Topological optimization for solids under heat and mass transfer using boundary element

Optimización topológica de sólidos en calor y transferencia de masa utilizando los elementos de contorno

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Abstract

The objective of this work is to present the implementation of a topological-shape sensitivity formulation in a BEM analysis for simultaneous heat and mass transfer optimization problems. The proposed approach uses a topological derivative in order to estimate the sensitivity to create a hole in the domain of the problem. Thus, it is evaluated at internal points, and the ones showing the lowest values are used to remove material by opening a circular cavity. As the iterative process evolves, the original domain has holes progressively punched out until a given stop criteria is achieved. Since the sensitivities for each of the differential equations are different, a penalization-type approach has been used to weight the sensitivities associated to each problem. This allows the imposition of distinct penalization factors for each problem, according to specified priorities. The results obtained showed good agreement with solutions available in the literature.

----------*Keywords:* Shape optimization, potential problems, boundary elements, topological derivative, mass transfer

Resumen

El objetivo de este trabajo es presentar la aplicación de una formulación para el análisis de sensibilidad de forma y topologia utilizando elemetos de contorno en problemas de optimización involucrando transferencia simultanea de calor y masa. El enfoque propuesto usa la derivada topológica para estimar la

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sensibilidad a crear un agujero en el domínio de definición del problema. De este modo, la misma se evalua en puntos internos y aquellos que presentan los valores más bajos se utilizan para eliminar material mediante la apertura de una cavidad circular. A medida que el proceso iterativo evoluciona, el dominio se modifica progresivamente con la incorporación de más agujeros hasta que se alcanza un criterio de parada determinado. Puesto que las sensibilidades de cada una de las ecuaciones diferenciales son diferentes, un enfoque tipo penalización ha sido utilizado para ponderar las sensibilidades asociadas a cada problema. Esto permite la imposición de factores de penalización distintos para cada problema, de acuerdo a prioridades especificadas. Los resultados obtenidos mostraron una buena concordancia con soluciones disponibles em la literatura.

---------- *Palabras clave:* Optimización de forma, problemas potenciales, elementos de contorno, derivada topológica, transferencia de masa

Introduction

Materials classified as porous are widely used in many applications in the engineering field. In the last years some efforts have been done in order to increase the material efficiency in different areas. A porous medium was defined by Kaviany [1] as a mixture of a heterogeneous solid matrix with its void with fluids. As a structural material a porous media has mechanical properties such as elasticity and strength.

The term "porous materials" is usually reserved to materials such as fibers, ceramic, concrete and porous rock as well. This kind of material is frequently present in a wide variety of devices or components. There are numerous scientific and engineering applications for porous materials. Some examples should be listed in order to give a panoramic view of the usage of these materials. For example, for Chemical engineering this material is found in reactors and static mixers, For Civil engineering, the concrete and the aquifers [2] (which consist of sand, gravel and fractured rock) are typical examples of porous materials, for mechanical engineering a layout of heat exchangers [3] and micro channel cooling [4] also can be modeled as a porous media, for biomedical engineering a good example are the bones, lungs and kidneys. In Dondero et al. [5]

a numerical methodology for the computation of the effective thermal conductivity (ETC) of random micro-heterogeneous materials using representative volume elements and the Fast Multipole Boundary Element Method (FMBEM) was introduced. This methodology was applied to solve a two-dimensional foam-like microstructure consisting of a random distribution of circular isolated holes. The final results showed that the proposed numerical methodology is effective for the computation of the ETC of random micro heterogeneous materials.

Obviously there are many others applications which are impossible to be cited herein. With this brief review was possible to expose the extension of the problems that involves the porous materials. In this sense the main objective of this work is focused in presenting a numerical methodology to combine heat and mass transfer designs in a resulting optimal solid shape for both problems. Materials which are in charge of transferring heat and mass simultaneously should be classified as porous materials. A strategy of compromise [6] that attributes weights to the respective equations will be employed in order to establish a relationship between both problems. A well-known topological derivative (D_T) approach [7, 8] was used to evaluate the sensitivities, as an alternative to the traditional homogenization methods [9]. The boundary

element method (BEM) was chosen to provide the numerical solution. Since the BEM does not require domain meshes, a significant reduction in the computational cost during the iterative optimization process can be achieved, in comparison to other traditional numerical methods. As the efforts will be straight to the solution of multi-objective optimization problems using the proposed methodology, this work will be structured as: Firstly, the D_T formulation for the Poisson equation is presented. Next, the optimization procedure employed herein for multi-criteria problems detailed. In order to access the formulation, a

case of simultaneous two-dimensional heat and mass transfer is optimized for mass reduction and discussed.

Topological derivative

A topological derivative for Poisson Equation is applied in this work. A simple example of applicability consists in a case where a small hole of radius (ε) is open inside the domain. The concept of topological derivative consists in to determine the sensitivity of a given function cost (ψ) when this small hole is increased or decreased (figure 1).
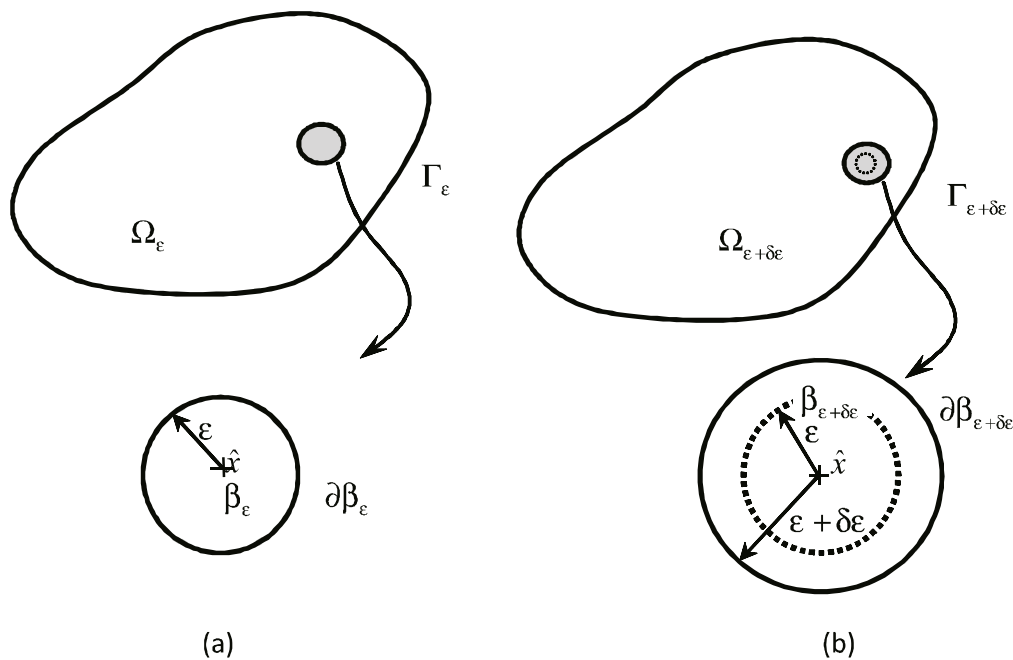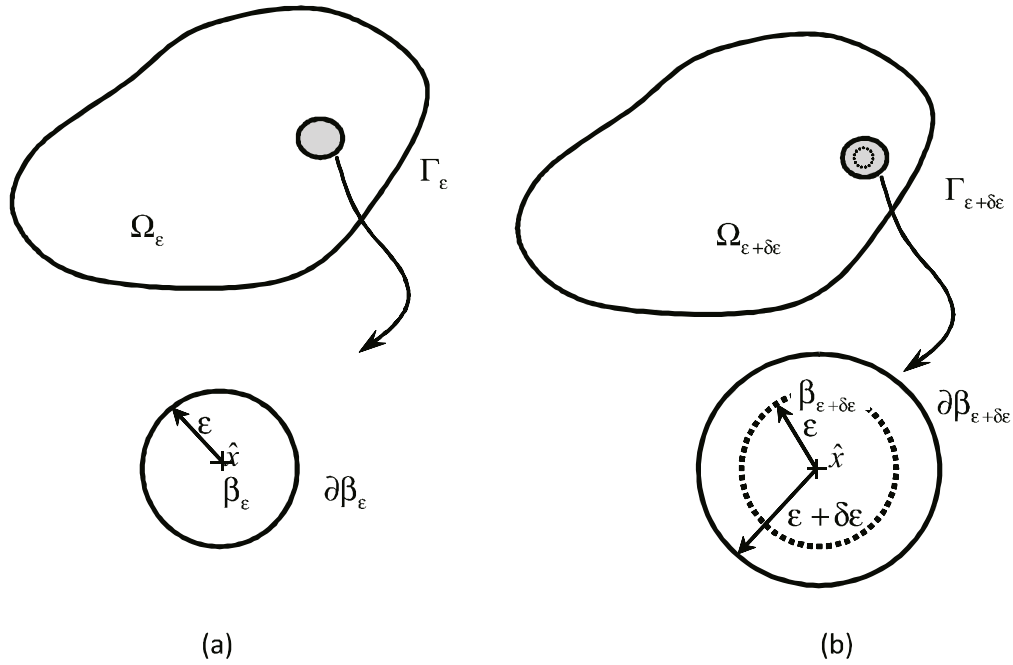

Figure 1 Topological derivative original concept: (a) Original Domain Ω and (b) Perturbed domain Ω_ε

The local value of D_T at a point ($\hat{x}$) inside the domain for this case is evaluated by:

$$\overset{*}{D_T}(\hat{x}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega)}{f(\varepsilon)} \qquad (1)$$

Where $\psi(\Omega)$ and $\psi(\varepsilon)$ are the cost function evaluated for the original and the perturbed

domain, respectively, and f is a problem dependent regularizing function. By equation (1) it is not possible to establish an isomorphism between domains with different topologies. This equation was modified introducing a mathematical idea that the creation of hole can be accomplished by single perturbing an existing one whose radius tends to zero, figure 2.

Figure 2 Topological Derivative with a new point of view. (a) Original Domain Ω and (b) Perturbed domain Ω_ε

This allows the restatement of the problem in such a way that it is possible to establish a mapping between each other [10].

$$D_T^*(\hat{x}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_{\varepsilon+\delta\varepsilon}) - \psi(\Omega_\varepsilon)}{f(\Omega_{\varepsilon+\delta\varepsilon}) - f(\Omega\varepsilon)} \qquad (2)$$

Where $\delta\varepsilon$ is a small perturbation on the holes's radius. Equation (2) gives a shape sensitivity

when the hole increase or decrease. It is also important to notice the both Eq. 1 e Eq. 2 are equivalent, as presented in [10].

The D_T for the steady state heat transfer will be briefly reviewed herein. In the case of linear heat transfer, the direct problem is stated as:

$$\text{Solve } \{u_\varepsilon \mid -k\Delta u_\varepsilon = b\} \text{ on } \Omega_\varepsilon \qquad (3)$$

Subjected to

$$\begin{cases} u_\varepsilon = \bar{u} & \text{on} \quad \Gamma_D \\ -k\dfrac{\partial u_\varepsilon}{\partial n} = \bar{q} & \text{on} \quad \Gamma_N \\ -k\dfrac{\partial u_\varepsilon}{\partial n} = h_c\left(u_\varepsilon - u_\infty\right) & \text{on} \quad \Gamma_R \end{cases} \qquad (4)$$

where

$$h(\alpha,\beta,\gamma) = \underbrace{\alpha\left(u_\varepsilon - \bar{u}^\varepsilon\right)}_{\text{Dirichlet b.c.}} + \underbrace{\beta\left(k\frac{\partial u_\varepsilon}{\partial n} + \bar{q}^\varepsilon\right)}_{\text{Neumann b.c.}} + \underbrace{\gamma\left(k\frac{\partial u_\varepsilon}{\partial n} + h_c^\varepsilon\left(u_\varepsilon - u_\infty^\varepsilon\right)\right)}_{\text{Robin b.c.}} = 0 \qquad (5)$$

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Is a function which takes into account the type of boundary condition on the holes to be created ($u_\varepsilon, \frac{\partial u_\varepsilon}{\partial n} = q_\varepsilon$ are the temperature and flux on the hole boundary, while u_∞^ε and h_c^ε are the hole's internal convection parameters, respectively).

Taking a general form for a cost function written as

$$\psi(\Omega_\tau) = \int_{\Omega_\tau} \phi_{\Omega_\tau}(u_\tau) d\Omega_\tau + \int_{\Gamma_\tau} \phi_{\Gamma_\tau}(u_\tau) d\Gamma_\tau \quad (6)$$

Where τ is a parameter associate to the shape change velocity, i.e., $x_\tau(x) = x + \tau v(x)$. The sensitivity of the cost function with respect to τ can be derived from the Gâteaux derivative.

$$\frac{d}{d\tau}\Psi(\Omega_\tau)_{\tau=0} = \lim_{\tau \to 0} \frac{\Psi(\Omega_\tau) - \Psi(\Omega_{\tau|\tau=0})}{\tau} h(\alpha, \beta, \gamma) = 0 \text{ on } \partial\beta_\varepsilon \quad (7)$$

Therefore the problem should be re-stated as:

Evaluate: $\dfrac{d}{d\tau}\Psi(\Omega_\tau) = 0$

Subject to

$$a_\tau(u_\tau, n_\tau) = l_\tau(n_\tau) \quad \forall n_\tau \in \beta_{\tau 1} \quad \forall \tau \geq 0 \quad (8)$$

Where a_τ is a continuous, coercive bilinear form, l_τ is a continuous linear functional and β_τ is the space of the admissible perturbation functions for the perturbed domain Ω_τ. Using the total potential energy as a cost function $\left(\Phi_\tau(u_\tau) := \frac{1}{2} a_\tau(u_\tau, u_\tau) - l_\tau(u_\tau)\right)$, the a_τ and l_τ functional are written as:

$$a_\varepsilon(u_\varepsilon, n_\varepsilon) := \int_{\Omega_\varepsilon} k\nabla u_\varepsilon \cdot \nabla \eta_\varepsilon d\Omega +$$
$$\int_{\Gamma_c} h_c u_\varepsilon \eta_\varepsilon d\Gamma + \int_{\partial\Lambda_\varepsilon} h_c^\varepsilon u_\varepsilon \eta_\varepsilon d\partial\Lambda$$

$$l_\varepsilon(\eta_\varepsilon) := \int_{\Omega_\varepsilon} b\eta_\varepsilon d\Omega - \int_\Gamma \bar{q}\eta_\varepsilon d\Gamma -$$
$$\int_{\Gamma_c} h_c u_\infty \eta_\varepsilon d\Gamma - \int_{\partial\Lambda_\varepsilon \bar{q}_\varepsilon} \eta_\varepsilon d\partial\Lambda + \gamma \int_{\partial\Lambda_\varepsilon} h_c^\varepsilon u_\infty \eta_\varepsilon d\partial\Lambda$$

Considering Eq. (8) one can derive the D_T expression particularized for the three classical boundary conditions prescribed on the holes.

Neumann boundary condition

For this case the eq. (5) is particularized as (α = 0, β = 1, γ = 0) and the D_T is obtained by taking the limit:

$$D_T(\hat{x}) = -\lim_{\varepsilon \to 0} \frac{1}{2f'(\varepsilon)}$$
$$\int_{\partial\Omega\varepsilon}\left[k\left(\frac{\partial u_\varepsilon}{\partial t}\right) - k\left(\frac{\partial u_\varepsilon}{\partial n}\right) - 2bu_\varepsilon - \frac{2}{\varepsilon}\bar{q}_\varepsilon u_\varepsilon\right] d\Omega\varepsilon \quad (9)$$

where t and n are the tangential and normal directions respectively.

Both cases of Neumann boundary conditions must be considered:

$$\bar{q}_\varepsilon = \left.\frac{\partial u_\varepsilon}{\partial n}\right|_{\partial\Omega_\varepsilon} = 0 \text{ com } f'(\varepsilon) = -\pi\varepsilon^2 \quad (10)$$

$$\bar{q}_\varepsilon = \left.\frac{\partial u_\varepsilon}{\partial n}\right|_{\partial\Omega_\varepsilon} \neq 0 \text{ com } f'(\varepsilon) = -2\pi\varepsilon \quad (11)$$

For homogeneous and non-homogeneous cases respectively.

Dirichlet boundary condition

For this case the eq. (5) is particularized as (α = 1, β = 0, γ = 0) and the D_T is obtained by taking the limit:

$$D_T(\hat{x}) = -\lim_{\varepsilon \to 0} \frac{1}{2f'(\varepsilon)}$$
$$\int_{\partial\Omega\varepsilon}\left[k\left(\frac{\partial u_\varepsilon}{\partial t}\right)^2 - k\left(\frac{\partial u_\varepsilon}{\partial n}\right)^2 - 2bu_\varepsilon\right] d\Omega\varepsilon \quad (12)$$

Being the conditions

$$u_\varepsilon = \overline{u}_\varepsilon \qquad \left.\frac{\partial u_\varepsilon}{\partial t}\right|_{\partial\Omega_\varepsilon} \neq 0 \qquad (13)$$

Used along with $f'(\varepsilon) = \dfrac{2\pi}{\mathrm{h}\,\varepsilon}$.

Robin boundary condition

In this case one has *(α = 0, β =0 , γ = 1)* and the D_T is obtained by taking the limit:

$$D_T(\hat{x}) = -\lim_{\varepsilon\to 0}\frac{1}{2f'(\varepsilon)}$$

$$\int_{\partial\Omega_\varepsilon}\left[k\left(\frac{\partial u_\varepsilon}{\partial t}\right)^2 - k\left(\frac{\partial u_\varepsilon}{\partial n}\right)^2 - 2bu_\varepsilon - \frac{2}{\varepsilon}h_c^\varepsilon\left(u_\varepsilon - 2u_{\varepsilon\infty}\right)\right]d\Omega\varepsilon \qquad (14)$$

Now the regularizing function for this case is $f'(\varepsilon) = -2\pi\varepsilon$.

Afterwards table 1 summarizes the final expressions for topological derivative, after apply the respective regularizing function for each boundary condition, under consideration in Eq. (9), Eq. (12) and Eq. (14). It is also important to inform that the same formulas presented as table 1 are used for determining the sensitivity of a domain governed by the Laplace equation.

Table 1 Topological derivative for the three b.c. prescribed on the holes

Boundary condition on the hole	Topological derivative	Evaluated at
Neumann homogeneous boundary condition (α = 0, β =1 , γ = 0)	$D_T(\hat{x}) = k\nabla u\nabla u - bu$	$\hat{x}\in\Omega\cup\Gamma$
Neumann non-homogeneous boundary condition (α = 0, β =1 , γ = 0)	$D_T(\hat{x}) = -q_\varepsilon u$	$\hat{x}\in\Omega\cup\Gamma$
Robin boundary condition (α = 0, β = 0, γ = 1)	$D_T(\hat{x}) = h_c^\varepsilon\left(u_\varepsilon - u_{\varepsilon\infty}\right)$	$\hat{x}\in\Omega\cup\Gamma$
Dirichlet boundary condition (α = 1, β = 0, γ = 0)	$D_T(\hat{x}) = -\frac{1}{2}k\left(u - \overline{u}_\varepsilon\right)$	$\hat{x}\in\Omega$
Dirichlet boundary condition (α = 1, β = 0, γ = 0)	$D_T(\hat{x}) = k\nabla u\nabla u - b\overline{u}_\varepsilon$	$\hat{x}\in\Gamma$

It is also important to take attention that D_T is evaluated by different expressions for interior and boundary points. Another remark relies on the fact that the expressions presented as Tab.1 are deduced taking the total potential energy as cost function.

Multi-criteria optimization procedure

The optimization of problems under more than one cost function is becoming quite common in engineering practice. For instance, in the electronic industry the miniaturization of components are leading to excessively slender designs, which demands new and efficient cooling devices, usually base on porous media. The successful design of such components imply in the optimization of both, heat and mass transfer. This technology presents two basic advantages [11]: (a) the porous heat sink provides more than 10 times the contact area of a smooth surface; and (b) the irregular structures of the porous heat sinks, at sufficient high velocities,

causes irregular fluid flow, increasing the thermal dispersion conductivity. This is a typical case where the heat conduction would lead to an optimum design, while the convection would lead to another one. Therefore, it is necessary to combine both optimization problems in a single one. Clearly, the adoption of one (single criteria) design could result in a less efficient performance of the product from the other criteria(s) point(s) of view.

In engineering design practice, it is usual for a thermal solid to be required to satisfy one of the following optimality criteria:

A   As uniform mass transfer rate as possible;

B   As uniform heat transfer rate as possible;

C   Maximum possible efficiency in both criteria A e B, simultaneously.

From the optimization point of view, the first two criteria mean the extremization of a single objective function. The satisfaction of criterion C needs the satisfaction of multiple design criteria, which is the goal of this work. After separate BEM heat and mass analysis, the heat flux and mass densities are determined at internal points. These values are used to evaluate the topological derivative. In order to estimate the relative material usage efficiencies at an internal point, two dimensionless factors are introduced as:

$$\alpha_M^i = \frac{D_T^M\big|_i}{D_T^M\big|_{max}} \qquad\qquad 0 \le \alpha_M^i \le 1 \qquad (15)$$

where α_M^i is the mass flux efficiency factor, $D_T^M\big|_i$ is the mass flux topological derivative at internal point i, and $D_T^M\big|_{max}$ is maximum value of $D_T^M\big|_i$. A heat flux efficiency factor α_H^i is derived accordingly. During the optimization process the basic goal is to remove material where if is less efficient. However, it may happen that for multi-criteria optimization (C), internal points with low heat fluxes does not necessarily will have low mass fluxes. In such cases it is necessary to apply a strategy to generate a compromise between both phenomena. Rosvany et al. [6] proposed a strategy of compromise in terms of weighted sums of α_H^i and α_M^i:

$$\alpha^i = w_M \alpha_M^i + w_H \alpha_H^i \qquad (16)$$

Where w_H and w_M are the weighting factors for the heat and the mass problems respectively. It is important to note that

$$w_M + w_H = 1 \qquad (17)$$

The weighting factors provide a meaningful way of assigning different levels of importance to each problem. Therefore, when $w_M = 1$ and $w_H = 0$ the criteria A is obtained as a special case, while $w_M = 0$ and $w_H = 1$ reduces the problem to a simple mass transfer optimization (criteria B). Figure 3 depicts a scheme in order to illustrate the multi-criteria optimization procedure.

$-\nabla^2 T = b$

Initial Design

$-\nabla^2 u = m$

BEM

DT

$$\alpha^i = w_M \alpha_M^i + w_H \alpha_H^i$$

Optimized design
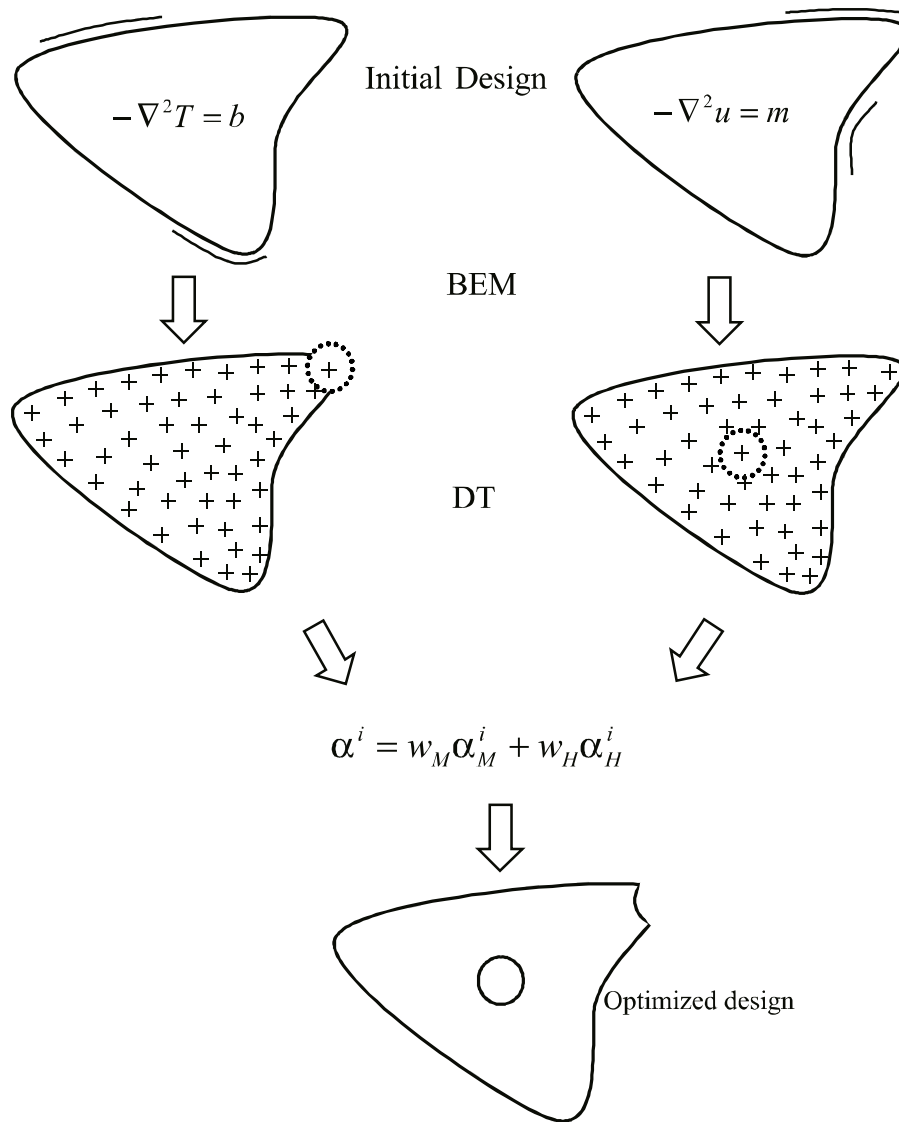
**Figure 3** Schematic view of multi-criteria optimization

Numerical example

The algorithm used in this work, for performing the numerical calculations, was developed using Matlab. This algorithm is composed by the subroutines: BEM (solver), D_T (sensitivity and geometric removal material) and multi-criteria procedure, as well. Using this algorithm, a porous square domain of dimension 20 ´ 20 is submitted to simultaneous heat and mass transfer. The geometry is discretised with 40 boundary elements integrated with 6 Gauss points. The

linear discontinuous elements will be adopted due the irregular boundaries resulted from the optimization process. The boundary conditions are depicted in figure 4. The heat transfer problem has a high temperature of 25°C at the right upper corner and a low temperature of 23°C at the mid lower side. The mass transfer problem has a high potential of 2 kg mol/m³ on the upper left corner and a low potential of 1 kg mol/m³ on the mid lower side. The remaining boundary is insulated, as well as all the holes open during the process. The conductivity and diffusivity coefficient

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are set as 1W/m°C and 1 m²/s, respectively. A regularly spaced grid of internal points was automatically generated, taking into account the radius of the holes created during each iteration. The radius was taken as a fraction of a reference dimension of the domain ($r = \alpha l_{ref}$)). Usually l_{ref} = min(height, width) was adopted. The objective in all cases is to minimize the material volume. The current volume of the domain (A_f) was checked at the end of each iteration until a reference value is achieved ($A_f = \beta A_0$, where A_0 represents the initial volume). This numerical example will be studied with $\alpha_M = 0.4$ and $\alpha_H = 0.6$, to illustrate a case where a higher priority is imposed to one of the problems. The values of α_M and α_H should be adjusted according to the priority set by the designer. Three internal control points were chosen in order to check temperature, mass concentration, heat and mass flux as the process evolves.
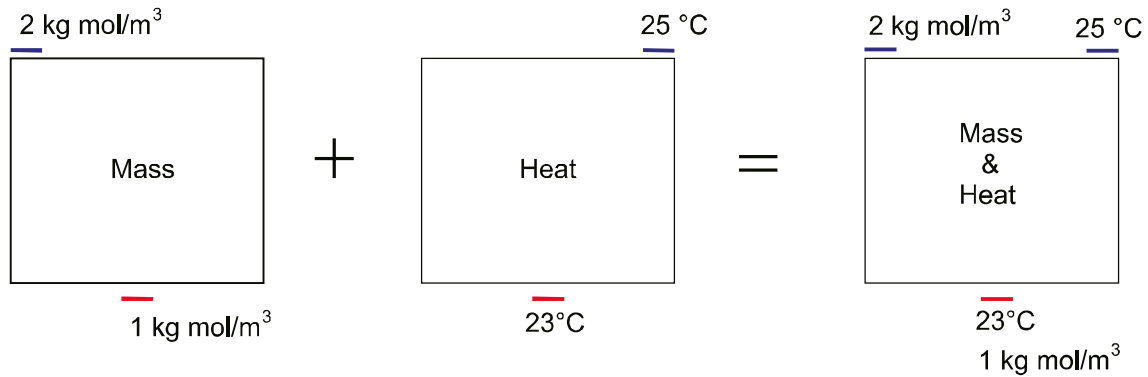
Figure 4 Initial boundary conditions

Fig. 5 illustrates the behavior of the topological derivative values calculated for mass (figure 5a) and heat transfer (figure 5b) inside the domain before the optimization process be initialized. Figure 5c represents the topological derivatives values for both problems obtained by equation (7).

Figure 6 depicts the topology evolution during the iterative process. It is clear the material removal where it is less necessary, according to the weighting factors used. The process iteration was halted when a remaining volume of 50 % was achieved. As explained before, three internal points of control were chosen ($p_1(10,6)$, $p_2(4.4,14)$ and $p_3(15.6,14)$), to account the internal physical parameters. A mean of the temperature and mass of the boundary elements were considered too.

Figure 7 and 8 show the history of temperature and heat flux at the three internal points. Analyzing the heat flux graph, it is possible to verify that the gradient at the points p_1 and p_2 are increasing as the process evolves, while at point p_3 there is a visible decrease of the gradient value. In figure 7, the point p_3 shows an increase of temperature due to the decrease of the gradient at that location. It is evident that the region which presents less efficiency is being removed. Consequently, the flux is maximized along the path connecting the points p_1 and p_2. figure 9 and 10 depict the history of mass concentration and mass flux at the three internal points. The mass flux at the points p_1 and p_2 drops after iteration 56, while it simultaneously increases at the point p_3. This occurs because after iteration 56 the D_T values at the internal points are gradually homogenized, making difficult to select locations with conspicuous lower values. The final geometry resulted in asymmetric Y-shaped design, with material concentrated at the right hand side, due to the weighting factors imposed. However, the mass flux is maximized from the point p_1 to p_3.
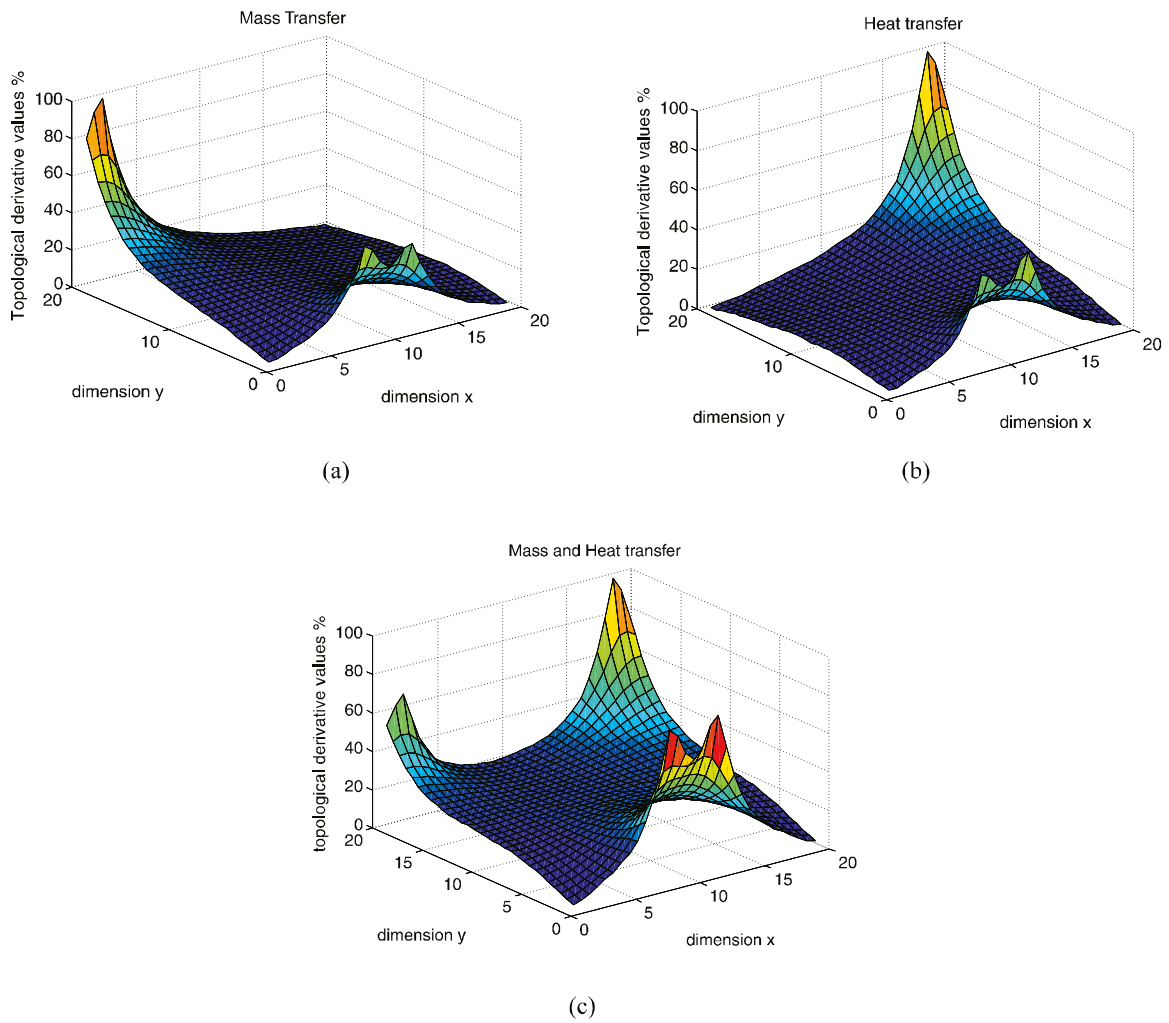
(a)

(b)

(c)

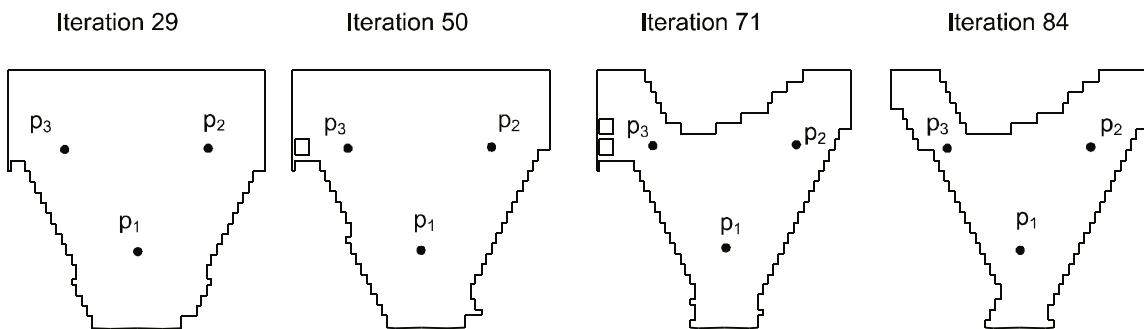**Figure 5** Initial D_T maps for $w_M = 0.4$ and $w_H = 0.6$
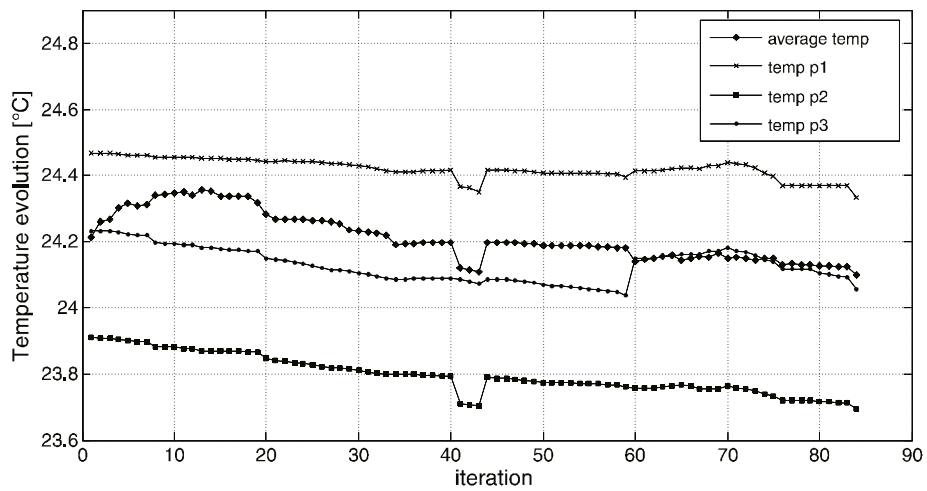

Figure 6 Topological evolution

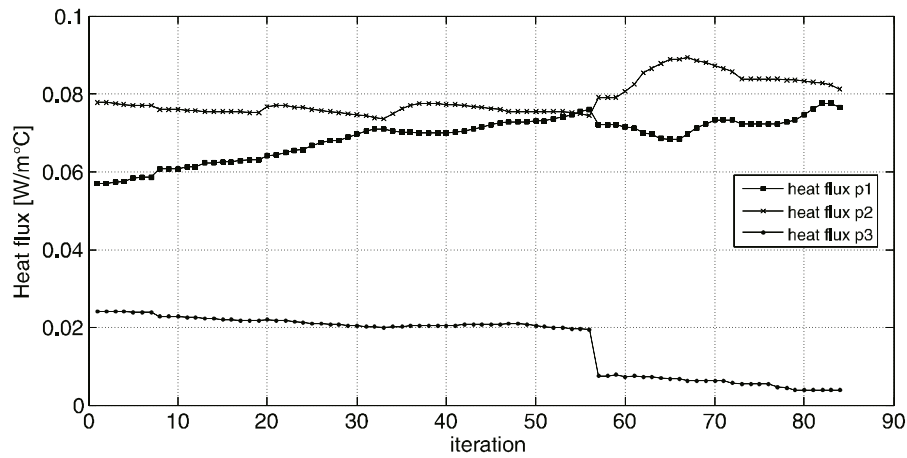**Figure 7** Temperature evolution per iteration for p_1, p_2 and p_3

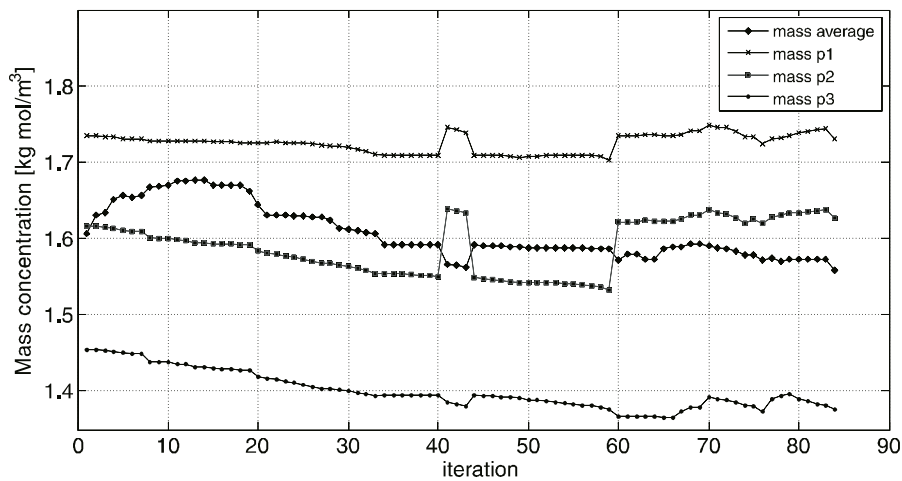**Figure 8** Heat flux evolution per iteration for p_1, p_2 and p_3

Figure 9 Mass evolution per iteration for p_1, p_2 and p_3
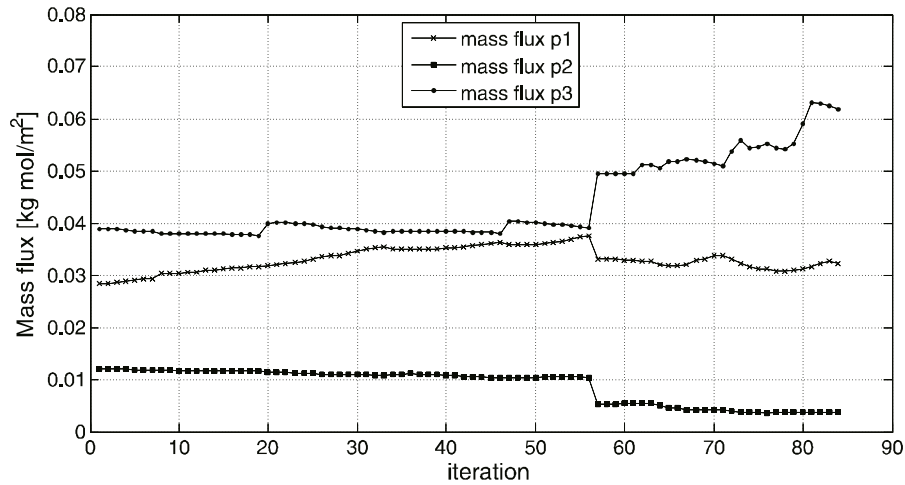
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Figure 10 Mass flux evolution per iteration for p_1, p_2 and p_3

Conclusions

The goal of this work was to extend the application of topological-shape sensitivity analysis to optimization problems governed simultaneously by two different equations, i.e., heat and mass transfer. In order to achieve this, a compromise optimization scheme was used, relying on topological derivative results for the problem. The BEM was used to provide the numerical solution. It is important to point out that D_T has the potential total energy as an implicit cost function. Therefore, the regions which store energy less efficiency are progressively removed. The final topology obtained for the numerical case showed the weighting factors influence for both problems (mass or heat transfer). It was shown that the present methodology can deliver optimal designs of solids in problems submitted to multi-criteria. It is also interesting to note the importance in specifying the priorities for both problems in order to reach physically meaningful solutions for materials porous.

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