evropský sociální fond v ČR
EVROPSKÁ UNIE
MINISTERSTVO ŠKOLSTVÍ, MLÁDEŽE A TĚLOVÝCHOVY
OP Vzdělávání pro konkurenceschopnost
INVESTICE DO ROZVOJE VZDĚLÁVÁNÍ

OPTIMIZATION OF COUPLED HEAT AND MASS TRANSPORT CONDITIONS WITHIN TEXTILE PRODUCTS

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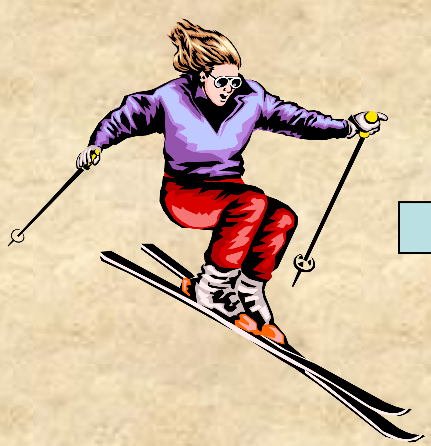
PROJEKT OPTIS PRO FT, reg. č.: CZ.1.07/2.2.00/28.0312 JE SPOLUFINANCOVÁN EVROPSKÝM SOCIÁLNÍM FONDEM A STÁTNÍM ROZPOČTEM ČESKÉ REPUBLIKY

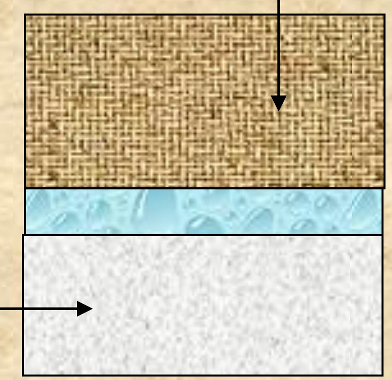
Practical motivation of the problem

Environmental conditions

interaction = balance within composite structure
(cf. textiles with the semi-permeable membrane)

Thermal comfort of the user

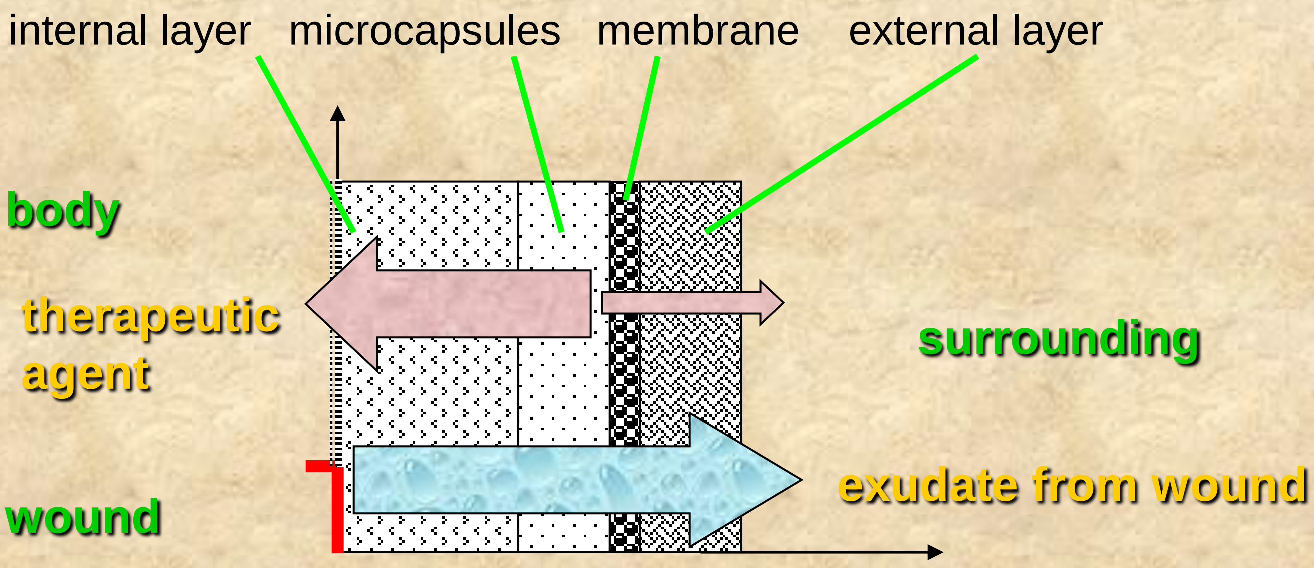




- Creation of the thermal comfort
- Improvement of the working conditions
- Lack of efficiently algorithms describing the 2D and 3D problems (only 1D model is sufficiently described)

Practical motivation of the problem

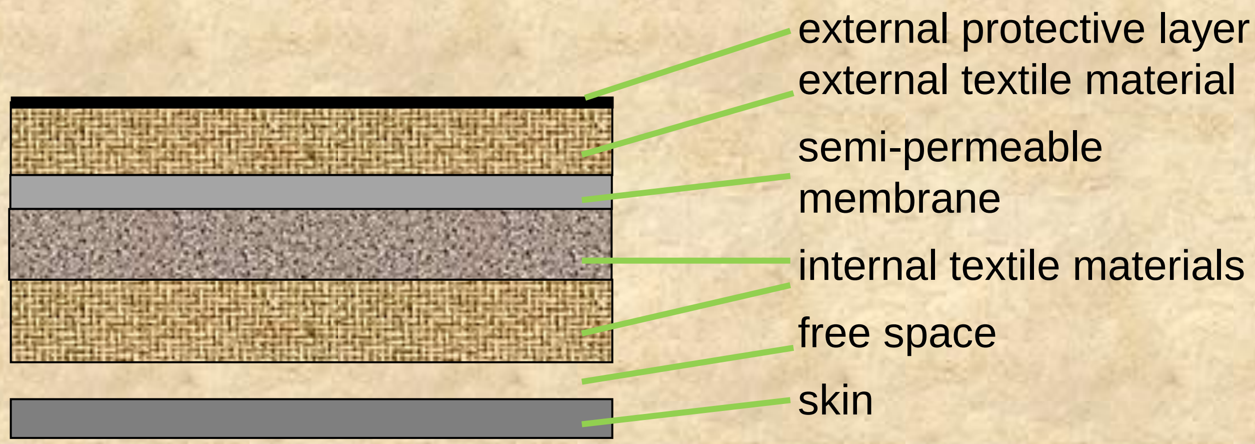
- Dressings on the textile structure with the microcapsulated terapeutic substance.



- Textile products subjected to the finishing procedure within the ironing machine.
- Press with the cooling and conditioning device for textile products.

Practical motivation of the problem

Heat and mass transport from the users body through the multilayer composite textile with the barrier effect, cf. firefighters protective clothing.



Solution strategy of the coupled problem

Primary problem. Initial conditions of coupled heat and mass transport.
Initial vector of design variables.

↓

Physical model. Definitions of material parameters. Homogenization.

↓

Mathematical model. General form of objective functional.
Determination of state variables for primary problem.

↓

Sensitivity analysis. Determination of state variables and sensitivity expressions by means of direct and adjoint approaches.

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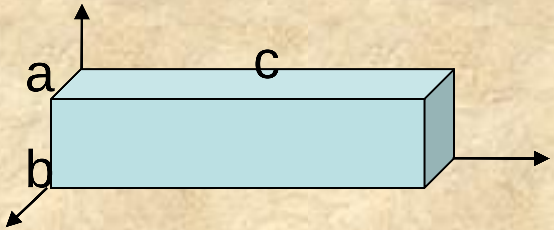
Shape optimization. Particular form of objective functional.
Numerical solution.

↓

Physical interpretation. Visualization = distribution maps of state variables.

Physical model. Homogenization



Problem of homogenization scale
(micro- and macroscale)

Comparable dimensions a, b, c: - 3D homogeneous textile structure
Negligible one dimension: - 2D homogeneous textile structure

Basic textile structures (yarn, ropes)
- macroscale: 1D

- microscale: 3D

Flat textiles
- macroscale: 2D

- microscale: 3D

Physical model. Homogenization

Textiles (woven fabrics, knitted fabrics, nonwovens) have the properties:
- the inhomogeneous, repeatable structure,
- the composite structure: matrix of fibers within the filling,
- some structures have the semi-permeable membrane.

Homogenization of textile structures
- creation of the homogeneous, orthotropic structure,
- average thermal and mass transfer conductivity coefficients for different materials of matrix and filling,

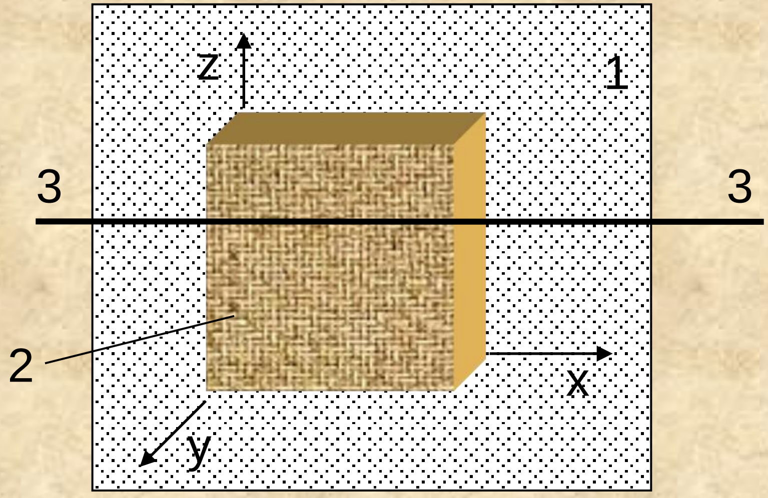
→ rule of mixture (Golanski,Terada,Kikuchi 1997)

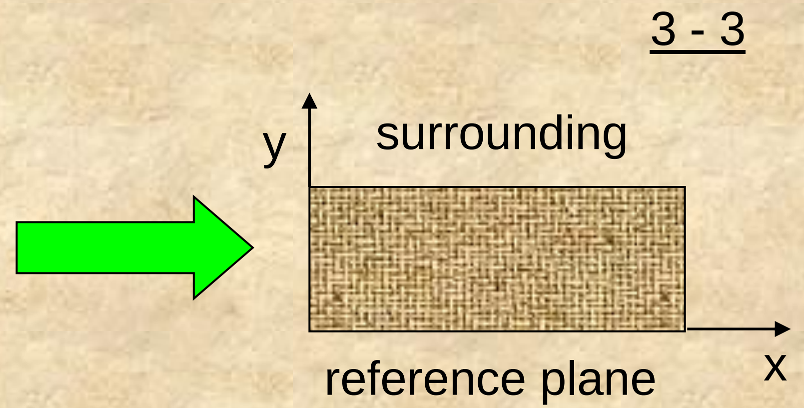
→ hydrostatic analogy by means of the Turner's Model (G, T, K, 1997)

→ proportional volume fraction for composite materials(Tomeczek 1999)

→ other metods (cf. solutions for porous structures, composites, etc.)

Physical model. Simplifications





1 – reference plane
2 – textile structure
3 – optional cross-section of textile structure

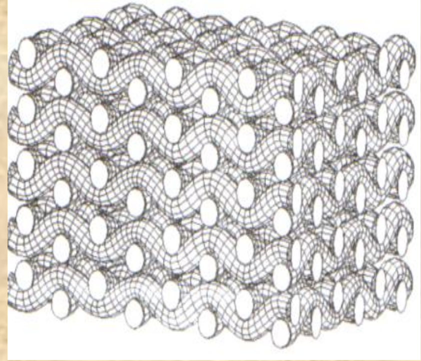
The same (i) shape, (ii) heat and mass transfer conditions in the structure:
Reduction 3D ---- 2D problem

Physical model.
Problem of primary transient heat and mass transfer

Input: flux density vector of

Heat $\mathbf{q}_1$

Moisture $\mathbf{q}_{w1}$



Output: flux density vector of

Heat $\mathbf{q}_2$

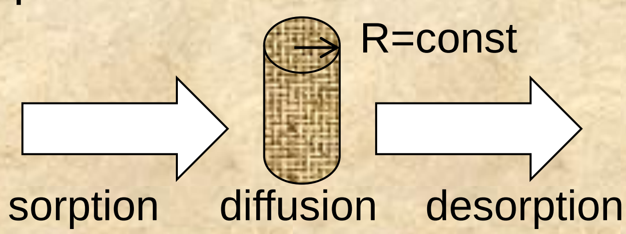
Moisture $\mathbf{q}_{w2}$

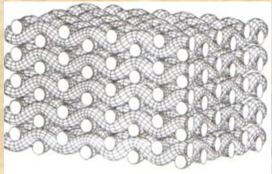
- Homogenized textile structure; multilayer textile composite = fibers + gas within the interfiber spaces.
- Different heat flux and moisture flux densities; i.e. gradients of temperature ∇T and moisture flux density $\nabla \mathbf{q}_w$ within the material.
- State variables:
  - water vapor concentration within fibers w_f
  - water vapor concentration in the void spaces between fibers w_a
  - temperature T

Physical model.
Problem of primary transient heat and mass transfer

Assumptions according Li(2001), Li and Luo(1999):

- Volume changes of fibers caused by moisture gradient can be neglected.
- Moisture is transferred through the fibers by sorption/desorption between the free spaces and the material as well as the diffusion within the fibres material.
- Orientation of fibers within the structure plays a minimum role in the mass transport; the diameters of the fibers are small and the water vapor travel much more rapidly in the air than in the fibers.
- Instantaneous thermal equilibrium between the fibers and gas in the interfiber spaces is achieved during the process of water vapor transfer.





Mathematical model.
Problem of primary transient heat and mass transfer

Necessary equations:

- Balance equations: heat and mass balances in the textile product.
- Constitutive equations: characterize the material during the coupled transfer, connect the heat and mass flux densities with the active forces generating the transport.
- State equations: correlations between state variables of system.
- Physic-chemical correlations: describe the properties of the particular material phase.

Heat balance formulation:

$$D_C + Z_C - O_C = A_C.$$

D_C – heat supplied with the water vapor to the material,
Z_C – heat emitted emitted by the source,
O_C – heat transported to the surrounding through the external boundary,
A_C – heat accumulated within the material.

Mathematical model.
Problem of primary transient heat and mass transfer

Heat supplied with the mass to the fibres, transported by sorpiton/desorption between fibres and the interfiber spaces

$$D_C = \int_{\Omega} \lambda_w (1-\varepsilon) \frac{dw_f}{dt} d\Omega$$

λ_w - heat sorption of water vapor by fibers i.e. the cross-transport coefficient,
ε - material porosity

Heat generated by the internal sources within the domain Ω

$$Z_C = \int_{\Omega} f(\mathbf{x},t) d\Omega$$

f - heat source capacity

Heat lost by the transport through the external surface Γ in time per unit

$$O_C = \int_{\Gamma} \mathbf{q}(\mathbf{x},t) d\Gamma \qquad \mathbf{q}(\mathbf{x},t) = \mathbf{A} \cdot \nabla T(\mathbf{x},t) + \mathbf{q}^*(\mathbf{x},t)$$

A - matrix of thermal conduction coefficients

Heat lost by accumulation within the material of the structure Ω

$$A_C = \int_{\Omega} \rho c \frac{dT}{dt} d\Omega$$

c - volumetric heat capacity
ρ - material density

Mathematical model.
Problem of primary transient heat and mass transfer

Heat balance in general form

$$\begin{cases} \rho c \dfrac{dT}{dt} - \lambda_w (1-\varepsilon) \dfrac{dw_f}{dt} = -\mathrm{div}\mathbf{q}(\mathbf{x},t) + f(\mathbf{x},t) \\ \mathbf{q}(\mathbf{x},t) = \mathbf{A} \cdot \nabla T(\mathbf{x},t) + \mathbf{q}^*(\mathbf{x},t) \end{cases}$$

Mathematical model.
Problem of primary transient heat and mass transfer

Mass generated by the sources within the domain Ω, cf. microcapsules

$$Z_M = \int_\Omega f_w(\mathbf{x},t)\,d\Omega$$

f_w- mass source capacity

Mass lost by the transport through the external surface Γ in time per unit

$$O_M = \int_\Gamma \mathbf{q}_w(\mathbf{x},t)\,d\Gamma; \quad \mathbf{q}_w(\mathbf{x},t) = D\,\nabla w_f(\mathbf{x},t) + \mathbf{q}_w^*(\mathbf{x},t)$$

D – mass diffusion coefficient

Mass lost by accumulation within the fibres

$$A_W = \int_\Omega (1-\varepsilon)\frac{dw_f}{dt}\,d\Omega$$

ε - material porosity

Mass lost by accumulation within the free spaces between fibres

$$A_P = \int_\Omega \varepsilon\frac{dw_a}{dt}\,d\Omega$$

Mathematical model.
Problem of primary transient heat and mass transfer

Mass balance formulation:

$$Z_M - O_M = A_C + A_P.$$

Z_M – mass generated by the sources,
O_M – mass transported to the surrounding through the external boundary,
A_C – mass accumulated within the fibres,
A_P – mass accumulated within the free spaces between fibres.

Mass balance in general form

$$\begin{cases} (1-\varepsilon)\dfrac{dw_f}{dt} + \varepsilon\dfrac{dw_a}{dt} = -\mathrm{div}\mathbf{q}_w(\mathbf{x},t) + f_w(\mathbf{x},t) \\ \mathbf{q}_w(\mathbf{x},t) = D\nabla w_f(\mathbf{x},t) + \mathbf{q}_w^*(\mathbf{x},t) \end{cases}$$

Mathematical model.
Problem of primary transient heat and mass transfer

Heat and mass transport equations

$$\begin{cases} (1-\varepsilon)\dfrac{dw_f}{dt} + \varepsilon\dfrac{dw_a}{dt} = -\mathrm{div}\mathbf{q}_w + f_w; \quad \mathbf{q}_w = D\nabla w_f + \mathbf{q}_w^*; \\ \rho c\dfrac{dT}{dt} - \lambda_w(1-\varepsilon)\dfrac{dw_f}{dt} = -\mathrm{div}\mathbf{q} + f; \quad \mathbf{q} = \mathbf{A}\cdot\nabla T + \mathbf{q}^*; \end{cases}$$

ε effective porosity of the textile material

$\mathbf{q}_w$ vector of mass flux density

$\mathbf{q}_w^*$ vector of initial mass flux density

f_w mass source capacity

$D = h_a\varepsilon/\zeta$ mass transport coefficient of the water vapor within the fibers

∇ gradient operator,

c volumetric heat capacity of fabric

λ_w cross coefficient (the heat sorption of water vapor by fibers)

$\mathbf{q}$ vector of heat flux density

$\mathbf{q}^*$ vector of initial heat flux density

f heat source capacity

t real time

2 equations – 3 state variables !!!!!!!!!!

Mathematical model.
Problem of primary transient heat and mass transfer

Third correlation acc. Li(2001) Li Luo(1999), Li Holcombe(1992):
- experimental equation,
- two-staged procedure described by the factor of proportionality p,
- first stage: Fick's diffusion; second stage: experimental correlation.

$$\frac{dw_f}{dt} = (1-p)R_1 + pR_2;$$

$p = 0$ when $w_a < 0{,}185$ and $t < t_{eq}$; $p = 0{,}5$ when $w_a \geq 0{,}185$ and $t < t_{eq}$;

$p = 1$ when $t > t_{eq}$;

Radial diffusion within fibres acc. to Fick's theory
R_1 sorption rate at the first stage

R_2 sorption rate at the second stage
experimental correlation

t_{eq} equilibrium time, variable for different textile structures, determined experimentally, cf. the wool fabric t_{eq}=540 s

Mathematical model.
Problem of primary transient heat and mass transfer

Sorption rate within fibres at the first stage of sorption process

$$R_1(\mathbf{x},t) = \frac{dw_f}{dt} = \frac{1}{r}\frac{d}{dr}\frac{\left(rD_f dw_f\right)}{dr}$$

$$w_f\left(\boldsymbol{x},R_1,t\right) = \rho\beta w_a;$$

$$\frac{dw_f}{dt} = \rho\beta\frac{dw_a}{dt}.$$

Transport equations at the first stage of sorption process

$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{\beta\rho}\right)\dfrac{dw_f}{dt} = -\mathrm{div}\mathbf{q}_w + f_w; & \mathbf{q}_w = D\,\nabla w_f + \mathbf{q}_w^*; \\ c\dfrac{dT}{dt} + \lambda_w(1-\varepsilon)\dfrac{dw_f}{dt} = -\mathrm{div}\mathbf{q} + f; & \mathbf{q} = \mathbf{A}\cdot\nabla T + \mathbf{q}^*. \end{cases}$$

Mathematical model.
Problem of primary transient heat and mass transfer

Sorption rate within fibres at the second stage of sorption process

$$R_2(\mathbf{x},t) = s_1 \,\mathrm{sign}(H_a - H_f)\exp\left(\frac{s_2}{|H_a - H_f|}\right);$$

s_1 s_2 material parameters
H relative humidity

- Functions H_1 H_2 (i.e. the material characteristics) should be known.
- Sorption/desorption process on the boundary fibres/interfiber spaces should be analyzed.

$$\frac{w_f}{w_a} = \frac{38582{,}80\,\frac{e_f}{T_f}}{38582{,}80\,\frac{e_a}{T_a}} = \frac{e_f}{e_a} = \eta \qquad \frac{H_f}{H_a} = \frac{\frac{e_f}{E_f}\cdot 100\%}{\frac{e_a}{E_a}\cdot 100\%} = \frac{e_f}{e_a} = \eta$$

$$E_a = E_f \qquad T_a = T_f$$

w absolute humidity, i.e. water vapor concentration
H realtive humidity
e water vapor pressure
E saturated water vapor pressure
η factor of proportionality, physical interpretation: absorption/desorption coefficient of the water vapor on the boundary fibres/interfiber spaces

Mathematical model.
Problem of primary transient heat and mass transfer

Transport equations at the second stage

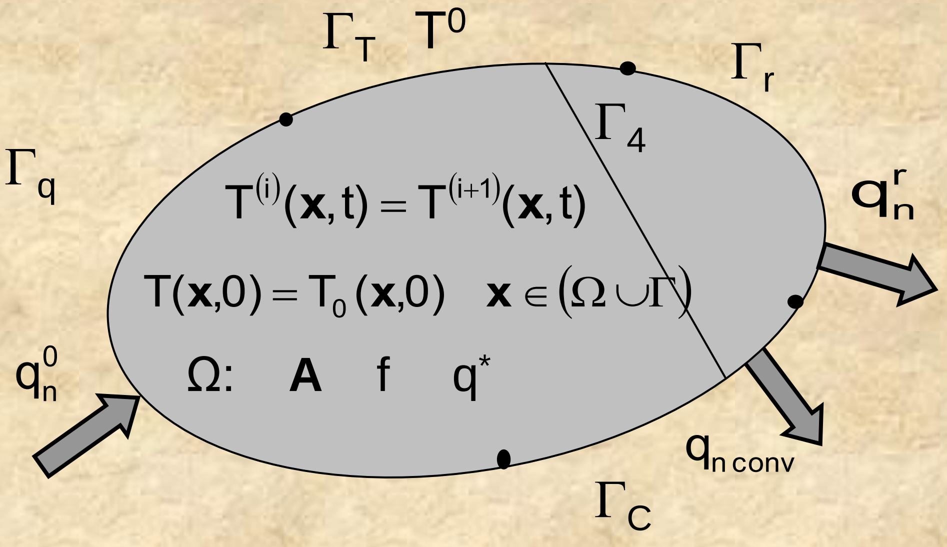
$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{\rho\eta}\right)\dfrac{dw_f}{dt} = -\mathrm{div}\,\mathbf{q}_w + f_w; \qquad \mathbf{q}_w = D\,\nabla w_f + \mathbf{q}_w^*; \\ c\dfrac{dT}{dt} + \lambda_w(1-\varepsilon)\dfrac{dw_f}{dt} = -\mathrm{div}\,\mathbf{q} + f; \qquad \mathbf{q} = \mathbf{A}\cdot\nabla T + \mathbf{q}^*. \end{cases}$$

Similar form of transport equations

Transport equations at the first stage

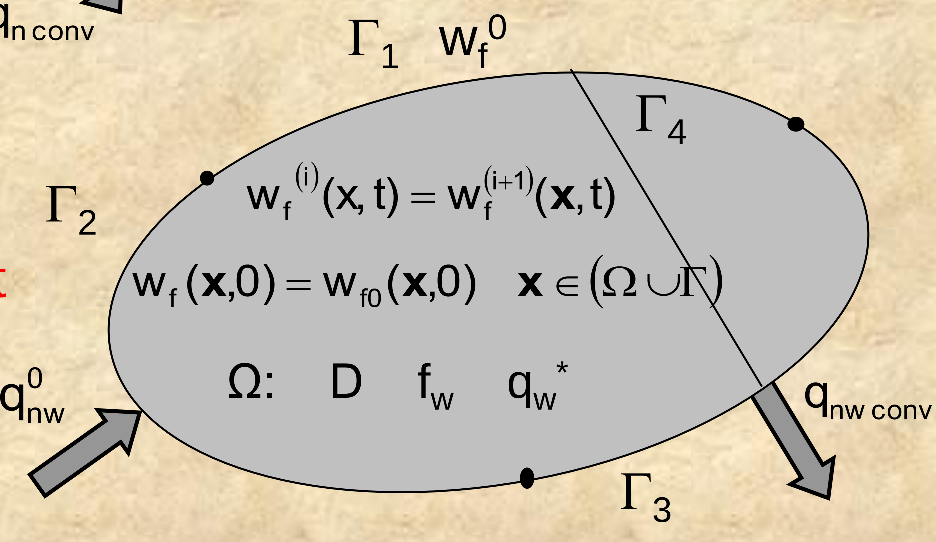
$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{\beta\rho}\right)\dfrac{dw_f}{dt} = -\mathrm{div}\,\mathbf{q}_w + f_w; \qquad \mathbf{q}_w = D\,\nabla w_f + \mathbf{q}_w^*; \\ c\dfrac{dT}{dt} + \lambda_w(1-\varepsilon)\dfrac{dw_f}{dt} = -\mathrm{div}\,\mathbf{q} + f; \qquad \mathbf{q} = \mathbf{A}\cdot\nabla T + \mathbf{q}^*. \end{cases}$$

Mathematical model.
Problem of primary transient heat and mass transfer



Heat transport

$\Gamma = \Gamma_T \cup \Gamma_q \cup \Gamma_c \cup \Gamma_r$



Moisture transport

$\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$

Mathematical model.
Problem of primary transient heat and mass transfer

Boundary conditions – mixed conditions

$$T(\mathbf{x},t) = T^0(\mathbf{x},t) \quad \mathbf{x} \in \Gamma_T; \quad w_f(\mathbf{x},t) = w_f^{\,0}(\mathbf{x},t) \quad \mathbf{x} \in \Gamma_1;$$

first-kind b.c.

$$q_n(\mathbf{x},t) = q_n^{\,0} \quad \mathbf{x} \in \Gamma_q; \quad q_{nw}(\mathbf{x},t) = q_{nw}^{\,0} \quad \mathbf{x} \in \Gamma_2;$$

second-kind b.c

$$q_n(\mathbf{x},t) = h\left[T(\mathbf{x},t) - T_\infty(\mathbf{x},t)\right] \quad \mathbf{x} \in \Gamma_C;$$

$$q_{nw}(\mathbf{x},t) = h_w\left[w_f(\mathbf{x},t) - w_{f\infty}(\mathbf{x},t)\right] \quad \mathbf{x} \in \Gamma_3;$$

third-kind b.c.

$$q_n^{\,r}(\mathbf{x},t) = \sigma T^4 \quad \mathbf{x} \in \Gamma_r;$$

radiation condit.

$$T^{(i)}(\mathbf{x},t) = T^{(i+1)}(\mathbf{x},t); \quad w_f^{\,(i)}(\mathbf{x},t) = w_f^{\,(i+1)}(\mathbf{x},t) \quad \mathbf{x} \in \Gamma_4;$$

fourth-kind b.c.

$$T(\mathbf{x},0) = T_0(\mathbf{x},0); \quad w_f(\mathbf{x},0) = w_{f0}(\mathbf{x},0) \quad \mathbf{x} \in (\Omega \cup \Gamma).$$

initial conditions

Mathematical model. Optional objective functional

The optional objective functional

$$F = F_1 + F_2 = \int_0^{t_f} \left[\int_{\Omega(\boldsymbol{b})} \Psi_1(T, \nabla T, f, \dot{T})\, d\Omega + \int_{\Gamma(\boldsymbol{b})} \gamma_1(T, q_n, T_\infty)\, d\Gamma \right] dt + \int_0^{t_f} \left[\int_{\Omega(\boldsymbol{b})} \Psi_2(w_f, \nabla w_f, f_w, \dot{w}_f)\, d\Omega + \int_{\Gamma(\boldsymbol{b})} \gamma_2(w_f, q_w, w_{f\infty})\, d\Gamma \right] dt;$$

Ψ_1, Ψ_2, γ_1, γ_2 continuous and differentiable functions of the arguments

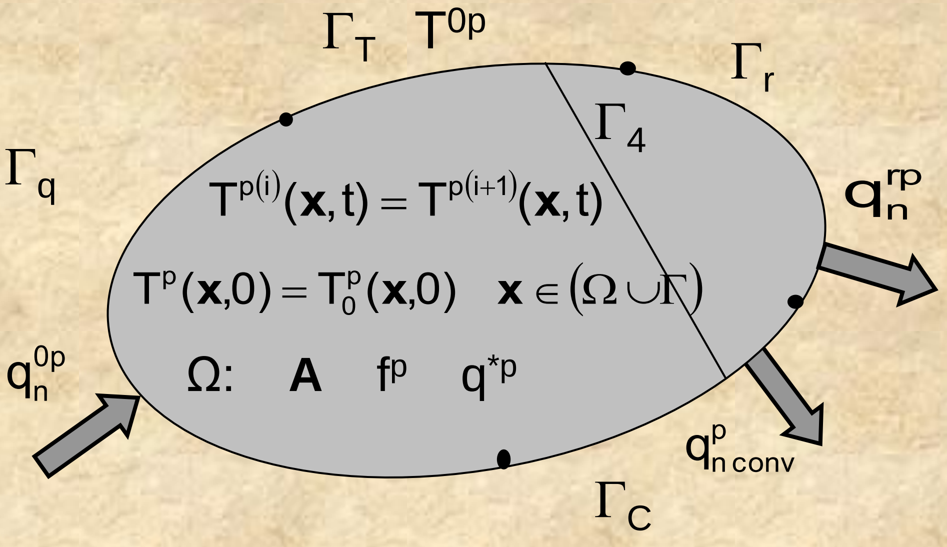
Material derivative concept:

1st order sensitivity with respect to design parameter:

$F_p = DF/Db_p \quad p = 1...P$

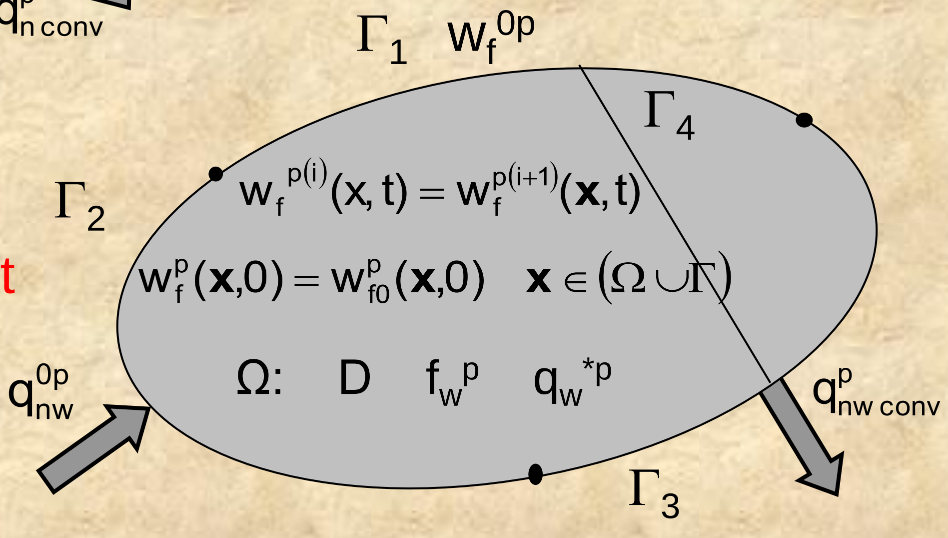
DIRECT APPROACH ADJOINT APPROACH

Sensitivity analysis. Direct approach



Heat transport

$\Gamma = \Gamma_T \cup \Gamma_q \cup \Gamma_c \cup \Gamma_r$



Moisture transport

$\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$

- The same: shapes, materials, heat and mass transport processes.
- Additional fields within the domain and on the boundaries.

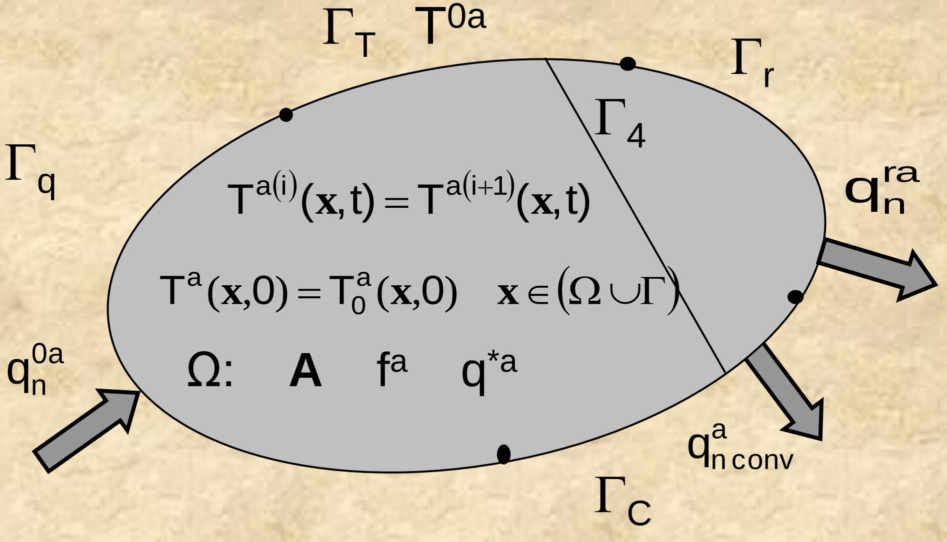
Sensitivity analysis. Direct approach

- The unknown fields = solutions of additional problems associated with each design parameter.
- Equations formulated by differentiation of equations for the primary problem.
- Differential transport equation

$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{Z}\right)\dfrac{dw_f^p}{dt} = -\mathrm{div}\,\mathbf{q}_w^p + f_w^p; \qquad \mathbf{q}_w^p = D\,\nabla w_f^p + \mathbf{q}_w^{*p}; \\ c\,\dfrac{dT^p}{dt} + \lambda_w \dfrac{dw_f^p}{dt} = -\mathrm{div}\,\mathbf{q}^p + f^p; \qquad \mathbf{q}^p = \mathbf{A}\cdot\nabla T^p + \mathbf{q}^{*p}. \end{cases}$$

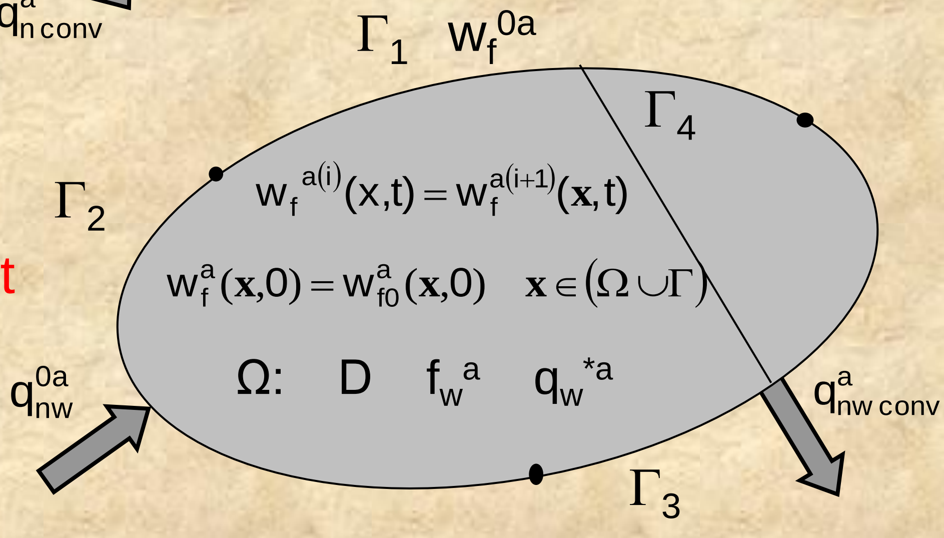
$$Z = \beta\rho \ \text{dla}\ p = 0; \quad Z = \beta\eta \ \text{dla}\ p > 0.$$

Sensitivity analysis. Adjoint approach



Heat transport

$\Gamma = \Gamma_T \cup \Gamma_q \cup \Gamma_c \cup \Gamma_r$



Moisture transport

$\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$

- The same: shapes, materials, heat and mass transport processes.
- Additional fields within the domain and on the boundaries.

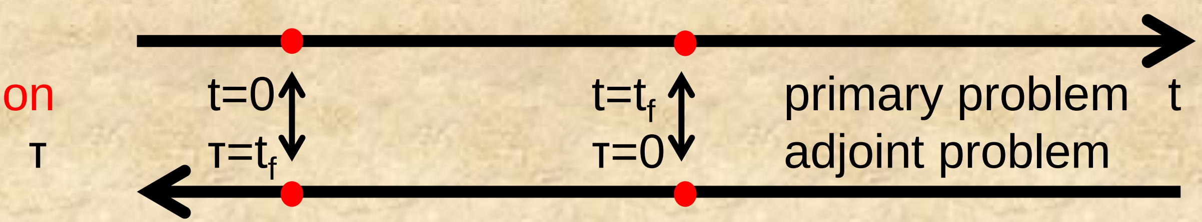
Sensitivity analysis. Adjoint approach

- Equations similar to the equations for the primary problem.
- Differential transport equation

$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{Z}\right)\dfrac{dw_f^a}{d\tau} = -\mathrm{div}\,\mathbf{q}_w^a + f_w^a; \qquad \mathbf{q}_w^a = D\,\nabla w_f^a + \mathbf{q}_w^{*a}; \\ c\,\dfrac{dT^a}{dt} + \lambda_w \dfrac{dw_f^a}{d\tau} = -\mathrm{div}\,\mathbf{q}^a + f^a; \qquad \mathbf{q}^a = A\cdot\nabla T^a + \mathbf{q}^{*a}. \end{cases}$$

$$Z = \beta\rho \;\; \text{for}\; p = 0; \quad Z = \beta\eta \;\; \text{for}\; p > 0.$$

Time transformation



Shape optimization problem

Creation of a new shape of the textile structure

Optimality conditions

$$\begin{cases} \min G \\ C - C_0 = 0 \end{cases} \quad \text{or} \quad \begin{cases} \max G = \min(-G) \\ C - C_0 = 0, \end{cases}$$

G, C optimization/constraint functionals.

Introducing the Lagrange functional = optimality conditions

$$\begin{cases} \dfrac{DG}{Db_p} = -\chi \dfrac{DC}{Db_p} \\ C - C_0 = 0. \end{cases}$$

DG/Db_p; DC/Db_p 1st order sensitivities of the optimization/constraint functionals with respect to design parameter b_p,

χ Lagrange multiplier.

Shape optimization problem. Functionals

- Heat and mass flux densities normal to the external boundary

$$G_1 = \int_0^{t_f} \left[\int_\Gamma q_n d\Gamma \right] dt; \qquad G_2 = \int_0^{t_f} \left[\int_\Gamma q_{nw} d\Gamma \right] dt; \; \Gamma \in \Gamma_{external}$$

Maximization = optimal radiator of heat and mass transport
Minimization = optimal isolator of heat and mass transport

- Amount of heat and mass generated within the domain

$$G_1 = \int_0^{t_f} \left[\int_\Omega f \, d\Omega \right] dt. \qquad G_2 = \int_0^{t_f} \left[\int_\Omega f_w d\Omega \right] dt.$$

Maximization = maximal amount of heat and mass generation
Minimization = minimal amount of heat and mass generation

Shape optimization problem. Functionals

- Measure of temperature and water vapor concentration

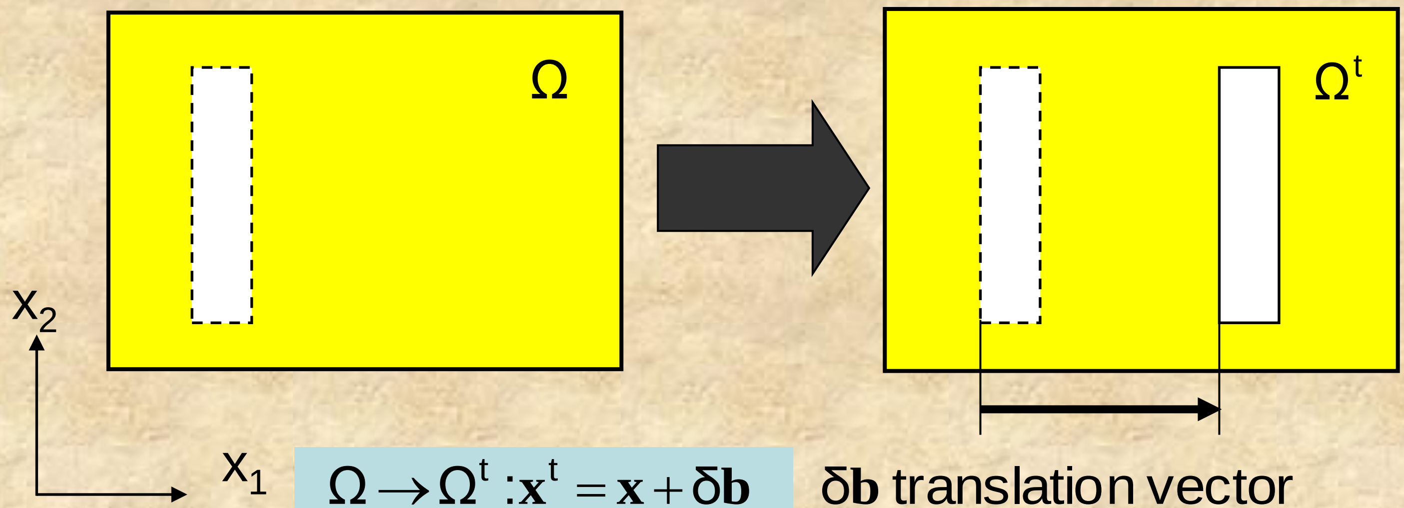
$$G_1 = \int_0^{t_f} \left\{ \left[\int_\Gamma \left(\frac{T}{T_0} \right)^n d\Gamma \right]^{\frac{1}{n}} \right\} dt \;\; ; \;\; n \to \infty; \quad G_2 = \int_0^{t_f} \left\{ \left[\int_\Gamma \left(\frac{w_f}{w_{f0}} \right)^n d\Gamma \right]^{\frac{1}{n}} \right\} dt \;\; ; \;\; n \to \infty \quad \Gamma \in \Gamma_{external}$$

T_0 w_{f0} assumed levels of state variables

Minimization of the functional =

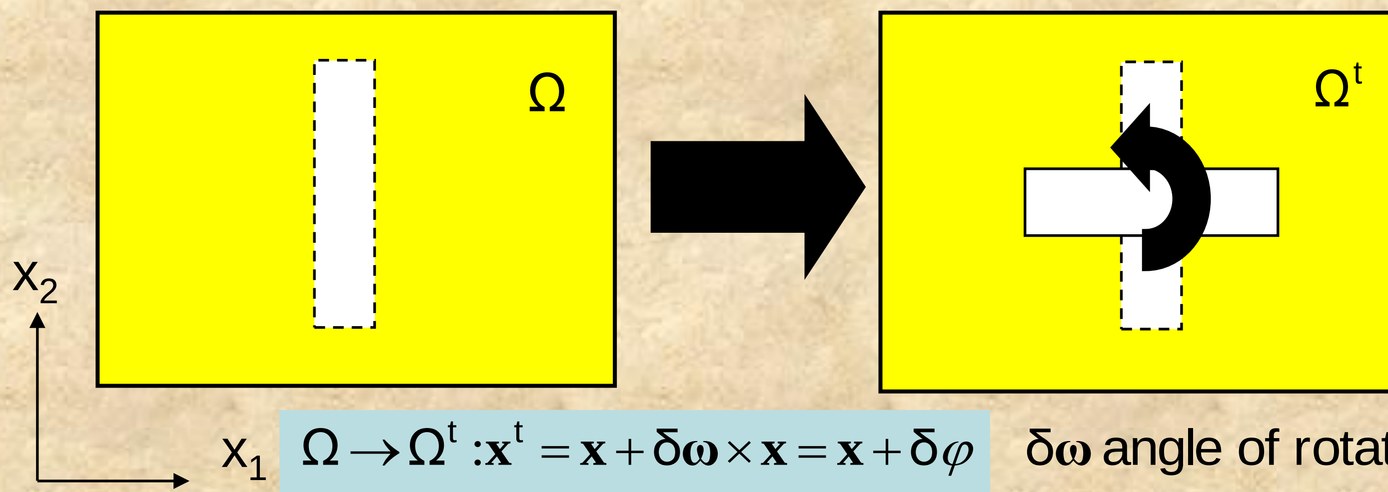
- distribution of state variables are equalized,
- maximal local values of state variables are minimized

Methods of shape modification



$$\Omega \to \Omega^t : \mathbf{x}^t = \mathbf{x} + \delta\mathbf{b}$$

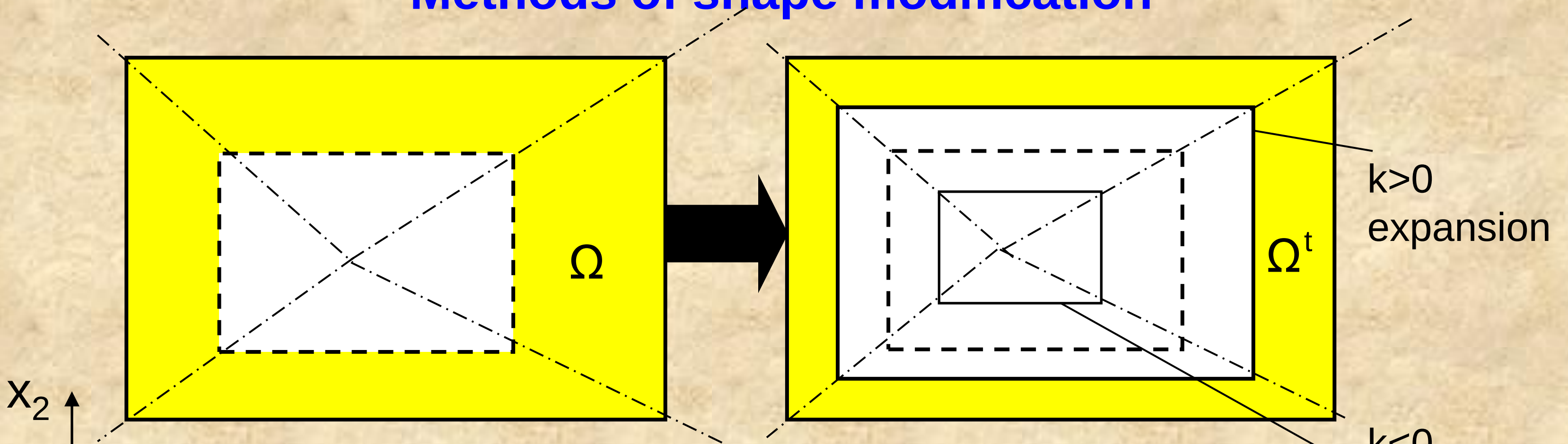
$\delta\mathbf{b}$ translation vector



$$\Omega \to \Omega^t : \mathbf{x}^t = \mathbf{x} + \delta\boldsymbol{\omega} \times \mathbf{x} = \mathbf{x} + \delta\varphi$$

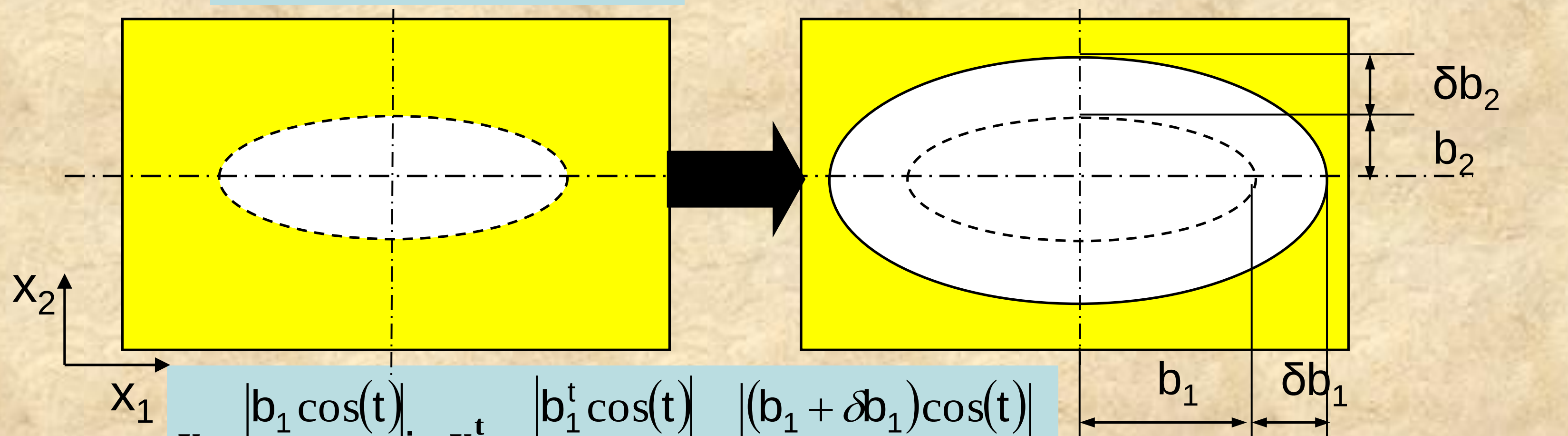
$\delta\boldsymbol{\omega}$ angle of rotation

Methods of shape modification



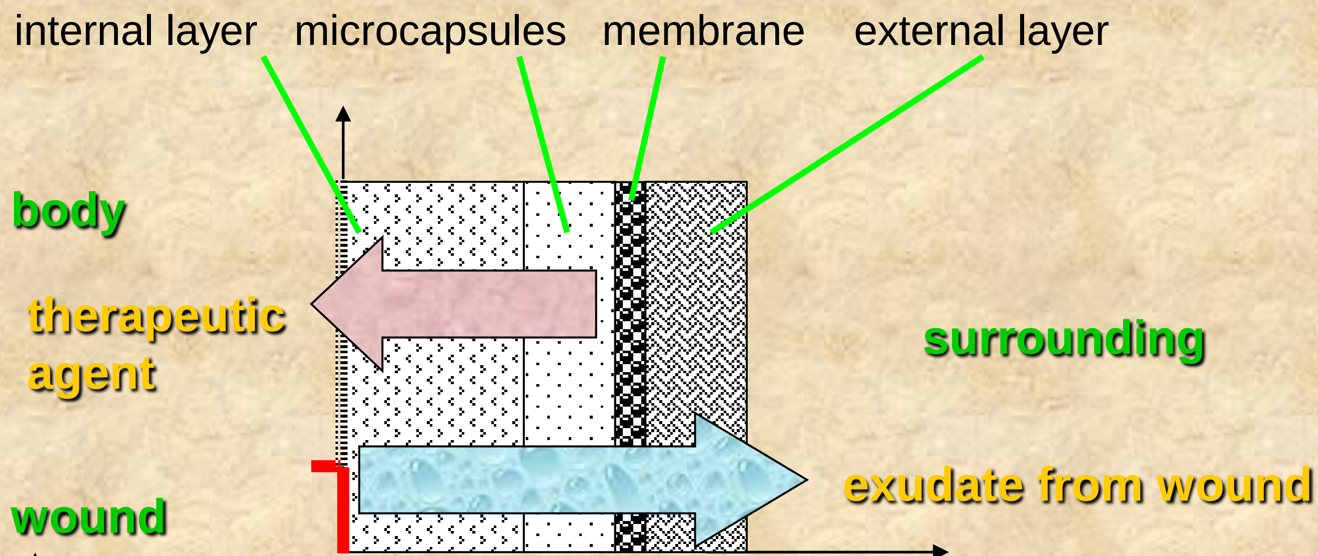
$$\Omega \to \Omega^{t} : \mathbf{x}^{t} = \mathbf{x} + \delta k\, \mathbf{x};$$

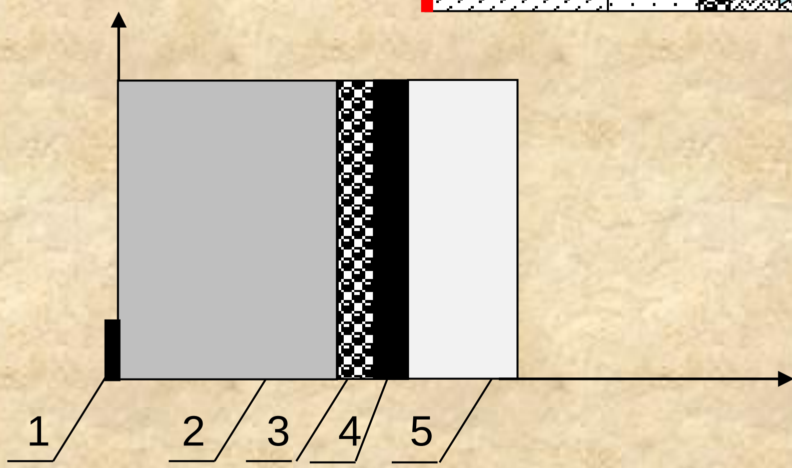
k scale change parameter



$$\mathbf{x} = \begin{vmatrix} b_1 \cos(t) \\ b_2 \sin(t) \end{vmatrix}; \quad \mathbf{x}^{t} = \begin{vmatrix} b_1^{t} \cos(t) \\ b_2^{t} \sin(t) \end{vmatrix} = \begin{vmatrix} (b_1 + \delta b_1)\cos(t) \\ (b_2 + \delta b_2)\sin(t) \end{vmatrix}$$

Numerical example: optimization of multilayer textile dressing with change phase material in terapeutic microcapsules

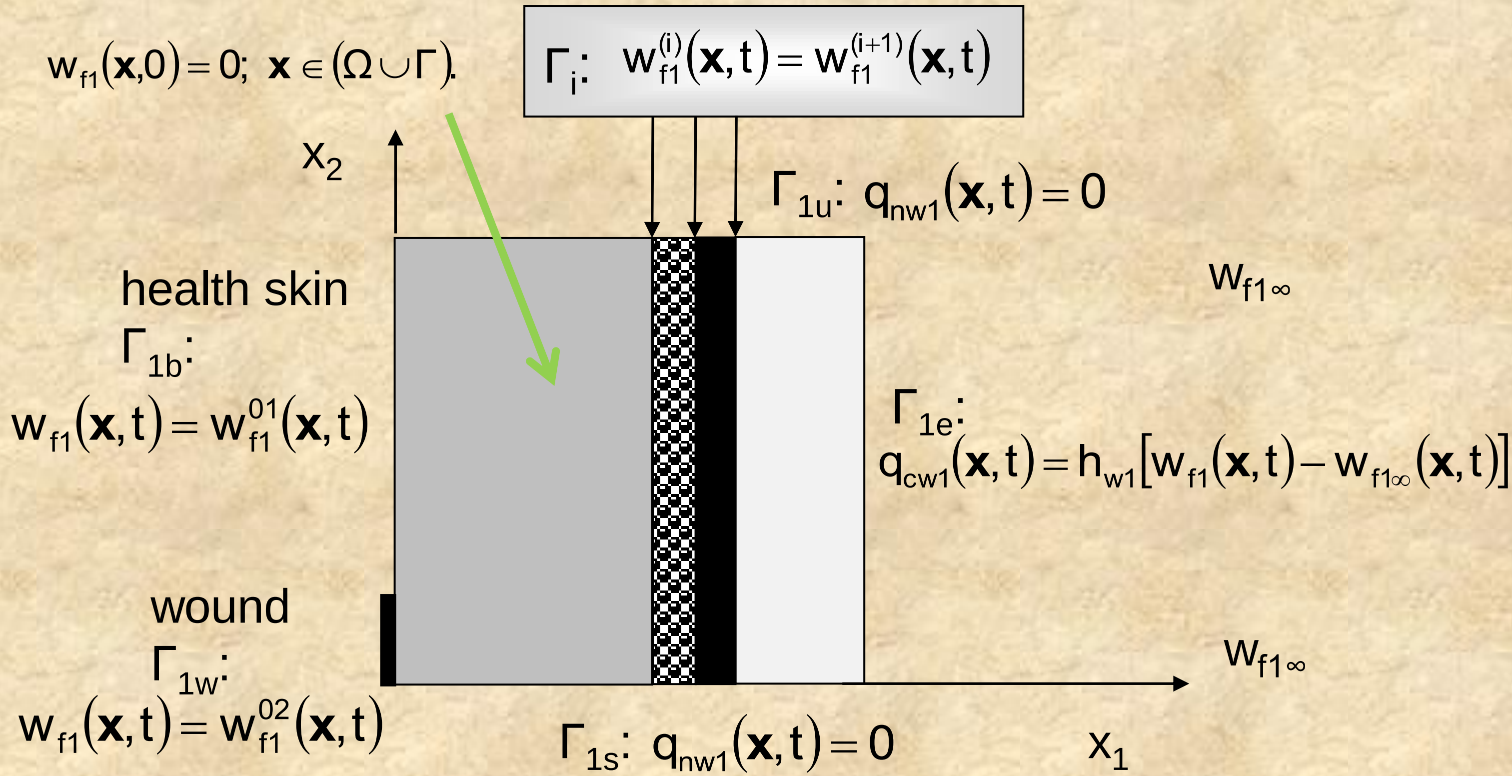




1 – wound,
2 – internal layer of nonwovens,
3 – nonwovens with microcapsules,
4 – membrane,
5 – external protective layer

Numerical example – primary problem

Transport of exudate from the wound to the surrounding – physical model

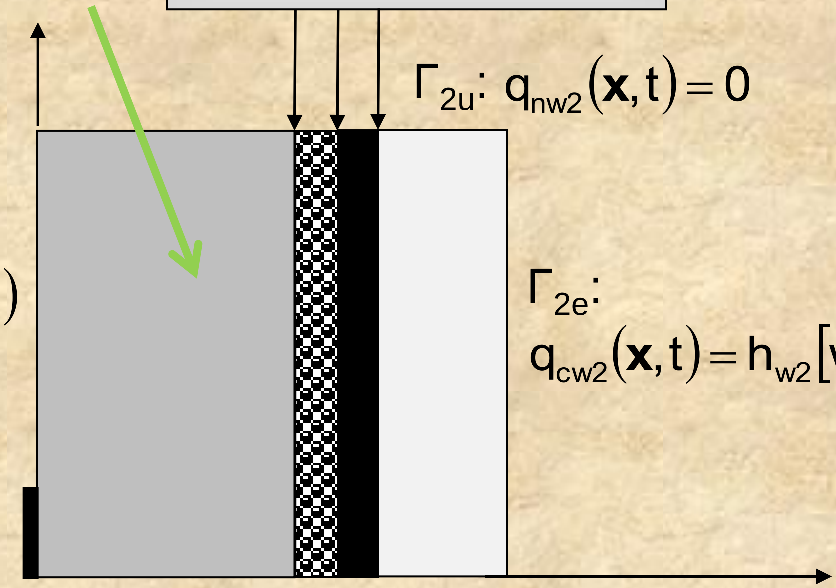


Numerical example – primary problem

Transport of therapeutic substance from the microcapsules to the skin – physical model

$w_{f2}(\mathbf{x},0)=0;\ \mathbf{x}\in(\Omega\cup\Gamma)$

$\Gamma_i:\ w_{f2}^{(i)}(\mathbf{x},t)=w_{f2}^{(i+1)}(\mathbf{x},t)$



$\Gamma_{2u}:\ q_{nw2}(\mathbf{x},t)=0$

$\Gamma_{2b}:$

$q_{nw2}(\mathbf{x},t)=q_{nw2}^{0}(\mathbf{x},t)$

$\Gamma_{2e}:$

$q_{cw2}(\mathbf{x},t)=h_{w2}\left[w_{f2}(\mathbf{x},t)-w_{f2\infty}\right]$

$\Gamma_{2s}:\ q_{nw2}(\mathbf{x},t)=0$

Numerical example – primary problem

Optimization problem:

- Real problem: Optimal mass transport from the dressing surface to the surrounding / the same heat conditions on the skin to secure the terapeutic effect.
- Physical model: Radiator of the mass diffusion, i.e. maximization of the mass flux densities of exudate and therapeutic agent on the external surface with the constant heat flux density on the skin.

Objective functional

$$F = \int_0^{t_f} \left[\int_{\Gamma_{1e}} q_{nw1}\, d\Gamma_{1e} + \int_{\Gamma_{2e}} q_{nw2}\, d\Gamma_{2e} \right] dt \to \max \Rightarrow$$

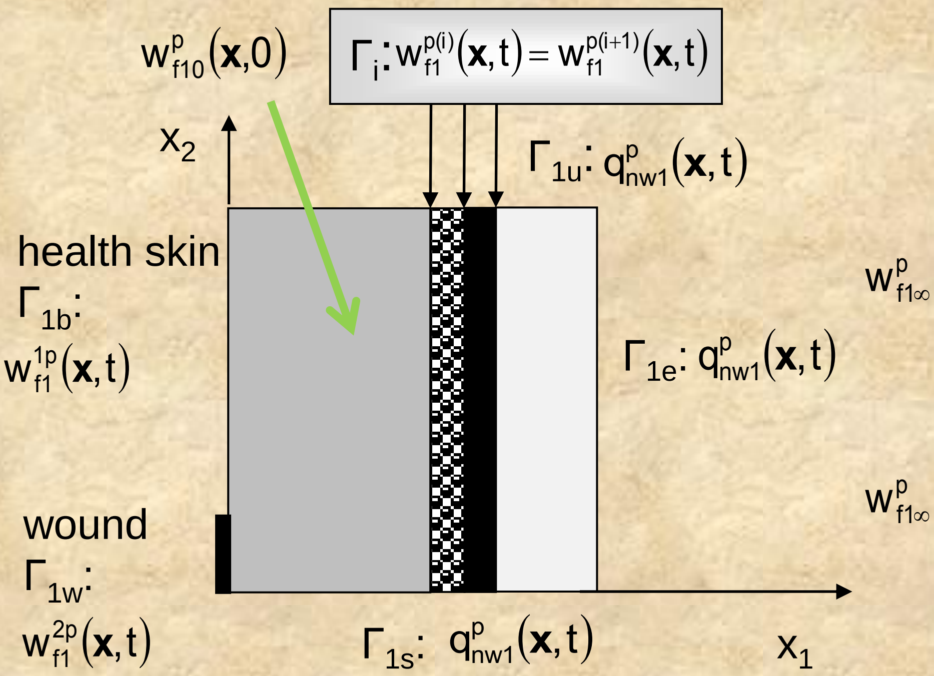
$$F = -\int_0^{t_f} \left[\int_{\Gamma_{1e}} q_{nw1}\, d\Gamma_{1e} + \int_{\Gamma_{2e}} q_{nw2}\, d\Gamma_{2e} \right] dt \to \min;$$

Constraints

$$\int_{\Gamma} q_n\, d\Gamma - q_n^0 = 0.$$

Numerical example – direct approach

Transport of exudate from the wound to the surrounding



Transport equation

$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{Z}\right)\dfrac{dw^{p(i)}_{f1}}{dt} = -\mathrm{div}\,\mathbf{q}^{p(i)}_{w1}; \\ \mathbf{q}^{p(i)}_{w1} = D^{(i)}\,\nabla w^{p(i)}_{f1} + \mathbf{q}^{*p(i)}_{w1}; \end{cases}$$

$$Z = \beta\rho \;\; \mathrm{dla}\; p = 0; \quad Z = \beta\eta \;\; \mathrm{dla}\; p > 0$$

Boundary conditions

$$w^p_{f1}(\mathbf{x},t) = -\nabla w^0_{f1}\cdot\mathbf{v}^p \quad \mathbf{x}\in\Gamma_{11}; \;\; \Gamma_{11} = \Gamma_{1b}\cup\Gamma_{1w};$$

$$q^p_{nw1}(\mathbf{x},t) = \mathbf{q}^0_{w1\Gamma}\cdot\nabla_\Gamma v^p_n - \nabla_\Gamma q^0_{nw1}\cdot\mathbf{v}^p_\Gamma - q^0_{nw1,n}v^p_n \quad \mathbf{x}\in\Gamma_{21}; \;\; \Gamma_{21} = \Gamma_{1s}\cup\Gamma_{1u};$$

$$q^p_{nw1}(\mathbf{x},t) = h_{w1}\left(w^p_{f1} - w^p_{f1\infty}\right) + \mathbf{q}_{w1\Gamma}\cdot\nabla_\Gamma v^p_n \quad \mathbf{x}\in\Gamma_{31}; \;\; \Gamma_{31} = \Gamma_{1e}$$

$$w^{p(i)}_{f1}(\mathbf{x},t) = w^{p(i)}_{f1}(\mathbf{x},t) \quad \mathbf{x}\in\Gamma_i;$$

$$w^p_{f10}(\mathbf{x},0) = -\nabla w_{f10}\cdot\mathbf{v}^p; \;\; \mathbf{x}\in(\Omega\cup\Gamma).$$

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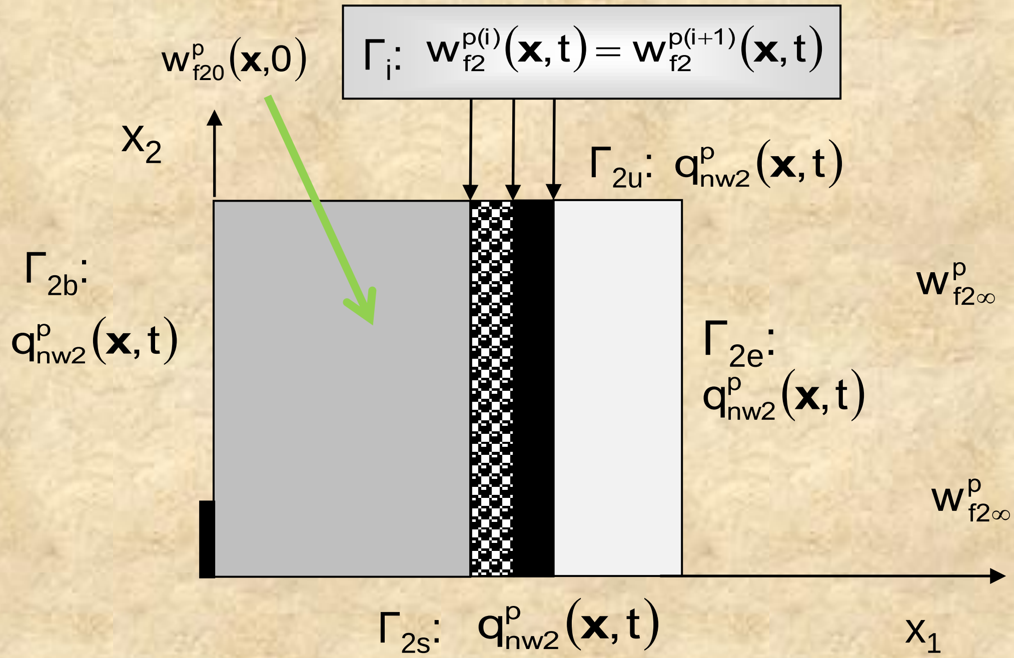
Department of Technical Mechanics and Informatics

Numerical example – direct approach

Transport of therapeutic substance from the microcapsules to the skin



Transport equation

$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{Z}\right)\dfrac{dw^{p(i)}_{f2}}{dt} = -\mathrm{div}\,\mathbf{q}^{p(i)}_{w2} + f^{p(i)}_{w}; \\ \mathbf{q}^{p(i)}_{w2} = D^{(i)}\,\nabla w^{p(i)}_{f2} + \mathbf{q}^{*p(i)}_{w2}; \end{cases}$$

$$Z = \beta\rho \;\; \mathrm{dla}\; p = 0; \quad Z = \beta\eta \;\; \mathrm{dla}\; p > 0$$

Boundary conditions

$$q^p_{nw2}(\mathbf{x},t) = \mathbf{q}^0_{w2\Gamma}\cdot\nabla_\Gamma v^p_n - \nabla_\Gamma q^0_{nw2}\cdot\mathbf{v}^p_\Gamma - q^0_{nw2,n}v^p_n \quad \mathbf{x}\in\Gamma_{22};\; \Gamma_{22} = \Gamma_{2b}\cup\Gamma_{2u}\cup\Gamma_{2s};$$

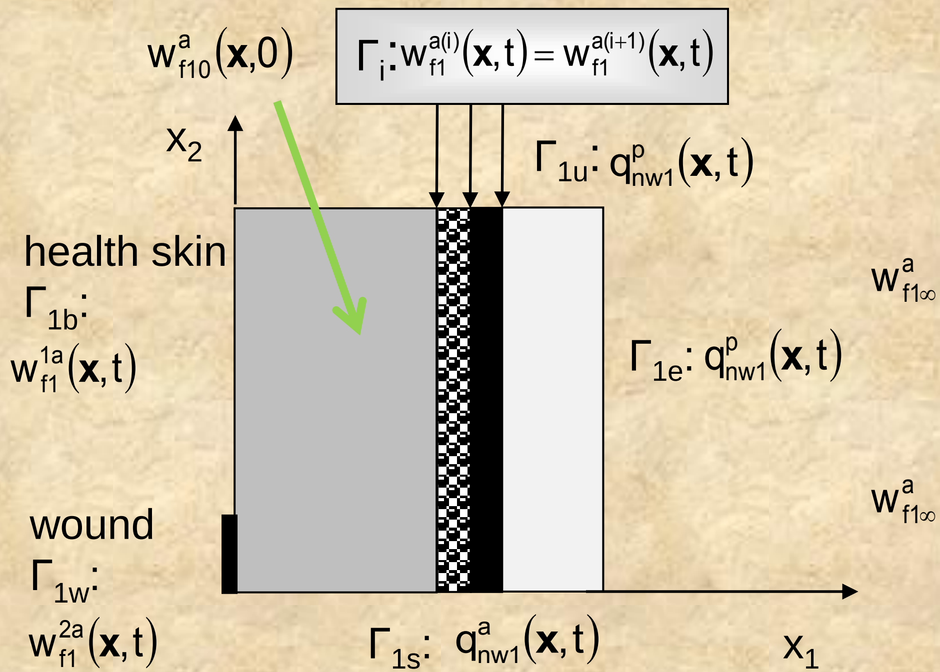
$$q^p_{nw2}(\mathbf{x},t) = h_{w2}\left(w^p_{f2} - w^p_{f2\infty}\right) + \mathbf{q}_{w2\Gamma}\cdot\nabla_\Gamma v^p_n \quad \mathbf{x}\in\Gamma_{32};\quad \Gamma_{32} = \Gamma_{2e}$$

$$w^{p(i)}_{f2}(\mathbf{x},t) = w^{p(i)}_{f2}(\mathbf{x},t) \quad \mathbf{x}\in\Gamma_i;$$

$$w^p_{f20}(\mathbf{x},0) = -\nabla w_{f20}\cdot\mathbf{v}^p;\;\; \mathbf{x}\in(\Omega\cup\Gamma).$$

Numerical example – adjoint approach

Transport of exudate from the wound to the surrounding



Transport equation

$$\begin{cases} \left(1-\varepsilon+\dfrac{\varepsilon}{Z}\right)\dfrac{dw^{a(i)}_{f1}}{dt} = -\operatorname{div}\mathbf{q}^{a(i)}_{w1}; \\ \mathbf{q}^{a(i)}_{w1} = D^{(i)}\,\nabla w^{a(i)}_{f1} + \mathbf{q}^{*a(i)}_{w1}; \end{cases}$$

$$Z = \beta\rho \ \text{dla}\ p = 0; \quad Z = \beta\eta \ \text{dla}\ p > 0$$

Boundary conditions

$$w^a_{f1}(\mathbf{x},\tau=0) = 0 \quad \mathbf{x}\in(\Omega\cup\Gamma); \qquad q^{*a}_{w1}(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Omega;$$

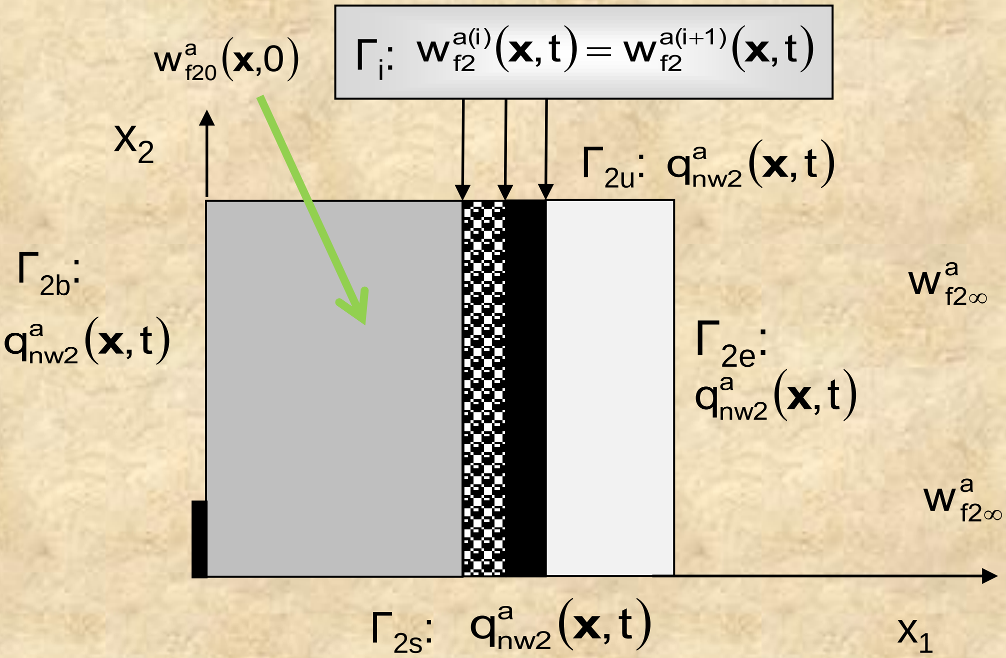
$$w^{0a}_{f1}(\mathbf{x},\tau) = -1 \quad \mathbf{x}\in\Gamma_{11}; \quad \Gamma_{11} = \Gamma_{1b}\cup\Gamma_{1w};$$

$$q^{0a}_{nw1}(\mathbf{x},\tau) = 0 \quad \mathbf{x}\in\Gamma_{21}; \quad \Gamma_{21} = \Gamma_{1s}\cup\Gamma_{1u};$$

$$w^a_{f1\infty}(\mathbf{x},\tau) = -1 \quad \mathbf{x}\in\Gamma_{31}; \ \Gamma_{31} = \Gamma_{1e}$$

Numerical example – adjoint approach

Transport of therapeutic substance from the microcapsules to the skin



Transport equation

$$\begin{cases}\left(1-\varepsilon+\dfrac{\varepsilon}{Z}\right)\dfrac{dw_{f2}^{a(i)}}{dt} = -\mathrm{div}\,\mathbf{q}_{w2}^{a(i)} + f_{w}^{a(i)};\\ \mathbf{q}_{w2}^{a(i)} = D^{(i)}\,\nabla w_{f2}^{a(i)} + \mathbf{q}_{w2}^{*a(i)};\end{cases}$$

$$Z=\beta\rho \text{ dla } p=0;\quad Z=\beta\eta \text{ dla } p>0$$

Boundary conditions

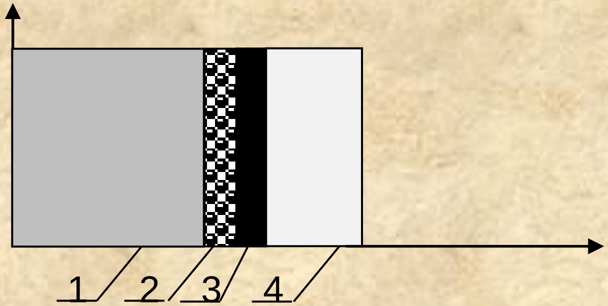
$$w_{f2}^{a}(\mathbf{x},\tau=0)=0 \qquad \mathbf{x}\in(\Omega\cup\Gamma); \qquad f_{w}^{a}(\mathbf{x},\tau)=0 \quad \mathbf{x}\in\Omega;$$

$$q_{w2}^{*a}(\mathbf{x},\tau)=0 \quad \mathbf{x}\in\Omega;$$

$$q_{nw2}^{0a}(\mathbf{x},\tau)=0 \quad \mathbf{x}\in\Gamma_{22};\ \Gamma_{22}=\Gamma_{2b}\cup\Gamma_{2u}\cup\Gamma_{2s};$$

$$w_{f2\infty}^{a}(\mathbf{x},\tau)=-1 \qquad \mathbf{x}\in\Gamma_{32};\ \Gamma_{32}=\Gamma_{2e}$$

Numerical example – material parameters



1 – internal layer of nonwovens,
2 – nonwovens with microcapsules,
3 – membrane,
4 – external protective layer

1,4 – nonwovens: porous acryl fibres (85% of fibres)

$\mathbf{A}^{(1)}=\mathbf{A}^{(1)}=28{,}8\cdot 10^{-3}\ \mathrm{kWm^{-1}K^{-1}}$ $\quad c^{(1)}=c^{(4)}=1610{,}9\ \mathrm{kJm^{-3}K}$ $\quad \eta^{(1)}=\eta^{(4)}=0{,}85$

$$D_f^{(1)}=D_f^{(4)}=\left[1{,}12-410\frac{w_f}{\rho}-8200\left(\frac{w_f}{\rho}\right)^2\right]\cdot 10^{-13};\quad t<540s;\ D_f^{(1)}=D_f^{(4)}=6{,}23\cdot 10^{-13};t\geq 540s$$

2 – nonwovens: porous acryl fibres with microcapsules (90% fibres)

$\mathbf{A}^{(2)}=27{,}5\cdot 10^{-3}\ \mathrm{kWm^{-1}K^{-1}}$ $\quad c^{(2)}=1600{,}0\ \mathrm{kJm^{-3}K}$ $\quad \eta^{(2)}=0{,}85$

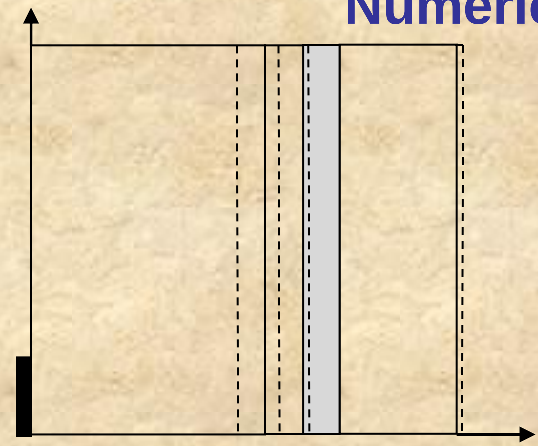
$$D_f^{(2)}=\left[0{,}896-328\frac{w_f}{\rho}-6560\left(\frac{w_f}{\rho}\right)^2\right]\cdot 10^{-13};\quad t<540s;\quad D_f^{(2)}=4{,}984\cdot 10^{-13};\quad t\geq 540s;$$

3 – semi-permeable membrane: polypropylene (95% of material)

$\mathbf{A}^{(3)}=51{,}8\cdot 10^{-3}\ \mathrm{kWm^{-1}K^{-1}}$ $\quad c^{(3)}=1715{,}0\ \mathrm{kJm^{-3}K}$ $\quad \eta^{(3)}=0{,}20$

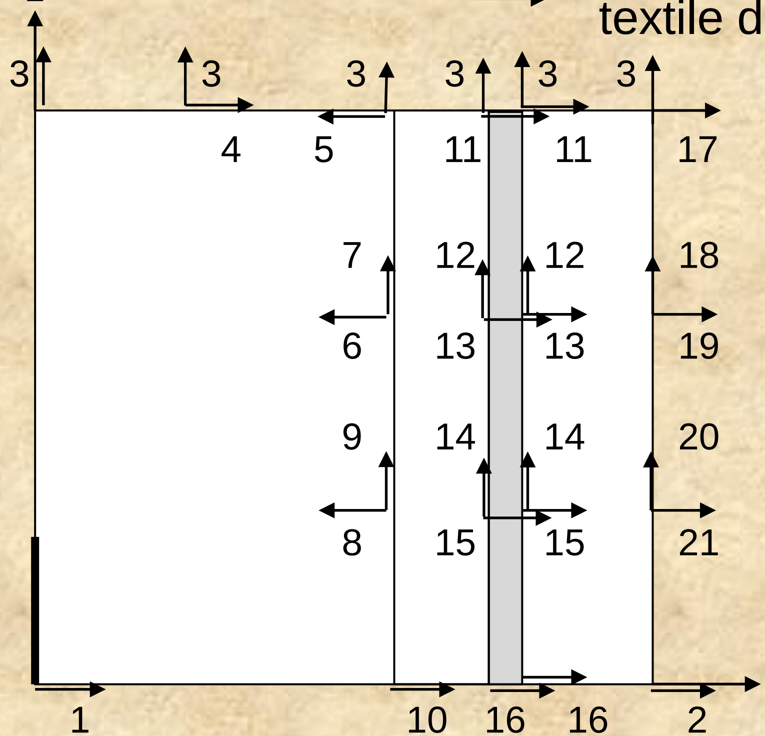
$$D_f^{(3)}=1{,}3e\cdot 10^{-13};\ t\ \text{optional}$$

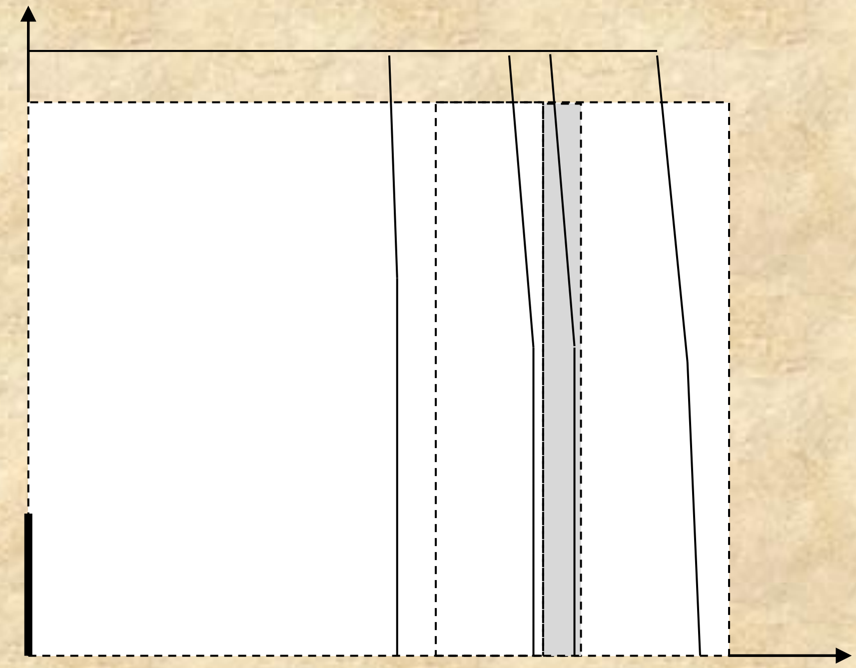
Numerical example – optimal shapes



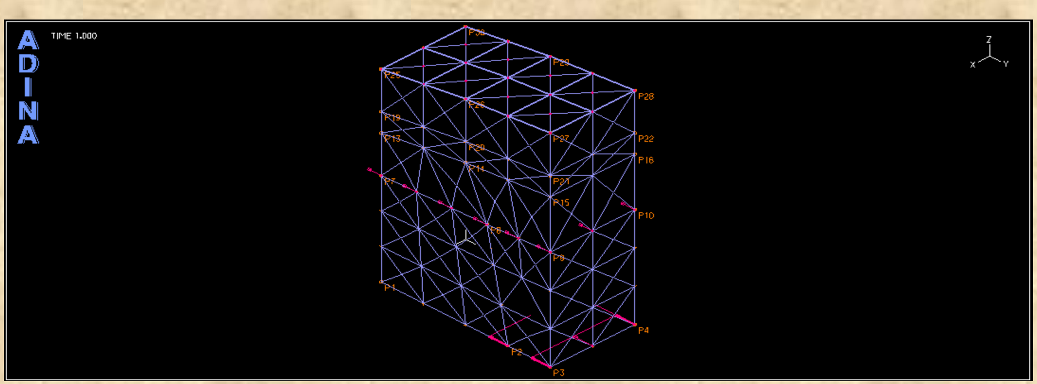
Initial / optimal thickness of layers in textile dressing

Design variables / initial shape / optimal shape of textile dressing for the variable shape of layers

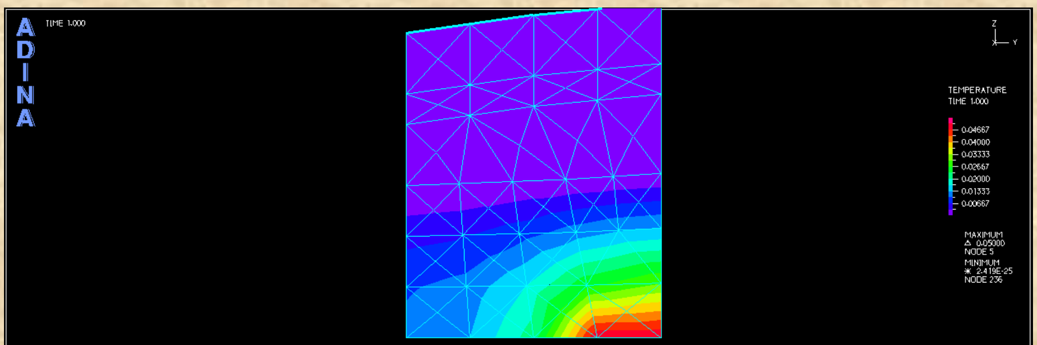




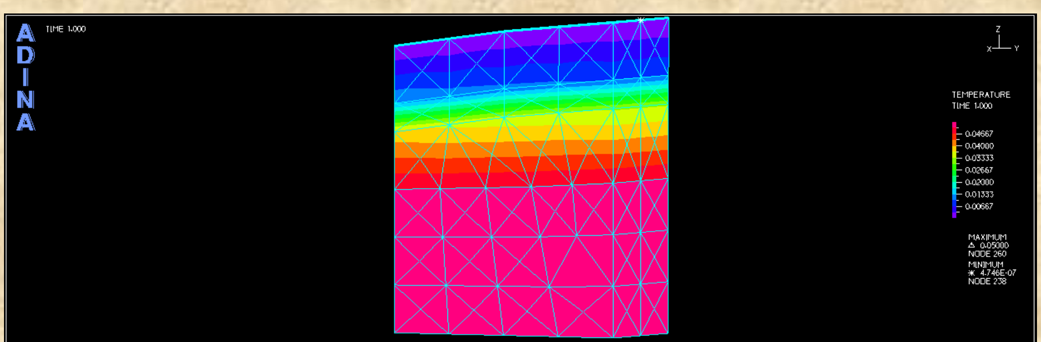
Numerical example – maps of state variables for optimal shapes



Finite Element Net

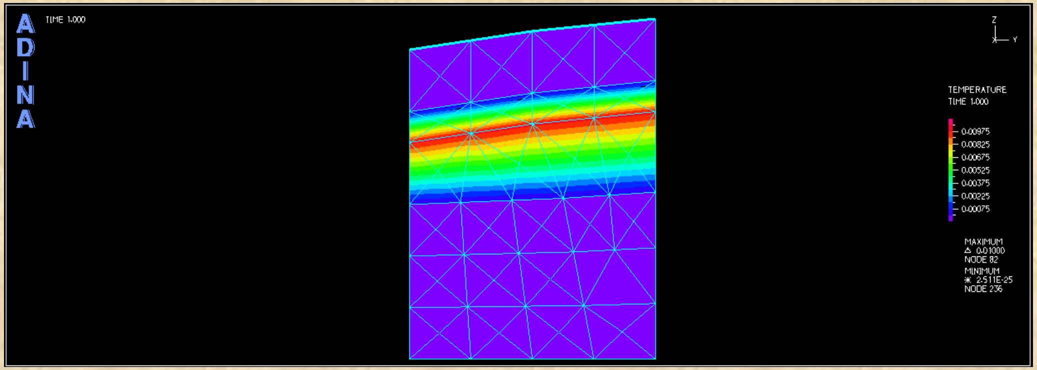


Exudate distribution
t=60s

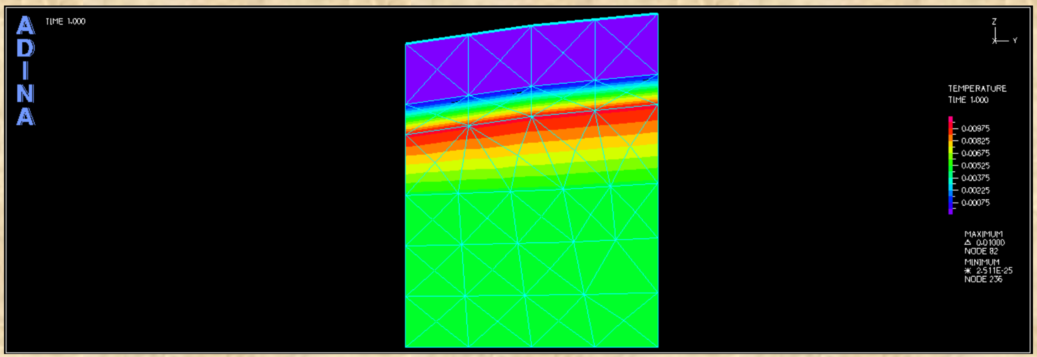


Exudate distribution
t=960s

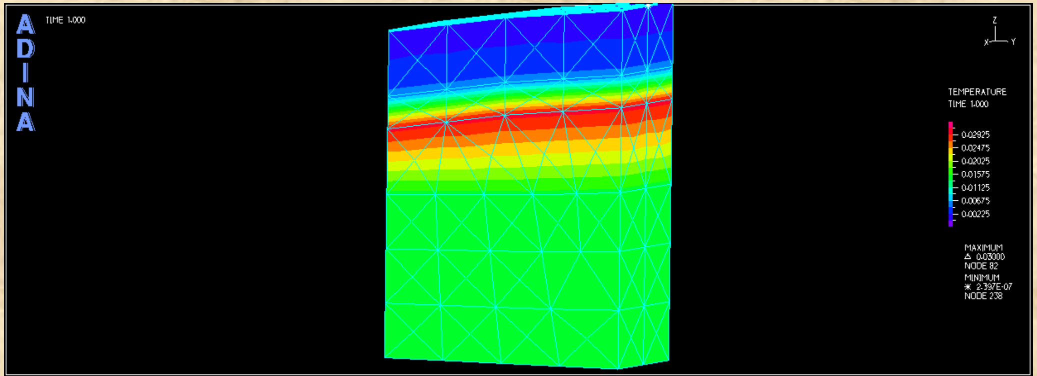
Numerical example – maps of state variables for optimal shapes



Therapeutic agent distribution t=60s



Therapeutic agent distribution t=360s



Therapeutic agent distribution t=960s

Conclusions

- The textile structures with the membranes and microcapsules are subjected to the coupled transport problems.
- The available literature does not contain the optimization of the similar problems for textile dressings by the sensitivity analysis.
- The effective optimization = the choice of criterion.
- Minimization of the objective functional = solution of the specified physical problem, the constraints = the permissible domain with respect to technological point of view.
- The physical model of the coupled transport is described by the state variables: temperature, the water vapor concentrations in fibres and within the free spaces between fibres.
- The mathematical model contains the transport equations, the boundary and the initial conditions.
- Numerical implementation shows that the discussed methods can be the effective and fast tools to create the optimal model of the textile structures during the coupled transport.