{0}_{n2,n} v^{p}_{n} \right) + \mathbf{q}^{0}_{2\Gamma} \cdot \nabla_{\Gamma} v^{p}_{n} \right] d\Gamma_{2b} + \int_{\Gamma_{1e}} q_{n1,n} v^{p}_{n} \, d\Gamma_{1e} +$$

$$\int_{\Gamma_{2e}} q_{n2,n} v^{p}_{n} \, d\Gamma_{2e} + \int_{\Sigma} \left] q_{n1} \mathbf{v}^{p} \cdot \boldsymbol{\upsilon} \right[+ \int_{\Sigma} \left] q_{n2} \mathbf{v}^{p} \cdot \boldsymbol{\upsilon} \right[\Big\} dt \, ; \qquad (42)$$

Let us analyze the example which shows the applicability of the theory to the real problems of oppositely directed diffusion.

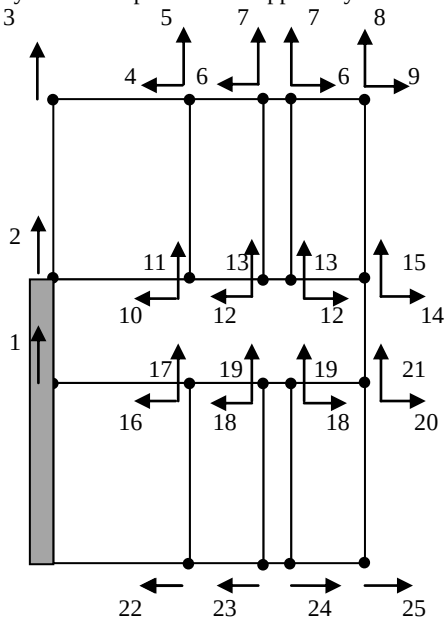

Figure 5: Design parameters of shape optimization problem

The independent design parameters are 25 coordinates of the selected, crucial points on the boundaries, depicted by the arrows $b_1 - b_{25}$ in Fig.5. Let us next introduce the additional constraints for the membrane, i.e. the coordinate changes should be not greater than 20% in relation to the initial location. The additional constraint is the same change of the dimensions for the central layer securing the exudate transport.

The iterative optimization algorithm introduces the analysis-synthesis procedure. The analysis step was performed by means of the Finite Element Method. The 2D structure domain was discretized by means of the Finite Elements Net of 4-nodal elements to determine the state variables. We should solve first the primary problem, next respectively the additional or the adjoint one. The final results are the sensitivity expressions within the domain and on the external boundary necessary to formulate the optimality conditions for the problem. At the synthesis stage we determine the increase of the coordinates of the nodal points of the Finite Element Net. The second-order Newton procedure, cf. for example Novruzzi, Roche [11], as well as the method of steepest descent are applied alternatively to find the directional minimum of the objective functional. The optimal shape of the textile dressing is shown in Fig.6. The optimal objective functional is equal to 82,17% the initial value.

We see at once that the optimal boundaries of the particular layers are located parallel to the initial shapes. Only one difference is the layer securing the exudate transport from the skin to the surrounding. This layer is much more wide than the initial one. The obtained shape simplify the transport of the exudate immediately to the surrounding.

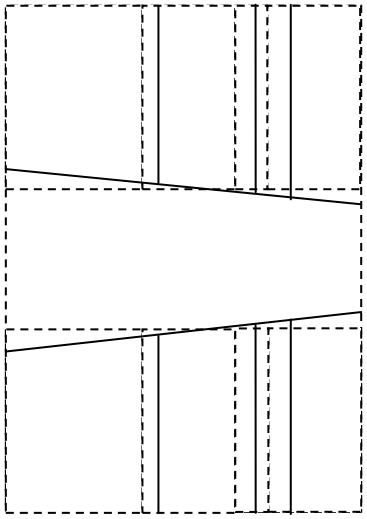

Figure 6: Initial and optimal shapes of textile dressing
------ initial shape ——— optimal shape

6. Numerical example of shape identification

Let us identify the obtained optimal shape of the textile dressing subjected to the oppositely directed diffusion. The primary problem is defined by means of the above discussed Eq.(25) – Eq.(36).

The objective functional is now the distance between the concentrations C_1 C_2 of the model and the real structure C_{1m} C_{2m} on the external boundary

$$F = \frac{1}{2} \int_0^{t_f} \left[\int_{\Gamma_{1e}} \left(C_1 - C_{1m} \right)^2 d\Gamma_{1e} + \int_{\Gamma_{2e}} \left(C_1 - C_{1m} \right)^2 d\Gamma_{1e} \right] dt \rightarrow \min \qquad (43)$$

Let us assume the piecewise linear portions, the main curvatures of the boundary are now negligible $H \rightarrow 0$.

The direct approach to sensitivity analysis is determined by the state equations for the exudate diffusion Eqs.(6) and the boundary conditions by Eqs.(38).

The state equation for the diffusion of the therapeutic agent are formulated by the Eqs.(8) and the boundary conditions by Eqs.(39).

Introducing the integrands according Eq.(43) and the first-order sensitivity correlation Eq.(10), we can formulate the following sensitivity vector

$$\mathbf{F}_p = \int_0^{t_f} \left[\int_{\Gamma_{1e}} \left(C_1 - C_{1m} \right) C_1^{p} \, d\Gamma_{1e} + \int_{\Gamma_{2e}} \left(C_2 - C_{2m} \right) C_2^{p} \, d\Gamma_{2e} \right] +$$

$$\frac{1}{2} \int_{\Gamma_{1e}} \left(C_1 - C_{1m} \right)^2_{,n} v^{p}_{n} \, d\Gamma_{1e} + \frac{1}{2} \int_{\Gamma_{2e}} \left(C_2 - C_{2m} \right)^2_{,n} v^{p}_{n} \, d\Gamma_{2e} +$$

$$\int_{\Sigma} \left] \frac{1}{2} \left(C_1 - C_{1m} \right)^2 \mathbf{v}^{p} \cdot \boldsymbol{\upsilon} \right[+ \int_{\Sigma} \left] \frac{1}{2} \left(C_2 - C_{2m} \right)^2 \mathbf{v}^{p} \cdot \boldsymbol{\upsilon} \right[\Big\} dt \, ;$$

$$p = 1, 2, \ldots P. \qquad (44)$$

The next is the adjoint problem. The state equations during the exudate diffusion are defined by Eq.(11) and the set of conditions in general form Eqs.(12). The adjoint problem of therapeutic agent is defined by means of Eqs.(13), the boundary and initial conditions by Eqs.(14). The sensitivity correlation Eqs.(37) can be simplified by means of the integrands acc. Eq.(43) to the following

$$C_1^{a}(\mathbf{x}, \tau = 0) = 0 \text{ within} (\Omega \cup \Gamma) \, ; \quad C_2^{a}(\mathbf{x}, \tau = 0) = 0 \text{ within} (\Omega \cup \Gamma) \, ;$$

$$\dot{R}_2^a(\mathbf{x},\tau)=0 \ \text{ within}\Omega; \qquad \mathbf{q}_1^{*a}(\mathbf{x},\tau)=0 \ \text{within}\Omega;$$
$$\mathbf{q}_2^{*a}(\mathbf{x},\tau)=0 \ \text{within}\Omega; \qquad C_1^{0a}(\mathbf{x},\tau)=0 \ \text{on}\,\Gamma_{1b} \ \text{and}\,\Gamma_{1w};$$
$$q_{n1}^{0a}(\mathbf{x},\tau)=0 \ \text{on}\,\Gamma_{1u} \ \text{and}\,\Gamma_{1s};$$
$$q_{n2}^{0a}(\mathbf{x},\tau)=0 \ \text{on}\,\Gamma_{2b} \ \text{and}\,\Gamma_{2u} \ \text{and}\,\Gamma_{2s};$$
$$C_{1\infty}^a(\mathbf{x},\tau)=\frac{1}{\beta_1}(C_1-C_{1m}) \ \text{on}\,\Gamma_{1e};$$
$$C_{2\infty}^a(\mathbf{x},\tau)=\frac{1}{\beta_2}(C_2-C_{2m}) \ \text{on}\,\Gamma_{2e}. \tag{45}$$

Defining the first-order sensitivity vector by means of Eq.(16) and introducing the integrands acc. Eq.(43), we obtain the sensitivity equation

$$F_p=-\left[\int_\Omega C_1^a(\nabla C_1\cdot\mathbf{v}^p)d\Omega\right]_{t=0}-\left[\int_\Omega C_2^a(\nabla C_2\cdot\mathbf{v}^p)d\Omega\right]_{t=0}+$$
$$\int_0^{t_f}\left\{\int_\Omega \nabla C_1^a\cdot\mathbf{q}_1^{*p}d\Omega+\int_\Omega\left[\nabla C_2^a\cdot\mathbf{q}_2^{*p}\right]d\Omega+\right.$$
$$-\int_{\Gamma_{1b}}\left[q_{n1}^a\left(\nabla_\Gamma C_1^{01}\cdot\mathbf{v}_\Gamma^p+C_{1,n}^{01}v_n^p\right)\right]d\Gamma_{1b}+$$
$$-\int_{\Gamma_{1w}}\left[q_{n1}^a\left(\nabla_\Gamma C_1^{02}\cdot\mathbf{v}_\Gamma^p+C_{1,n}^{02}v_n^p\right)\right]d\Gamma_{1w}+$$
$$-\int_{\Gamma_{2b}}\left[C_2^a\left(\nabla_\Gamma q_{n2}^0\cdot\mathbf{v}_\Gamma^p+q_{n2,n}^0v_n^p\right)+\mathbf{q}_{2\Gamma}^0\cdot\nabla_\Gamma v_n^p\right]d\Gamma_{2b}+$$
$$-\int_{\Gamma_{1e}}C_1^a\mathbf{q}_{1\Gamma}\cdot\nabla_\Gamma v_n^p d\Gamma_{1e}-\int_{\Gamma_{2e}}C_2^a\mathbf{q}_{2\Gamma}\cdot\nabla_\Gamma v_n^p d\Gamma_{2e}$$
$$\frac{1}{2}\int_{\Gamma_{1e}}(C_1-C_{1m})^2{}_{,n}\,v_n^p\,d\Gamma_{1e}+\frac{1}{2}\int_{\Gamma_{2e}}(C_2-C_{2m})^2{}_{,n}\,v_n^p\,d\Gamma_{2e}+$$
$$\left.\int_\Sigma\right]\frac{1}{2}(C_1-C_{1m})^2\mathbf{v}^p\cdot\boldsymbol{\upsilon}\left[+\int_\Sigma\right]\frac{1}{2}(C_2-C_{2m})^2\mathbf{v}^p\cdot\boldsymbol{\upsilon}\left.\right\}dt \tag{46}$$

The identified shape of the identification process is the optimal one from the optimization, cf. Fig.6. The shape was identified in 6 iterations, see Fig.7. The location of membrane is fixed during the identification process.

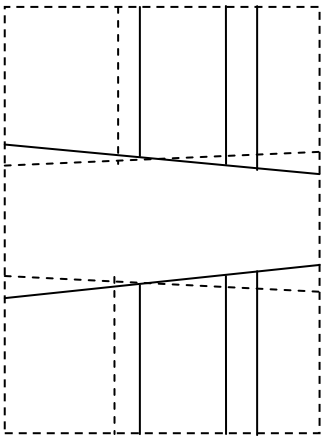

Figure 7: Initial and identified shapes of textile dressing
------ initial shape ——— identified shape

7. Conclusions

Therapeutically speaking, shape optimization process is the important problem of the dressing design. Thus, we secure the optimal shape of the dressing with respect to the different physical phenomena. The discussed case secures the optimal exudate transport to the surrounding. A part of the exudate diffuses into the material and dissolves the microcapsules with the therapeutic agent. The membrane prevents to transport this agent to the surrounding only a part is transported with the exudate along the special part immediately to the surrounding.

We see at once that the discussed methods can be applied to determine the optimal shape of the textile dressing with respect to the different criteria. The discussed case is the typical one for the dressings but we can apply a few objective functionals as well as the wide spectrum of different shapes. Thus, the methods presented can be an effective tool to generate the new structures of textile products.

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