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# Shape Optimization and Shape Identification for Transient Diffusion Problems in Textile Structures

**Abstract**
*The equation of substance balance and the set of boundary and initial conditions determine the transient diffusion problem within the homogenized textile structure. Introducing an arbitrary behavioral functional, its first-order sensitivity expressions can be stated using the material derivative concept and both the direct and the adjoint approaches. Shape optimization and identification problems are then formulated applying the sensitivity expressions. Simple numerical examples of shape identification and optimization of textile structures are presented.*

**Key words:** *diffusion, textile structures, sensitivity analysis, shape optimisation, shape identification.*

## Introduction

Diffusion is an important phenomenon in practical textile engineering. Typical examples are moisture transport through textiles, sweat diffusion through the clothing layers, gas diffusion through protective clothing on the workplace, etc. The problem of diffusion is characterised by the equation of substance balance, and particularly by the diffusion coefficient within the fabric. The main difficulty is to describe diffusion within a material. The general and classical works here include Crank [1], Tomeczek [2], and Li [3]. The classical diffusion equation is applied to each diffusing species. Physically speaking, some researches characterise the diffusion of ionic species using a diffusion coefficient tensor, cf. Tyrrell & Harris [4], or introducing the agglomerated diffusion coefficient, cf. Rubinstein [5]. Diffusion parameters in textile structures have been introduced using different descriptions, as for instance in Ekstein [6]. Kulish & Lage [7] discussed diffusion within a porous medium with randomly distributed heat sinks described by the differential diffusion equation, which is a typical structure of the new interactive clothing. The structure consists of a solid porous matrix with pores filled with capsules containing a phase-changing material. The analysed forms of the boundary and the initial conditions are determined for many particular problems, each characterised by a set of governing equations; see for example Kącki [8]. Fan & Longtin [9] present a non-contact laser-based thermoreflective technique to measure the changes in concentration on a surface, which can help to determine the boundary conditions of the fabric. The technique can be used over a wide range of time scales, ranging from micro-seconds to minutes. For another interesting method of description, the reader is referred to Li [10], where the moisture exchange between fibre and air is discussed. The drying of fabrics is divided into two processes, the evaporation-condensation process and the moisture sorption & desorption. In addition, the boundary conditions and the physical properties of fibres and fabric are given. The moisture transport was considered by Więźlak et al. [11] to formulate a microclimate under a clothing pack. A textile membrane inserted into a cylinder is treated as a system of the fibres and surrounding air.

Compact and inhomogeneous textiles should at first be homogenised. In fact, the mean values of the diffusion coefficient within the textile structure are determined. This paper will introduce the classical rule of mixture as well as a hydrostatic analogy, both according to Golanski, Terada & Kikuchi [12]. Any textile structure is a composite material containing fibres with the surrounding filling. The diffusion coefficient can be formulated introducing the volume fraction of the fibres, cf. Tomeczek [2].

The presented form of the formal description is similar to that shown for the thermal problems. Fuller treatments can be found in Dems et al. [13], Dems & Rousselet [14], Dems & Korycki [15], and Korycki [16,17]. The first-order sensitivities of an arbitrary behavioural functional are formulated as a function of the transformation velocity field and solutions of primary, direct and adjoint diffusion problems. The main goal of the presented paper is to introduce the first-order sensitivity expressions to the problems of design and identification which are associated with diffusion within textile structures. Thus, the above structures can be designed and identified more effectively and rapidly, using the procedures proposed. This class of problems has not yet been introduced in the studied literature. Of course, the physical interpretation and the detailed analysis of diffusion problem is different, and immediately follows the form of the obtained expressions.

The problems considered can be discussed and solved using different numerical methods, cf. Roche & Sokołowski [18]. They gave more information about the numerical methods applied in the practice of identification and optimisation. Haji-Sheikh & Massena [19] present a generalised method for the integral solution of the diffusion equation in regions with irregular boundaries. The solution for the diffusion equation was decomposed into two parts, one with homogeneous and the other with inhomogeneous boundary conditions.

## Primary problem formulation

The boundary shape of the structure is described using a vector of design parameters **b**, whereas the state variable is now the component concentration C during the diffusion. Let us introduce the transient diffusion problem within a diffusive anisotropic domain Ω stated by the equation of substance balance and the set of boundary and initial conditions. It is assumed that the solution containing the diffusive component is immovable, and according to [2, 8] (cf. Figure 1) the state equations are presented as Equations 1 where C denotes the component concentration, $t$ is the time of the primary structure, $\dot{C}$ is the time derivative of the component concentration, $\nabla$ is the gradient operator, $\boldsymbol{q}$ is the vector of the diffusion flux density, $\boldsymbol{q}^*$ is the vector of the initial diffusion flux density, $\dot{R}$ denotes the chemical reaction rate of the component during diffusion, i.e. the diffusion generation source, D is the diffusion coefficient, $q_n = \boldsymbol{n} \cdot \boldsymbol{q}$ is the diffusion flux density normal to the boundary, $\boldsymbol{n}$ is the normal unit vector directed outwards on the external boundary Γ, β denotes the convective diffusion coefficient and $C_\infty$ is the surrounding component concentration.

Let us next modify the shape of the domain Ω together with the surrounding external boundary Γ. Due to an infinitesimal transformation process, the shape variation has the form of Equation (2) where $\varphi(\boldsymbol{x}, \boldsymbol{b}, t)$ denotes a given function of the defined parameters, $v^p(\boldsymbol{x}, \boldsymbol{b}, t)$ is a transformation velocity field associated with the parameter $b_p$; $p = 1...P$, treated as a time-like parameter.

Let us introduce an arbitrary behavioural functional associated with the unsteady diffusion problem, in the form of Equation (3) where Ψ and γ are continuous and differentiable functions of their arguments. According to [20], the material derivative of the above functional $F$ with respect to the design parameter $b_p$ is defined as being the first-order sensitivity $F_p$ in the basic form of (4).

The unknown sensitivities of the state fields appearing in Equation (4) can be derived using the direct approach to sensitivity analysis, or can be eliminated from Equation (4) using the adjoint state fields, alternatively obtained as the result of the solution of the adjoint diffusion problem.

The problem of component diffusion remains a difficult problem to deal with, primarily because of the physical interpretation of the existing phenomena. As might be expected, most of the governing equations for the diffusion problem can be determined using the same assumptions, description and methods as introduced previously for the question of heat transfer.

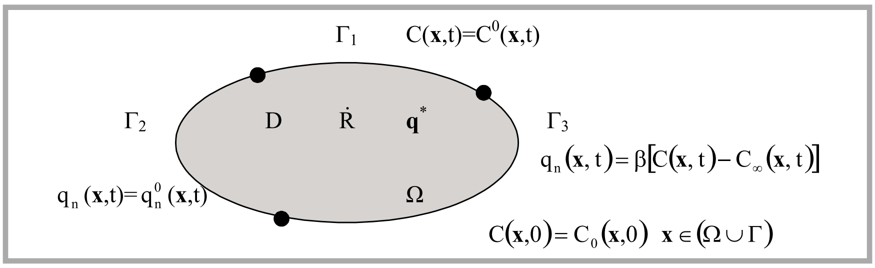


***Figure 1.*** *Primary diffusion problem.*

$$\left.\begin{aligned} &-\operatorname{div}\mathbf{q} + \dot{R} = \dot{C} \\ &\mathbf{q} = D\,\nabla C + \mathbf{q}^* \\ &\dot{C} = \frac{dC}{dt}\;;\; \dot{R} = \frac{dR}{dt} \end{aligned}\right\} \mathbf{x} \in \Omega; \quad \begin{aligned} &C(\mathbf{x},t) = C^0(\mathbf{x},t)\;\; \mathbf{x}\in\Gamma_1\;;\;\; q_n(\mathbf{x},t) = \mathbf{n}\cdot\mathbf{q} = q_n^0(\mathbf{x},t)\;\; \mathbf{x}\in\Gamma_2; \\ &q_n(\mathbf{x},t) = \beta\left[C(\mathbf{x},t) - C_\infty(\mathbf{x},t)\right]\;\; \mathbf{x}\in\Gamma_3\;; \\ &C(\mathbf{x},0) = C_0(\mathbf{x},0)\;\; \mathbf{x}\in(\Omega\cup\Gamma), \end{aligned} \tag{1}$$

$$\Omega \to \Omega^* : \quad \mathbf{x}^* = \mathbf{x} + \delta\varphi(\mathbf{x},\mathbf{b},t) = \mathbf{x} + \frac{\partial\varphi(\mathbf{x},\mathbf{b},t)}{\partial b_p}\delta b_p = \mathbf{x} + \mathbf{v}^p(\mathbf{x},\mathbf{b},t)\delta b_p \tag{2}$$

$$F = \int_0^{t_f}\left[\int_\Omega \Psi(C,\nabla C,\mathbf{q},\dot{R},\dot{C})\,d\Omega + \int_\Gamma \gamma\,(C,q_n,C_\infty)\,d\Gamma\right]dt \tag{3}$$

$$\begin{aligned} F_p = \frac{DF}{Db_p} = &\int_0^{t_f}\int_\Omega \left[\Psi,_C C_p + \nabla_{\nabla C}\Psi(\nabla C)_p + \Psi,_{\mathbf{q}}\cdot\mathbf{q}_p + \Psi,_{\dot{R}}(\dot{R})_p + \Psi,_{\dot{C}}\dot{C}_p + \Psi\operatorname{div}\mathbf{v}^p\right]d\Omega\,dt\, + \\ &+ \int_0^{t_f}\int_\Gamma\left[\gamma,_C C_p + \gamma,_{q_n}(q_n)_p + \gamma,_{C_\infty}(C_\infty)_p + \gamma\left(\operatorname{div}_\Gamma\mathbf{v}^p - 2Hv_n^p\right)\right]d\Gamma\,dt, \end{aligned} \tag{4}$$

where $\Psi,_C = \frac{\partial\Psi}{\partial C};\;\; \Psi,_{\mathbf{q}} = \frac{\partial\Psi}{\partial\mathbf{q}};\;\; \nabla_{\nabla C}\Psi = \left|\frac{\partial\Psi}{\partial C,_1};\frac{\partial\Psi}{\partial C,_2};\frac{\partial\Psi}{\partial C,_3}\right|;\;\; \gamma,_C = \frac{\partial\gamma}{\partial C};\;\; \mathbf{q}_p = \frac{D\mathbf{q}}{Db_p};$ etc.

***Equations: 1, 2, 3, and 4.***

## Direct approach to sensitivity analysis

It is easily seen that the direct approach is most convenient for obtaining sensitivities with respect to a few of the design variables (Figure 2). The additional structure has the same shape and diffusion properties as the primary body, and is characterised by the equation of substance balance, the boundary and the initial conditions. The necessary equations are obtained by differentiation of equations for primary structure with respect to the design parameters and presented as Equation (5).

Thus, the first-order sensitivity expression is similar to the equation obtained for the thermal problems. The external boundary of the additional structure is composed of three portions $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ , and the

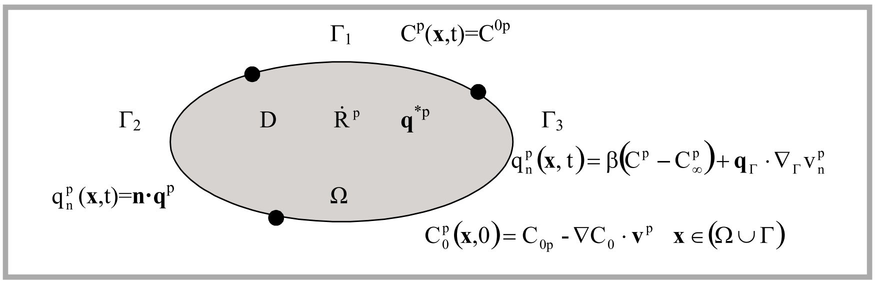


***Figure 2.*** *Additional diffusion problem.*

$$\left.\begin{aligned} &-\operatorname{div}\mathbf{q}^p + \dot{R}^p = \dot{C}^p \\ &\mathbf{q}^p = D\,\nabla C^p + \mathbf{q}^{*p} \end{aligned}\right\}\mathbf{x}\in\Omega \qquad \dot{C}^p = \frac{dC^p}{dt}$$

$$\begin{aligned} &C^p = C^{0p} = C_p^0 - \nabla C^0\cdot\mathbf{v}^p\;\; \mathbf{x}\in\Gamma_1 \\ &q_n^p = \mathbf{n}\cdot\mathbf{q}^p = q_{np}^0 + q_\Gamma^0\cdot\nabla_\Gamma v_n^p - \nabla_\Gamma q_n^0\cdot\mathbf{v}_\Gamma^p - q_{n,n}^0 v_n^p\;\; \mathbf{x}\in\Gamma_2 \\ &q_n^p = \mathbf{n}\cdot\mathbf{q}^p = \beta[C^p - C_\infty^p] + q_\Gamma\cdot\nabla_\Gamma v_n^p\;\; \mathbf{x}\in\Gamma_3 \\ &C_0^p(\mathbf{x},0) = C_{0p} - \nabla C_0\cdot\mathbf{v}^p\;\; \mathbf{x}\in(\Omega\cup\Gamma) \end{aligned} \tag{5}$$

***Equations: 5.***

first-order sensitivity of the functional *F* are adapted as presented by Equation (6).

Thus, the total derivatives $C^0_p$ on $\Gamma_1$ and $(q^0_n)_p$ on $\Gamma_2$ are known in advance. The first-order sensitivity expression is a sum of integrals of time as well as within the structural domain Ω, on the whole external boundary Γ, on parts of the external boundary $\Gamma_1$, $\Gamma_2$, $\Gamma_3$, and along the curve Σ between two adjacent parts of the piecewise smooth boundary Γ. The diffusive state fields of the additional structure are now $C^p$, $q^p$ and $q^p_n$, i.e. all the local sensitivities of the state fields for the primary body. These parameters can be determined from additional diffusion problems associated with the design parameter $b_p$ which are given by Equation (5). The direct method requires the solution (*P*+1) problems for the existing *P* design parameters.

$$F_p = \left[\int_\Omega \Psi_{,\dot{C}} C^p d\Omega\right]_0^{t_f} + \int_0^{t_f}\left\{\int_\Omega\left[\left(\Psi_{,C} - \frac{d}{dt}\left(\Psi_{,\dot{C}}\right)\right)C^p + \nabla_{\nabla C}\Psi\cdot\nabla C^p + \Psi_{,\mathbf{q}}\cdot\mathbf{q}^p + \Psi_{,\dot{R}}\dot{R}^p\right]d\Omega\ + \right.$$
$$+\int_{\Gamma_1}\left[\gamma_{,C}\left(C^0_p - \nabla_\Gamma C^0\cdot\mathbf{v}^p_\Gamma - C^0_{,n} v^p_n\right) + \gamma_{,q_n}\left(q^p_n - \mathbf{q}_\Gamma\cdot\nabla_\Gamma v^p_n\right)\right] d\Gamma_1 +$$
$$+\int_{\Gamma_2}\left[\gamma_{,C} C^p + \gamma_{,q_n}\left(q^0_{np} - \nabla_\Gamma q^0_n\cdot\mathbf{v}^p_\Gamma - q^0_{n,n} v^p_n\right)\right] d\Gamma_2 + \int_\Gamma \gamma_{,C_\infty} C^p_\infty\, d\Gamma + \qquad (6)$$
$$\left.+\int_{\Gamma_3}\left[\gamma_{,C} C^p + \gamma_{,q_n}\beta\left(C^p - C^p_\infty\right)\right]d\Gamma_3 + \int_\Gamma\left(\Psi + \gamma_{,n} - 2H\gamma\right)v^p_n d\Gamma + \int_\Sigma \left]\gamma\,\mathbf{v}^p\cdot\boldsymbol{\nu}\right[ d\Sigma\right\}dt;\ p = 1...P$$

***Equation: 6.***

problems in the form $\tau = t_f - t$. The final time $t = t_f$ determined for the primary and the additional problem is the starting time for the adjoint problem τ = 0. Under the above assumption, the time derivatives of temperature existing in Equation (8) are stated as

$$dT^a/d\tau = -\ dT^a/dt.$$

Let us next introduce Equation (8) into the right-hand side of Equation (6). Thus, the sum of specified integrals vanishes if the following boundary-value conditions are specified as Equation (9).

Applying Equation (9) in the right-hand side of Equation (6), the first-order sensitivity vector can be specified in the form of Equation (10) - see page 46.

This expression is a sum of integrals of time as well as within the domain Ω, on the whole external boundary Γ, on the boundary portions $\Gamma_1$, $\Gamma_2$, $\Gamma_3$, and along the discontinuity curve Σ. The diffusive state fields of the additional structure $C^a$, $q^a$ and $q^a_n$ can be determined from Equations (7) and (9) respectively.

## Adjoint approach to sensitivity analysis

In order to determine the first-order sensitivity vector $F_p$ one must calculate the primary and the adjoint diffusion problem for the one objective functional, i.e. only two diffusive problems, cf. Figure 3. If the number of functionals is equal to *N*, then *N*+1 diffusive problems should be considered. Both the adjoint and the primary structure have the same shape and diffusion properties, but the adjoint body is subject to boundary conditions and domain diffusion sources depending on the considered objective functional. The diffusion equation and the conditions for the adjoint structure state the transient adjoint problem Equation (7) where $C^a$ denotes the component concentration for adjoint structure, τ is the time of the adjoint structure, $\dot{C}^a$ is the time derivative of the component concentration, $\mathbf{q}^a$ denotes the vector of the diffusion flux density, $\mathbf{q}^{*a}$ is the vector of the initial diffusion flux density, $\dot{R}^a$ denotes the diffusion generation source of the adjoint structure, and $C^a_\infty$ is the surrounding component concentration. The state variable of the adjoint problem is the component concentration $C^a$.

In order to formulate the conditions for adjoint structure, the identity as Equation (8) is introduced using the diffusion equation (see Equation 7).

Let us take the transformation of time τ of the adjoint problem with respect to the time *t* of the primary and the additional

## The shape optimisation problem and optimisation functionals

The shape optimisation problem can be introduced by minimising or maximising

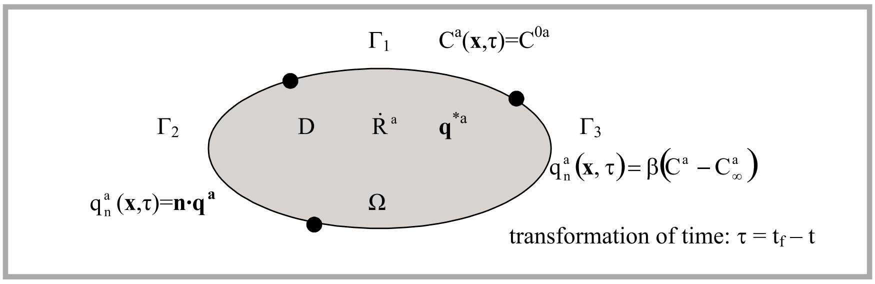


***Figure 3.*** *Adjoint diffusion problem.*

$$\left.\begin{aligned} -\operatorname{div}\mathbf{q}^a + \dot{R}^a &= \dot{C}^a \\ \mathbf{q}^a &= D\nabla C^a + \mathbf{q}^{*a}\end{aligned}\right\}\mathbf{x}\in\Omega;\quad \dot{C}^a = \frac{dC^a}{d\tau};\quad \begin{aligned} &C^a(\mathbf{x},\tau) = C^{0a}(\mathbf{x},\tau)\ \ \mathbf{x}\in\Gamma_1; \\ &q^a_n(\mathbf{x},\tau) = \mathbf{n}\cdot\mathbf{q}^a = q^{0a}_n(\mathbf{x},\tau)\ \ \mathbf{x}\in\Gamma_2; \\ &q^a_n(\mathbf{x},\tau) = \beta[C^a(\mathbf{x},\tau) - C^a_\infty(\mathbf{x},\tau)]\ \ \mathbf{x}\in\Gamma_3;\end{aligned} \qquad (7)$$

$$\left[\int_\Omega C^a C^p d\Omega\right]_{t=t_f} + \int_0^{t_f}\int_\Omega\left(C^p\dot{R}^a + \nabla C^p\cdot\mathbf{q}^{*a}\right)d\Omega dt + \int_0^{t_f}\int_{\Gamma_1} C^{0a} q^p_n\, d\Gamma_1 dt - \int_0^{t_f}\int_{\Gamma_2} C^p q^{0a}_n\, d\Gamma_2 dt +$$
$$+\int_0^{t_f}\int_{\Gamma_3}\beta C^p C^a_\infty\, d\Gamma_3 dt - \int_0^{t_f}\int_\Omega C^p\frac{dC^a}{dt}d\Omega dt - \int_0^{t_f}\int_\Omega C^p\frac{dC^a}{d\tau}d\Omega dt = \left[\int_\Omega C^a C^p d\Omega\right]_{t=0} + \qquad (8)$$
$$+\int_0^{t_f}\int_\Omega\left(C^a\dot{R}^p + \nabla C^a\cdot\mathbf{q}^{*p}\right)d\Omega dt + \int_0^{t_f}\int_{\Gamma_1} C^{0p} q^a_n\, d\Gamma_1 dt - \int_0^{t_f}\int_{\Gamma_2} C^a q^{0p}_n\, d\Gamma_2 dt + \int_0^{t_f}\int_{\Gamma_3} C^a\left(\beta C^p_\infty - \mathbf{q}_\Gamma\cdot\nabla_\Gamma v^p_n\right)d\Gamma_3 dt.$$

$$C^a(\mathbf{x},\tau=0) = \Psi_{,\dot{C}}(\mathbf{x},t=t_f)\ \ \mathbf{x}\in(\Omega\cup\Gamma);\qquad \dot{R}^a(\mathbf{x},\tau) = \Psi_{,C}(\mathbf{x},t) - \frac{d}{dt}\Psi_{,C}(\mathbf{x},t)\ \ \mathbf{x}\in\Omega;$$
$$\mathbf{q}^{*a}(\mathbf{x},\tau) = \nabla_{\nabla C}\Psi(\mathbf{x},t) + \nabla_{\mathbf{q}}\Psi(\mathbf{x},t)\cdot\mathbf{A}(\mathbf{x})\ \ \mathbf{x}\in\Omega;\qquad C^{0a}(\mathbf{x},\tau) = \gamma_{,q_n}(\mathbf{x},t)\ \ \mathbf{x}\in\Gamma_1; \qquad (9)$$
$$q^{0a}_n(\mathbf{x},\tau) = -\gamma_{,C}(\mathbf{x},t)\ \ \mathbf{x}\in\Gamma_2;\qquad C^a_\infty(\mathbf{x},\tau) = \frac{1}{\beta}\gamma_{,C}(\mathbf{x},t) + \gamma_{,q_n}(\mathbf{x},t)\ \ \mathbf{x}\in\Gamma_3;$$

***Equations: 7, 8, and 9.***

the objective functional with the imposed constraint on the structural cost $K \le K_0$, where $K_0$ is the assumed structural cost. The structural cost for the homogeneous structure can be assumed to be proportional to the optimised domain Ω. Let us next consider the Lagrange functional given for the inequality constraints in the form [13] $F' = F + \chi(K - K_0 + \zeta^2)$, where the Lagrange multiplier χ can be an optional real number, and $\xi^2$ is an additional variable. This variable denotes the slack variable, and Dems [13] gives its possible interpretation. Considering the stationarity of the above functional, the following optimality conditions can be obtained:

$$\begin{cases} \dfrac{DF}{Db_p} = -\chi \int_\Omega u\, v_n^p\, d\Gamma \\ \int_\Omega u\, d\Omega - K_0 + \xi^2 = 0. \end{cases} \tag{11}$$

where u is the unit material cost. The optimisation procedure was solved using the variational formulation of the Finite Element Method. This assumption ensures the choice of the objective functionals of a clear physical interpretation. Some of the possible functionals are presented underneath.

It is convenient to assume that the optimisation functional is the diffusive flux density through the assumed boundary portion or the whole external boundary:

$$F = \int_0^{t_f} \left( \int_\Gamma q_n\, d\Gamma \right) dt; \;\; \Gamma \in \Gamma_{external} \quad . \tag{12}$$

Minimising the above functional corresponds to the shape design of the optimal diffusive isolator; in other words, the diffusive transport through the assumed boundary portion is reduced. Regarding a model of the diffusive emitter, the above functional should be maximised.

The alternative objective functional can be associated with the intensity of chemical reaction within the structural domain, which can be denoted as follows:

$$F = \int_0^{t_f} \left( \int_\Gamma \dot{R}\, d\Gamma \right) dt \quad . \tag{13}$$

The optimal shape of the regarded structure can be determined from the point of view of maximising or minimising the above functional.

The functional $F$ can be a global measure of the local maximum concentration of the diffusive component within the structural domain or along its boundary. The structural optimisation causes the minimising of the component distribution in the following form:

$$\begin{aligned} F_p = &-\left[ \int_\Omega \left( \Psi,_{\dot{C}} - C^a \right)\left( C_p - \nabla C \cdot \mathbf{v}^p \right) d\Omega \right]_{t=0} + \int_0^{t_f} \Bigg\{ \int_\Omega \left[ \left( \nabla_q \Psi + \nabla C^a \right) \cdot \mathbf{q}^{*p} + \left( \Psi,_{\dot{R}} + C^a \right) \dot{R}^p \right] d\Omega + \\ &+ \int_{\Gamma_1} \left[ \left( \gamma,_C + q_n^a \right) \left( C_p^0 - \nabla_\Gamma C^0 \cdot \mathbf{v}_\Gamma^p - C,_n^0 v_n^p \right) - \gamma,_{q_n} \mathbf{q}_\Gamma \cdot \nabla_\Gamma v_n^p \right] d\Gamma_1 + \\ &+ \int_{\Gamma_2} \left[ \left( \gamma,_{q_n} - C^a \right) \left( q_{np}^0 - \nabla_\Gamma q_n^0 \cdot \mathbf{v}_\Gamma^p - q_n^0,_n v_n^p \right) - C^a \mathbf{q}_\Gamma^0 \cdot \nabla_\Gamma v_n^p \right] d\Gamma_2 + \\ &+ \int_{\Gamma_3} \left[ C^a \beta C_\infty^p - C^a \mathbf{q}_\Gamma \cdot \nabla_\Gamma v_n^p - \gamma,_{q_n} \beta C_\infty^p \right] d\Gamma_3 + \int_\Gamma \left( \Psi + \gamma,_n - 2H\gamma \right) v_n^p\, d\Gamma + \\ &+ \int_\Gamma \gamma,_{C_\infty} C_\infty^p\, d\Gamma + \int_\Sigma \left( \gamma \mathbf{v}^p \cdot \nu \right) d\Sigma \Bigg\} dt \end{aligned} \tag{10}$$

***Equation: 10.***

$$F = \int_0^{t_f} \left[ \int_\Gamma \left( \frac{C}{C_0} \right)^n d\Gamma \right]^{\frac{1}{n}} dt; \tag{14}$$

$$n \to \infty; \;\; \Gamma \in \Gamma_{external}$$

where $C_0$ is the assumed level of the component concentration. For $n \to \infty$, the functional F represents the global measure of the maximum local concentration of the diffusive component within the domain.

## The shape identification problem and identification functionals

The shape identification problem is defined as minimising the introduced objective functional without constraint. The stationarity conditions can be denoted as follows $F \to \min \Rightarrow F_p = \dfrac{DF}{Db_p} = 0.$

The most popular form of the objective functional is the 'distance' between the component concentration C of the identified model and the concentration $C_m$ of the real existing structure, stated on the external boundary part $\Gamma_m$ in the form

$$F = \frac{1}{2} \int_0^{t_f} \left[ \int_{\Gamma_m} (C - C_m)^2 d\Gamma_m \right] dt \, . \tag{15}$$

The alternative form of the objective functional can be introduced as the following measure of the component concentration:

$$F = \int_0^{t_f} \left\{ \left[ \int_{\Gamma_m} \left( \frac{C}{C_m} \right)^n d\Gamma_m \right]^{\frac{1}{n}} \right\} dt; \;\; n \to \infty. \tag{16}$$

This homogeneous functional can be used during the expansion or contraction of the modified boundary. Minimising the functional reduces the 'distance' between the component concentrations C and $C_m$ and minimises the maximum local value of the concentration.

The functional F can be a simple adaptation of the Damage Location Assurance Criterion existing in mechanical problems, cf. Messina et al. [21]. The objective functional can now be expressed as Equation (17).

The range of correlation between the component concentrations of the identified model C and the real existing structure $C_m$ is from zero (no correlation) to one (the full correlation).

The solution of both optimality equations given by Equation (11) as well as stationarity conditions require knowledge of the first-order sensitivities of the objective functional. Their derivation was discussed in the above sections and formulated using the direct approach (cf. Equation (6)), as well as the adjoint approach (cf. Equation 10).

In the next section, some applications of the derived expressions and objective functionals presented will be indicated, and simple numerical examples will be presented.

$$F = \int_0^{t_f} \left[ \left( \int_{\Gamma_m} C_m C\, d\Gamma_m \right)^2 \left( \int_{\Gamma_m} C_m C_m\, d\Gamma_m \right)^{-1} \left( \int_{\Gamma_m} C C\, d\Gamma_m \right)^{-1} \right] dt \tag{17}$$

***Equation: 17.***

## Numerical examples

### Shape identification problem

The expressions discussed can be applied to the two-dimensional shape optimisation of the segment of an item of interactive thermal clothing. The structure of the clothing is sequential, whereas the thermal protection can be improved using empty, hermetic spaces within the fabric. The main idea of interactive clothing is to adapt to an acting external impulse, such as temperature changes. The impulse causes a rapid change in volume by filling the spaces within the segments of the clothing with gas, air or alternatively using the mechanical element with shape memory. This kind of clothing was analysed by Szosland [22].

For this reason, the transient diffusion within the textile material is here considered. Of course, only one segment can be considered at a time. Let us assume that the medium within the hole contains moisture, and we must solve a two-dimensional shape identification problem, cf. Figure 4.

The lower part of the external boundary contacts the control surface. This part of the external boundary $\Gamma_1$ has the prescribed component concentration changed in time according to the function $C = C^0 = 500 + 100\sin(\Pi \cdot t/10)$. The calculations were performed for $t_0 = 0$; $t_k = 240$ s; $\Delta t = 60$ s. Additionally, on this portion of the external boundary, the component concentration of the real existing structure $C_m$ should be measured. The left and right sides of the external disc boundary are diffusively isolated, i.e. the diffusion flux density normal to these portions $\Gamma_2$ is equal to zero $q_n = 0$. The upper part of the external boundary is the portion $\Gamma_3$, with the diffusive convection characterised by the convection coefficient $\beta = 10^{-3}$ m. The surrounding component concentration of the moisture is assumed as equal to $C_\infty = 0.1C_{\Gamma 3}$, i.e. 10% of the component concentration on the above portion $\Gamma_3$. The diffusion within the fabric can be characterised as moisture diffusion within a solid material. The activated energy is assumed, according to Ekstein [6], to be equal to E = 12.14 kJ/kmol whereas the exponential coefficient equals $K = 2 \cdot 10^{-7}$ m$^2$/s. The diffusion coefficient within the fabric can be described according to [2] $D = K\exp(-E/(R_g T)) = 1.9904 \cdot 10^{-7}$ m$^2$/s. On the boundary of the hole, the diffusion flux density normal to the portion $\Gamma_2$ is prescribed, as changed in time according to the function $q_n = q_n^0 = 500(2.718)^{-0.1t}$. The calculations were performed for the same time parameters as on the boundary $\Gamma_1$. Let us next assume $R = 0$, $q^* = 0$. The primary problem can be introduced in view of Equations (1), as Equation (18).

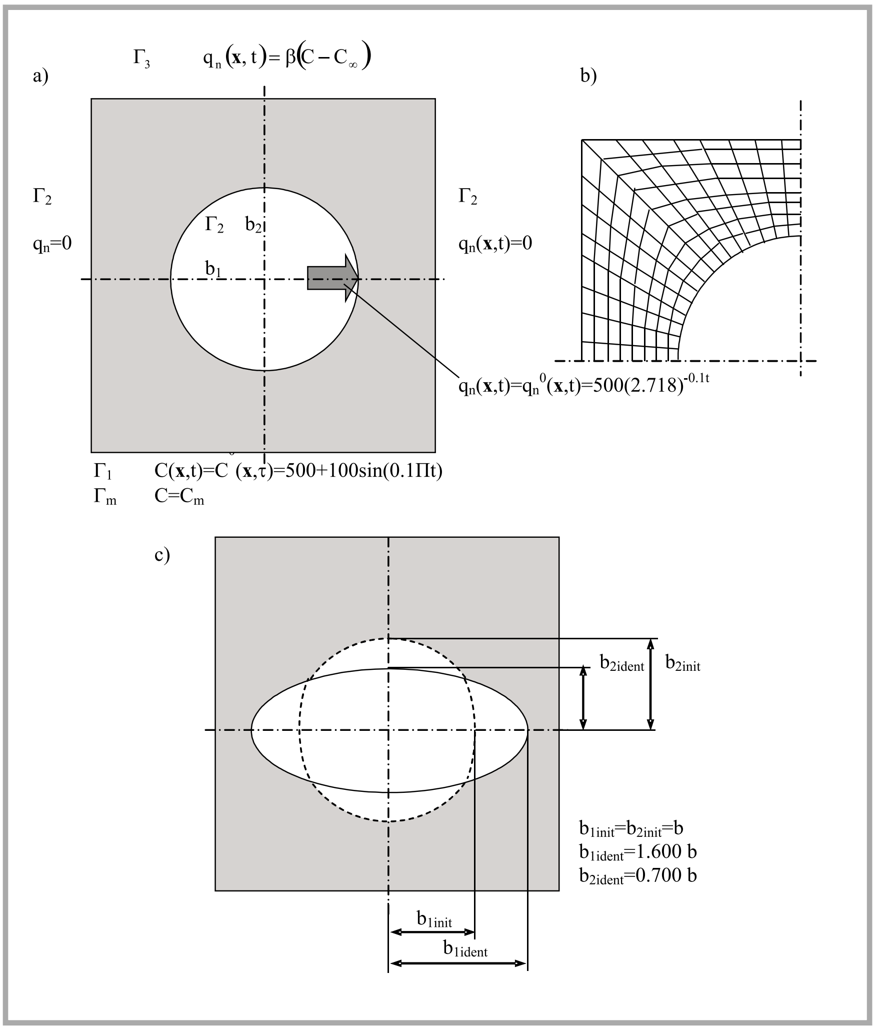

***Figure 4.*** *Shape identification of the diffusive structure.*

Let us state the objective functional according to Equation (15). First the direct approach is discussed. Using Equation (1), Equation (5) and Equation (15), as well as assuming the material derivatives $C_\Gamma^{0p}$ on $\Gamma_1$; $q_{n\Gamma}^{0p}$ on $\Gamma_2$ and $C_{0p}$ on $(\Omega \cup \Gamma)$ as known in advance, the governing equations for additional structure have the form of Equation (19).

$$\left.\begin{aligned} -\operatorname{div}\mathbf{q} &= \dot{C} \\ \mathbf{q} = D\nabla C \ ; \ \dot{C} &= \frac{dC}{dt} \end{aligned}\right\} \ \mathbf{x} \in \Omega;$$
$$C(\mathbf{x},t) = C^0(\mathbf{x},t) = 500 + 100\sin\frac{\Pi t}{10} \ \ \mathbf{x} \in \Gamma_1; \ \ q_n(\mathbf{x},t) = q_n^0(\mathbf{x},t) = 0 \ \ \mathbf{x} \in \Gamma_2 \text{ (external)};$$
$$q_n(\mathbf{x},t) = q_n^0(\mathbf{x},t) = 500(2.718)^{-0.1t} \ \ \mathbf{x} \in \Gamma_2 \text{ (hole)};$$
$$q_n(\mathbf{x},t) = \beta[C(\mathbf{x},t) - C_\infty(\mathbf{x},t)] \ \ \mathbf{x} \in \Gamma_3; \quad C(\mathbf{x},0) = C_0(\mathbf{x},0) \ \ \mathbf{x} \in (\Omega \cup \Gamma) \ . \tag{18}$$

$$\left.\begin{aligned} -\operatorname{div}\mathbf{q}^p &= \dot{C}^p \\ \mathbf{q}^p &= D\nabla C^p \end{aligned}\right\} \mathbf{x} \in \Omega \qquad \dot{C}^p = \frac{dC^p}{dt}$$
$$\begin{aligned} C^p &= C^{0p} = -\nabla C^0 \cdot \mathbf{v}^p \ \ \mathbf{x} \in \Gamma_1 \\ q_n^p &= \mathbf{n} \cdot \mathbf{q}^p = 0 \ \ \mathbf{x} \in \Gamma_2 \\ q_n^p &= \mathbf{n} \cdot \mathbf{q}^p = \beta[C^p - C_\infty^p] + q_\Gamma \cdot \nabla_\Gamma v_n^p \ \ \mathbf{x} \in \Gamma_3 \\ C_0^p(\mathbf{x},0) &= -\nabla C_0 \cdot \mathbf{v}^p \ \ \mathbf{x} \in (\Omega \cup \Gamma) \end{aligned} \tag{19}$$

***Equations: 18 and 19.***

To determine the first-order sensitivity expressions, it is necessary to use Equation (6) and Equation (15).

Our next goal is to formulate the equations for adjoint approach to sensitivity analysis. Now introducing Equation (7), Equation (9) and Equation (15), the adjoint problem can be formulated as Equation (20).

The first-order sensitivity expression can be stated in view of Equation (10) and Equation (15).

It is assumed that the length of both semi-axes describes the shape of the hole. Thus, we also have only two independent design parameters, depicted by the lengths $b_1$ and $b_2$ on Figure 4a. The analysis step of the identification procedure was performed using the Finite Element Method, and the domain was discretised using the 4-nodal elements net (cf. Figure 4b). The solution is iterative. The first step of each analysis was the solution of the primary problem, and then the additional problems or the adjoint problem were solved. The results obtained are first-order sensitivities, which are considered at the synthesis stage of the identification procedure. Thus, the first-order Method of Steepest Descent is applied in order to find the directional minimum. The initial shape and the shape identified in four iterations are shown in Figure 4c.

The problem described by Equations (18) to (20) is time-dependent, i.e. the unsteady diffusion problem must be solved. Physically speaking, the problem is a simple generalisation of the steady moisture transport, see for example Zienkiewicz [23] and Huebner [24]. Thus, additional time-dependent terms of the state variable are considered in the standard FEM-equation. Zienkiewicz [23] discussed these additional terms, the matrixes for different two-dimensional problems and the solution methods. In this case, the transient component concentration was found using recurrence relations, cf. Huebner [24].

### Shape optimisation problem

The first-order sensitivity expressions can be applied alternatively to the two-dimensional shape optimisation of the diffusive textile structure. The primary problem is the same as described by Equations (18). The objective functional

$$\left.\begin{aligned} -\operatorname{div}\mathbf{q}^a &= \dot{C}^a \\ \mathbf{q}^a &= D\,\nabla C^a \end{aligned}\right\}\mathbf{x}\in\Omega;\quad \dot{C}^a = \frac{dC^a}{d\tau}; \qquad \begin{aligned} &C^a(\mathbf{x},\tau) = C^{0a}(\mathbf{x},\tau) \quad \mathbf{x}\in\Gamma_1; \\ &q_n^a(\mathbf{x},\tau) = \mathbf{n}\cdot\mathbf{q}^a = q_n^{0a}(\mathbf{x},\tau) \quad \mathbf{x}\in\Gamma_2; \\ &q_n^a(\mathbf{x},\tau) = \beta[C^a(\mathbf{x},\tau) - C_\infty^a(\mathbf{x},\tau)] \quad \mathbf{x}\in\Gamma_3; \end{aligned} \tag{20}$$

$$C^a(\mathbf{x},\tau=0) = 0 \quad \mathbf{x}\in(\Omega\cup\Gamma); \qquad \dot{R}^a(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Omega; \qquad \mathbf{q}^{*a}(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Omega;$$

$$C^{0a}(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Gamma_1; \qquad q_n^{0a}(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Gamma_2; \qquad C_\infty^a(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Gamma_3;$$

***Equations: 20.***

is assumed to be the diffusive flux density normal to the lower part of the external boundary, according to Equation (12), cf. Figure 5. Let us compose the external boundary using 8 piecewise linear portions; the main curvatures of the boundary are now H→0. The additional structure is characterised by Equations (19), whereas the first-order sensitivity expression can be determined using Equation (6) and Equation (12).

The adjoint approach to sensitivity analysis can be stated using Equation (7), Equation (9) and Equation (12) in the form (21).

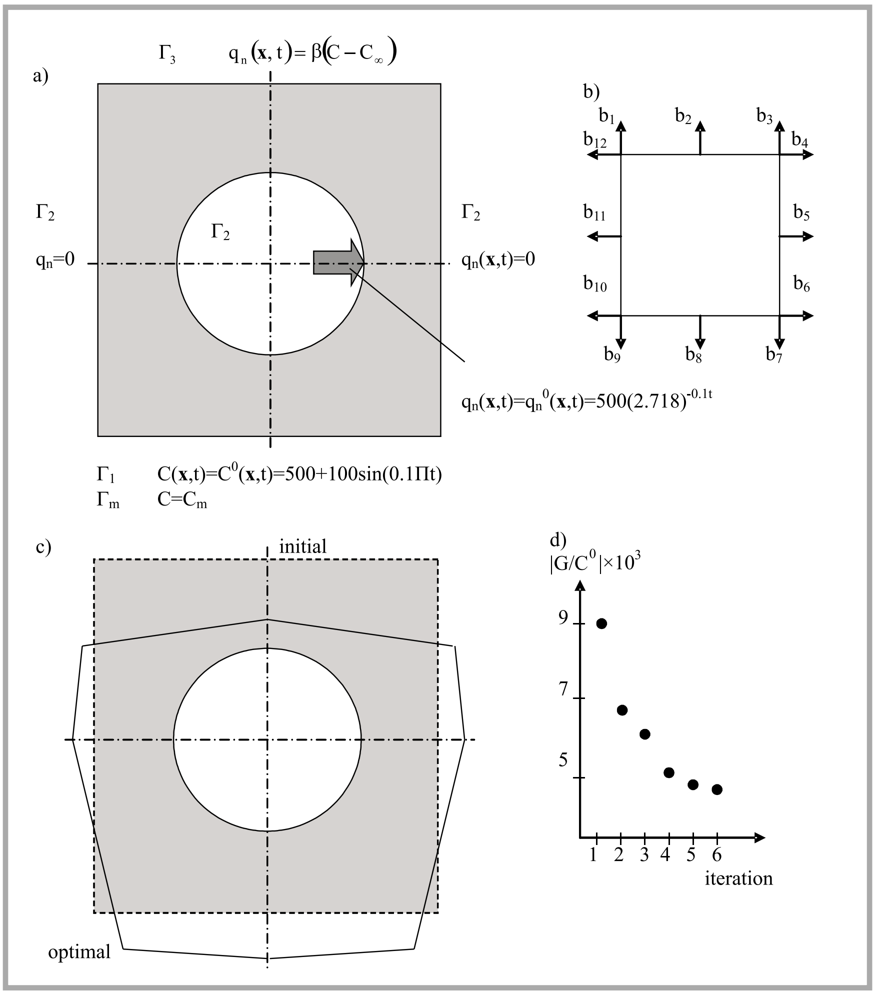


***Figure 5.*** *Shape optimisation of the diffusive structure.*

$$\left.\begin{aligned} -\operatorname{div}\mathbf{q}^a &= \dot{C}^a \\ \mathbf{q}^a &= D\,\nabla C^a \end{aligned}\right\}\mathbf{x}\in\Omega;\quad \dot{C}^a = \frac{dC^a}{d\tau}; \qquad \begin{aligned} &C^a(\mathbf{x},\tau) = C^{0a}(\mathbf{x},\tau) \quad \mathbf{x}\in\Gamma_1; \\ &q_n^a(\mathbf{x},\tau) = \mathbf{n}\cdot\mathbf{q}^a = q_n^{0a}(\mathbf{x},\tau) \quad \mathbf{x}\in\Gamma_2; \\ &q_n^a(\mathbf{x},\tau) = \beta[C^a(\mathbf{x},\tau) - C_\infty^a(\mathbf{x},\tau)] \quad \mathbf{x}\in\Gamma_3; \end{aligned} \tag{21}$$

$$C^a(\mathbf{x},\tau=0) = 0 \quad \mathbf{x}\in(\Omega\cup\Gamma); \qquad \dot{R}^a(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Omega; \qquad \mathbf{q}^{*a}(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Omega;$$

$$C^{0a}(\mathbf{x},\tau) = 1 \quad \mathbf{x}\in\Gamma_1; \qquad q_n^{0a}(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Gamma_2; \qquad C_\infty^a(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Gamma_3;$$

***Equations: 21.***

The independent shape designing parameters are now 12 coordinates of the selected points on the external boundary, which is depicted by the arrows $b_1 - b_{12}$ in Figure 5b. Thus, the shape of the external boundary is optimised, whereas the boundary of the hole is stationary. In this case, the structural cost is assumed as a constant during the optimisation process.

The analysis step of the optimisation procedure was performed using the Finite Element Method, and the structure was discretised by applying the 4-nodal element net (cf. Figure 4b). The solution procedure is iterative, similar to the shape identification problem. At first the primary, additional and adjoint problems should be solved. The obtained sensitivities are applied into the Method of Steepest Descent. The initial and the optimal shapes of the structure are shown in Figure 5c. The optimal boundary is located very far from the hole with the diffusive medium. The history of optimisation process is shown in Figure 5d, and the changes are plotted in terms of the iteration number.

## Conclusion

The main objective of this paper was to present the application of the direct and adjoint approaches to sensitivity analysis in the transient diffusion problems within the textile structures. The formal description of the governing equations characterising the diffusion is similar to that for heat transfer problems. Physically speaking, the interpretation of the expressions obtained is different, and follows the diffusive phenomena.

The first-order sensitivity vectors were formulated using the material derivative concept as well as direct and adjoint approaches to sensitivity analysis. Both approaches can be chosen alternatively, and the expressions obtained can be introduced into the existing optimisation and identification methods in order to find the directional minimum of the objective functional. The presented analysis allows us to introduce the inequality constraints imposed on the structural cost, which is typical of engineering problems existing in the real world.

The numerical examples presented prove that the analysis can be an effective tool for determining the optimal boundary shapes for the optimal design problems, redesign procedures and identification problems in textile engineering.

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