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# How to insulate a pipe?

Fabien Caubet\*, Carlos Conca<sup>†</sup>, Marc Dambrine<sup>‡</sup> and Rodrigo Zelada<sup>§</sup>

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## Abstract

This paper focuses on the problem of finding the optimal distribution of a thermal insulator around a pipe. We consider the framework of one fluid inside a pipe of thin width and surrounded by a thermal insulator. We use an asymptotic model to avoid dealing with the thin layer, leading to non-standard transmission conditions which involve discontinuities and second order tangential derivatives. We thus consider the shape optimization problem that aims to minimize the heat flux outside an insulator with a given volume. Then we characterize the shape derivative of the objective functional and perform 3D numerical simulations using the level set evolution method.

**Keywords:** Shape optimization, asymptotic model, Ventcel conditions, transmission conditions, Navier-Stokes equations, thermal insulation

**AMS Classification:** 49Q10, 35Q79, 80M50, 76D55

## 1 Introduction and setting of the problem

### 1.1 Motivations

In our daily lives, reducing heat loss is of great importance from an ecological perspective. Indeed this problem appears in various contexts and applications such as hot water pipes, buildings, or electric kettles, for example. A typical question involves optimizing the thermal insulation around a pipe containing hot water, subject to a volume constraint on the insulator. Insulation problems have been studied for a long time. Here are a few recent advances (see, e.g., [7, 8]). In particular, in [7], two thermal insulation problems were addressed by parametrizing the insulator material by means of the tangential and normal coordinates on the boundary of the hot body (not a fluid) and minimizing with respect to the variable thickness: it was shown that under certain conditions, when the hot body is inside a ball, then the optimal insulator is a ball. Regarding the numerics, in [29], different configurations were compared and a heuristic was proposed to optimize a polygon satisfying certain geometrical constraints, providing insights into how the insulator should be configured.

In this work, we aim to provide practical numerical solutions of the optimal insulator. We therefore first perform a theoretical sensitivity analysis of the problem of insulating a pipe containing a hot fluid and then implement a descent method -here the null-space algorithm [20]- using the level set framework (see, e.g., [3]).

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In many practical applications (see figure 1) the wall thickness of the tube (in red in the figure) is very small compared to its length and also small compared to the insulator thickness. For



Figure 1: The thermal insulation of a pipe (photo by Sönke Kraft aka Arnulf zu Linden on commons.wikimedia.org).

obvious computational reasons, it makes sense not to mesh it. One possibility would be to ignore it. In this work, we propose to take it into account by means of an interface condition written at the edge of the domain occupied by the fluid, obtained by an asymptotic model of order one with respect to the small parameter (i.e. the ratio between this thickness and the length of the pipe). The novelties of this work are: first, the model takes into account the motion of the fluid and thus a convection term appears in the heat equation in the fluid zone; second, the pipe is considered through an interface term rather than with the usual model of insulation.

## 1.2 The physical context

As previously mentioned, we consider in this work a given pipe, with a known geometry on which the thickness of the wall of the pipe is very small compared to the length of the pipe. Moreover, we assume that this pipe is surrounded by an insulator.

More precisely, the problem can be stated as follows. Let  $\epsilon > 0$  the given thickness of the wall of the pipe. Let  $\Omega_1^\epsilon, \Omega_m^\epsilon, \Omega_2^\epsilon$  open bounded domains in  $\mathbb{R}^d$  ( $d = 2, 3$ ), such that the whole domain is  $\Omega^\epsilon := \overline{\Omega_1^\epsilon} \cup \overline{\Omega_m^\epsilon} \cup \overline{\Omega_2^\epsilon}$ . The subset  $\Omega_1^\epsilon$  is the part physically occupied by the fluid,  $\Omega_m^\epsilon$  corresponds to the wall of the pipe, and finally  $\Omega_2^\epsilon$  corresponds to the insulating material we will be looking to place to reduce heat loss. The interfaces between the domains have two connected components denoted by  $\Gamma_i^\epsilon := \overline{\partial\Omega_i^\epsilon} \cap \overline{\partial\Omega_m^\epsilon}$ ,  $i = 1, 2$ , and we also assume that  $\Gamma_1^\epsilon \cap \Gamma_2^\epsilon = \emptyset$ . Figure 2a illustrates the geometry of our problem.

As the pipe may have a complex geometry, the flow of the heat transfer fluid is described by the Navier-Stokes equations (rather than the Stokes equations). We precise that we consider here the steady state case and we denote by  $\mathbf{u}^\epsilon$  the velocity of the fluid and  $p^\epsilon$  the pressure. Let  $\nu > 0$  be

the kinematic viscosity. The boundary of the fluid region  $\Omega_1^\epsilon$  is assumed to be composed by three disjoint regions:  $\partial\Omega_1^\epsilon =: \Gamma_D^\epsilon \cup \Gamma_1^\epsilon \cup \Gamma_N^\epsilon$ , where  $\Gamma_D^\epsilon$  is the input of the fluid with a given velocity (non homogeneous Dirichlet boundary condition) and where  $\Gamma_N^\epsilon$  contains the outlet-pressure condition (Neumann boundary condition). The classical non-slip condition  $\mathbf{u}^\epsilon = 0$  is imposed on  $\Gamma_1^\epsilon$ . To summarize, the motion of the fluid is described by the following equations:

$$\left\{ \begin{array}{ll} -\nu\Delta\mathbf{u}^\epsilon + (\nabla\mathbf{u}^\epsilon)\mathbf{u}^\epsilon + \nabla p^\epsilon = 0 & \text{in } \Omega_1^\epsilon, \\ \operatorname{div}(\mathbf{u}^\epsilon) = 0 & \text{in } \Omega_1^\epsilon, \\ \mathbf{u}^\epsilon = \mathbf{u}_D & \text{on } \Gamma_D^\epsilon, \\ \sigma(\mathbf{u}^\epsilon, p^\epsilon)\mathbf{n} = 0 & \text{on } \Gamma_N^\epsilon, \\ \mathbf{u}^\epsilon = 0 & \text{on } \Gamma_1^\epsilon, \end{array} \right. \quad (1.1)$$

where  $\mathbf{u}_D$  is a given inlet velocity, where  $\mathbf{n}$  denotes the exterior unit normal, and where  $\sigma(\mathbf{u}, p)$  is the fluid stress tensor defined by

$$\sigma(\mathbf{u}, p) := 2\nu\varepsilon(\mathbf{u}) - p\mathbf{I},$$

with  $\varepsilon(\mathbf{u}) := \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^t)$  the symmetric gradient and  $\mathbf{I}$  the identity matrix, and where the superscript  $t$  denotes the transpose matrix.

Concerning the temperature, we consider the stationary heat equation in the whole domain  $\Omega^\epsilon$  with a Fourier-Robin condition on the outer boundary of the insulating material stating that the heat flux there is proportional to the gap of temperatures with a given rate  $\alpha > 0$ . Notice that the temperature field inside the pipe  $\Omega_1^\epsilon$  is determined in terms of the velocity  $\mathbf{u}^\epsilon$  through a convection-diffusion equation. It is convenient to decompose the temperature field into

$$\mathbb{T}^\epsilon = \mathbb{T}_1^\epsilon \mathbb{1}_{\Omega_1^\epsilon} + \mathbb{T}_m^\epsilon \mathbb{1}_{\Omega_m^\epsilon} + \mathbb{T}_2^\epsilon \mathbb{1}_{\Omega_2^\epsilon},$$

where  $\mathbb{T}^\epsilon$  is the solution of the stationary convection-diffusion equation in  $\Omega^\epsilon$  and where  $\mathbb{T}_i^\epsilon$  is its restriction to  $\Omega_i^\epsilon$ , for  $i = 1, 2, m$ . Here  $\mathbb{1}$  denotes the indicator function of a domain. The physical parameters are the given thermal diffusivity  $\kappa_1, \kappa_2, \kappa_m$  that are assumed to be positive numbers. The boundary of  $\Omega_2^\epsilon$  is the disjoint union  $\partial\Omega_2^\epsilon =: \Gamma_2^\epsilon \cup \Gamma_R^\epsilon$  and the boundary of  $\Omega_m^\epsilon$  is given by  $\partial\Omega_m^\epsilon =: \Gamma_1^\epsilon \cup \Gamma_2^\epsilon \cup \Gamma_{m,N}^\epsilon$ . On the Dirichlet part  $\Gamma_D^\epsilon$ , a given temperature is imposed, and the previously mentioned Fourier-Robin condition is imposed on  $\Gamma_R^\epsilon$ . Moreover, we impose Neumann boundary conditions on  $\Gamma_{m,N}^\epsilon \cup \Gamma_N^\epsilon$ . Finally, classical transmission conditions are assumed on  $\Gamma_1^\epsilon \cup \Gamma_2^\epsilon$  and we obtain the following system:

$$\left\{ \begin{array}{ll} -\operatorname{div}(\kappa_1\nabla\mathbb{T}_1^\epsilon) + \mathbf{u}^\epsilon \cdot \nabla\mathbb{T}_1^\epsilon = 0 & \text{in } \Omega_1^\epsilon, \\ -\operatorname{div}(\kappa_m\nabla\mathbb{T}_m^\epsilon) = 0 & \text{in } \Omega_m^\epsilon, \\ -\operatorname{div}(\kappa_2\nabla\mathbb{T}_2^\epsilon) = 0 & \text{in } \Omega_2^\epsilon, \\ \mathbb{T}_1^\epsilon = \mathbb{T}_D & \text{on } \Gamma_D^\epsilon, \\ \kappa_1 \frac{\partial\mathbb{T}_1^\epsilon}{\partial\mathbf{n}} = 0 & \text{on } \Gamma_{m,N}^\epsilon \cup \Gamma_N^\epsilon, \\ \kappa_2 \frac{\partial\mathbb{T}_2^\epsilon}{\partial\mathbf{n}} + \alpha\mathbb{T}_2^\epsilon = \alpha\mathbb{T}_{\text{ext}} & \text{on } \Gamma_R^\epsilon, \\ \mathbb{T}_1^\epsilon = \mathbb{T}_m^\epsilon & \text{on } \Gamma_1^\epsilon, \\ \mathbb{T}_2^\epsilon = \mathbb{T}_m^\epsilon & \text{on } \Gamma_2^\epsilon, \\ \kappa_1 \frac{\partial\mathbb{T}_1^\epsilon}{\partial\mathbf{n}} = \kappa_m \frac{\partial\mathbb{T}_m^\epsilon}{\partial\mathbf{n}} & \text{on } \Gamma_1^\epsilon, \\ \kappa_2 \frac{\partial\mathbb{T}_2^\epsilon}{\partial\mathbf{n}} = \kappa_m \frac{\partial\mathbb{T}_m^\epsilon}{\partial\mathbf{n}} & \text{on } \Gamma_2^\epsilon, \end{array} \right. \quad (1.2)$$

where  $\mathbb{T}_D$  is a given input temperature and  $\mathbb{T}_{\text{ext}}$  is the given exterior temperature.

### 1.3 Setting of the approximated and the shape optimization problems

As exposed above, the actual configuration involves three inseparable parts: the fluid, the wall of the pipe, and the insulator. However, the wall thickness is very small compared to the other dimensions, and keeping this wall in a numerical model requires the use of very refined and therefore very expensive meshes, especially in dimension three, to compute the temperature field.

**The approximated domains.** We therefore propose, in a classical way since the work of Enquist and Nedelec [17], to forget this zone in the geometrical description of the problem, but to take into account its impact on the thermal properties through artificial transmission conditions at the new fluid-insulator interface. We thus obtain, at the cost of a systematic model error, an approximate solution whose calculation is much less costly since it only requires a much coarser mesh (adapted to the internal diameter of the pipe and no longer to the wall thickness). Our idea is to use this inexpensive approximate model to optimize the shape of the insulation around the pipe. Figure 2 illustrates this geometric approximation.

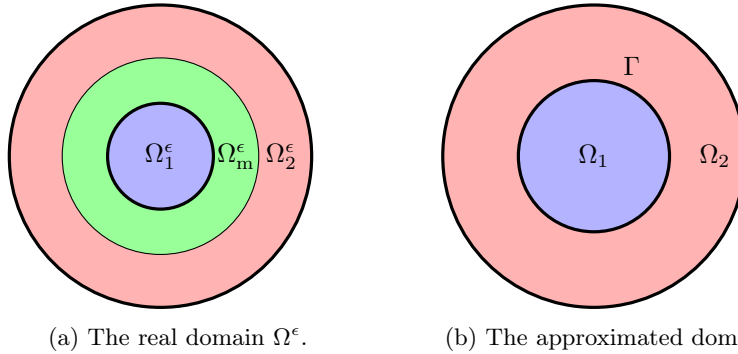


Figure 2: Approximation of the domain from three to two layers (cross-section view)

Thus, in the following, we only consider a two layer domain: one occupied by the fluid (denoted by  $\Omega_1$ ) and one by the insulator (denoted by  $\Omega_2$ ), separated by the interface  $\Gamma := \partial\Omega_1 \cap \partial\Omega_2$  (see Figure 2b). We then define  $\Omega := \Omega_1 \cup \Omega_2$ . All along the paper, the domains are assumed to be smooth. In a similar way to above,  $\partial\Omega_1$  and  $\partial\Omega_2$  are respectively decomposed as  $\partial\Omega_1 =: \Gamma_D \cup \Gamma \cup \Gamma_N$  and  $\partial\Omega_2 =: \Gamma \cup \Gamma_R$ . Moreover, we assume that  $\bar{\Gamma} \cap \bar{\Gamma}_D \neq \emptyset$  and  $\bar{\Gamma} \cap \bar{\Gamma}_N \neq \emptyset$ . Finally we assume in the following that  $\mathbf{n}_{\Gamma_N}$  and  $\mathbf{n}_{\Gamma_D}$  are respectively unit tangent vectors to  $\Gamma$  on  $\partial\Gamma \cap \partial\Gamma_N$  and  $\partial\Gamma \cap \partial\Gamma_D$ . Figure 3 illustrates our configuration.

**The approximated equations.** We can now specify the boundary values problems that we will consider in the following. Concerning the fluid, the system is similar since the equations are not affected by this reduction of the domain. Hence, we consider

$$\left\{ \begin{array}{ll} -\nu\Delta\mathbf{u} + (\nabla\mathbf{u})\mathbf{u} + \nabla p = 0 & \text{in } \Omega_1, \\ \operatorname{div}(\mathbf{u}) = 0 & \text{in } \Omega_1, \\ \mathbf{u} = \mathbf{u}_D & \text{on } \Gamma_D, \\ \sigma(\mathbf{u}, p)\mathbf{n} = 0 & \text{on } \Gamma_N, \\ \mathbf{u} = 0 & \text{on } \Gamma, \end{array} \right. \quad (1.3)$$

where  $\mathbf{u}_D \in H^{1/2}(\Gamma_D)^d$  is the given inlet velocity. It is well-known that these stationary Navier-Stokes equations are well-posed if  $\nu$  is large enough (see, e.g., [21, 28]), which we will assume in the remainder of this work.

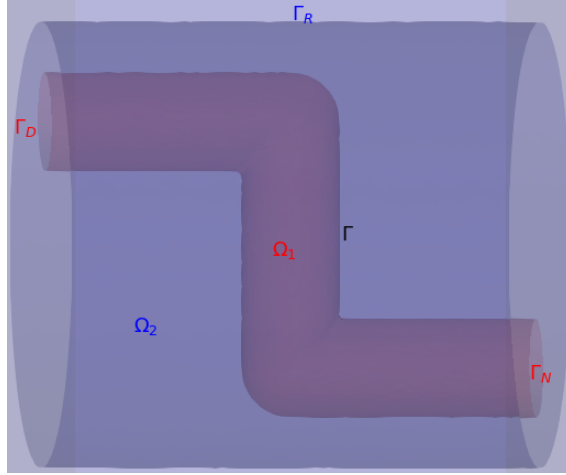


Figure 3: Configuration of the 3D thermal insulation problem

As far as the thermal equations are concerned, the omission of the wall of the pipe has a significant impact on the equations. We use the approach introduced in [17] based on now classic asymptotic techniques. This approach and technical implementation are explained in detail and pedagogically in Vial's thesis [30]. We also mention the work [13] dealing with generalized boundary conditions for an interface problem. As previously, we use the following decomposition:

$$\mathbb{T} = \mathbb{T}_1 \mathbb{1}_{\Omega_1} + \mathbb{T}_2 \mathbb{1}_{\Omega_2}, \kappa = \kappa_1 \mathbb{1}_{\Omega_1} + \kappa_2 \mathbb{1}_{\Omega_2}.$$

Then doing similar computations to what we have done in [11], when  $\epsilon$  is sufficiently small, the following approximate problem of order one is obtained:

$$\left\{ \begin{array}{ll} -\operatorname{div}(\kappa_1 \nabla \mathbb{T}_1) + \mathbf{u} \cdot \nabla \mathbb{T}_1 = 0 & \text{in } \Omega_1, \\ -\operatorname{div}(\kappa_2 \nabla \mathbb{T}_2) = 0 & \text{in } \Omega_2, \\ \mathbb{T}_1 = \mathbb{T}_D & \text{on } \Gamma_D, \\ \kappa_1 \frac{\partial \mathbb{T}_1}{\partial \mathbf{n}} = 0 & \text{on } \Gamma_N, \\ \kappa_2 \frac{\partial \mathbb{T}_2}{\partial \mathbf{n}} + \alpha \mathbb{T}_2 = \alpha \mathbb{T}_0 & \text{on } \Gamma_R, \\ \left\langle \kappa \frac{\partial \mathbb{T}}{\partial \mathbf{n}} \right\rangle = -\kappa_m \epsilon^{-1} [\mathbb{T}] & \text{on } \Gamma, \\ \left[ \kappa \frac{\partial \mathbb{T}}{\partial \mathbf{n}} \right] = \epsilon \operatorname{div}_\tau (\kappa_m \nabla_\tau \langle \mathbb{T} \rangle) - \kappa_m H[\mathbb{T}] & \text{on } \Gamma, \end{array} \right. \quad (1.4)$$

where  $\mathbb{T}_D \in \mathbb{H}_0^{1/2}(\Gamma_D) := \{\mathbb{S}|_{\Gamma_D}, \mathbb{S} \in \mathbb{H}^{1/2}(\partial\Omega_2), \mathbb{S}|_{\partial\Omega_2 \setminus \Gamma_D} = 0\}$  is the given input temperature and  $\mathbb{T}_0 \in \mathbb{H}^{1/2}(\Gamma_R)$  is the given exterior temperature, and where  $\mathbf{u}$  solves the Navier-Stokes system (1.3). In the previous equations,  $\operatorname{div}_\tau$  and  $\nabla_\tau$  are respectively the tangential divergence and gradient operator, and  $H$  is the mean curvature of  $\Gamma$ . Since the jumps are not zero, we need to orientate the normal at the interface: we choose the outer unit normal  $\mathbf{n}$  at  $\Gamma$  oriented towards  $\Omega_2$ , this is  $\mathbf{n} := \mathbf{n}_1 = -\mathbf{n}_2$  at  $\Gamma$ , where  $\mathbf{n}_i$  is the exterior normal of  $\Omega_i$ . The jump and mean across the interface  $\Gamma$  are defined, for a function  $\phi$ , as

$$[\phi] := \phi_1 - \phi_2 \quad \text{and} \quad \langle \phi \rangle := \frac{1}{2} (\phi_1 + \phi_2).$$

The well-posedness of this system is proved below (see Theorem 2.1).

**Remark 1.1.** *It should be pointed out that the solution  $\mathbb{T}$  of the approximated problem obviously depends on the parameter  $\epsilon$ . It is then necessary to justify that the model error committed by using  $\mathbb{T}$  instead of  $\mathbb{T}^\epsilon$  is of order  $\epsilon$  in  $H^1$  norm. This is a little technical, as the two functions are not defined on the same set. Nevertheless, it is a classic result. That is not the point of our work, so we refer the reader to [13] for example where a similar result is demonstrated and just comment on it. Obviously, the systematic error committed by approximating  $\mathbb{T}^\epsilon$  by  $\mathbb{T}$  is weaker than that committed by just looking at the limit problem obtained formally by resolving the heat equation in  $\Omega_1 \cup \Gamma \cup \Omega_2$ , i.e. with no source term at the  $\Gamma$  interface.*

*Strictly speaking, this dependence of the solution of the approximated problem on the small parameter  $\epsilon$  should be explicitly mentioned. As this would make the notations much heavier, we chose to simply denote  $\mathbb{T}$  the solution of the previous approximated problem.*

**The shape optimization problem.** We can now set out the main question that we are going to study in this work: *given a pipe with a known fixed geometry and a given quantity of insulation, how should the insulation be positioned to minimize heat loss to the outside world, whose temperature is known?* In other words, the domain  $\Omega_1$  being fixed, we are looking for a domain  $\Omega_2$  of prescribed volume so that the heat flux across the interface with the outside, i.e.  $\Gamma_R$ , is as small as possible. We therefore define the criterion  $J$  by

$$J(\Omega_2) := \int_{\Gamma_R} \left( \kappa_2 \frac{\partial \mathbb{T}_2}{\partial \mathbf{n}} \right)^2 ds = \int_{\Gamma_R} \alpha^2 (\mathbb{T}_2 - \mathbb{T}_0)^2 ds, \quad (1.5)$$

where the temperature  $\mathbb{T}$  solves the approximated convection-diffusion problem (1.4).

We thus consider the following shape optimization problem: *given a prescribed volume  $V_0 > 0$ , minimize  $J$  under the constraint*

$$G(\Omega_2) = V_0, \quad \text{where } G(\Omega_2) := \int_{\Omega_2} dx.$$

The fundamental questions of the existence of optimal domains and their regularity have been studied in the work of Bucur *et al.* [8] in a simplified setting (no pipe wall and no fluid circulation just a heated body). This is not the topic of the present work to study these questions. We will here focus on the numerical computation of such a solution, and to this end prove the existence and compute the shape derivatives in this framework.

## 2 Main results

In this section, we claim the main results of our work. All the proofs are detailed in the following section.

### 2.1 Functional spaces and well posedness of the approximated problem (1.4)

We consider the following affine spaces associated to the non-homogeneous Dirichlet boundary data  $\mathbf{u}_D \in H^{1/2}(\Gamma_D)^d$  and  $\mathbb{T}_D \in H_0^{1/2}(\Gamma_D)$ :

$$\mathcal{V}_{\mathbf{u}_D} := \{ \mathbf{w} \in H^1(\Omega_1)^d; \mathbf{w} = \mathbf{u}_D \text{ on } \Gamma_D, \mathbf{w} = 0 \text{ on } \Gamma \},$$

$$\mathcal{H}_{\mathbb{T}_D} := \{ \mathbb{S} = (\mathbb{S}_1, \mathbb{S}_2) \in H^1(\Omega_1, \Gamma) \times H^1(\Omega_2, \Gamma); \mathbb{S}_1 = \mathbb{T}_D \text{ on } \Gamma_D; \mathbb{S}_2 = \mathbb{T}_D \text{ on } \Gamma \cap \Gamma_D \},$$

where, for  $i = 1, 2$ ,

$$H^1(\Omega_i, \Gamma) := \{S \in H^1(\Omega_i); S|_\Gamma \in H^1(\Gamma)\}.$$

The spaces  $\mathcal{V}_0$  and  $\mathcal{H}_0$  are Hilbert spaces when they are equipped with the respective norms:

$$\|\mathbf{w}\|_{\mathcal{V}_0} := \|\mathbf{w}\|_{H^1(\Omega_1)^d} \quad \text{and} \quad \|S\|_{\mathcal{H}_0} := \left( \|\nabla S\|_{L^2(\Omega)^d}^2 + \|\nabla_\tau \langle S \rangle\|_{L^2(\Gamma)^{d-1}}^2 + \|[S]\|_{L^2(\Gamma)}^2 \right)^{1/2}.$$

Then the Navier-Stokes equations (1.3) have the following variational formulation

$$\begin{cases} \text{Find } (\mathbf{u}, p) \in \mathcal{V}_{\mathbf{u}_D} \times L^2(\Omega_1) \text{ such that, for all } (\mathbf{w}, r) \in \mathcal{V}_0 \times L^2(\Omega_1), \\ \int_{\Omega_1} (2\nu\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{w}) + \rho(\nabla\mathbf{u})\mathbf{u} \cdot \mathbf{w} - p \operatorname{div}(\mathbf{w}) - r \operatorname{div}(\mathbf{u})) \, dx = 0. \end{cases} \quad (2.1)$$

As previously mentioned, we assume that the viscosity  $\nu$  is large enough so that the problem (1.3) is well-posed: it has a unique weak solution  $(\mathbf{u}, p) \in \mathcal{V}_{\mathbf{u}_D} \times L^2(\Omega_1)$ . For the remainder of this work, we assume that the velocity of the fluid at the outlet, i.e. at the boundary  $\Gamma_N$ , actually causes it to exit: there is no recirculation at the outlet. This assumption on the velocity is written as

$$\mathbf{u} \cdot \mathbf{n} \geq 0 \quad \text{on } \Gamma_N. \quad (2.2)$$

For the temperature, the corresponding variational formulation of the approximated problem (1.4) is given by

$$\text{Find } T \in \mathcal{H}_{T_D} \text{ such that, for all } S \in \mathcal{H}_0, \quad a(T, S) = l(S), \quad (2.3)$$

where the bilinear and linear forms are respectively

$$\begin{aligned} a(T, S) &:= \int_{\Omega_1 \cup \Omega_2} \kappa \nabla T \cdot \nabla S \, dx + \int_{\Omega_1} S \mathbf{u} \cdot \nabla T \, dx + \int_{\Gamma_R} \alpha T S \, ds \\ &\quad + \int_{\Gamma} \left( \epsilon \kappa_m \nabla_\tau \langle T \rangle \cdot \nabla_\tau \langle S \rangle + \kappa_m H[T] \langle S \rangle + \frac{\kappa_m}{\epsilon} [T][S] \right) \, ds, \\ l(S) &:= \int_{\Gamma_R} \alpha T_{\text{ext}} S \, dx. \end{aligned}$$

Then the following result claims that this problem is well-posed.

**Theorem 2.1** (Well-posedness of the state equation for temperature). *Assume that the exit condition (2.2) holds. There exists a positive real number  $\epsilon_0$  such that, if  $0 < \epsilon < \epsilon_0$ , then the convection-diffusion problem (2.3) has a unique solution  $T \in \mathcal{H}_{T_D}$ .*

## 2.2 Shape sensitivity analysis

Now we aim to perform a shape sensitivity analysis and compute the shape derivative of the objective functional  $J$  given in (1.5). To do this, we rely on the Hadamard shape derivative (see [26, 27, 23, 4]). We suppose  $\Omega_2$  to be smooth enough (at least  $\mathcal{C}^2$ ). The main idea is to perturb the domain  $\Omega_2$  (in particular, the free boundary  $\Gamma_R$ ) using a vector deformation field  $\boldsymbol{\theta} \in \mathcal{C}^{1,\infty}(\Omega)^d := \mathcal{C}^1 \cap W^{1,\infty}(\Omega)^d$  with  $\|\boldsymbol{\theta}\|_{W^{1,\infty}(\Omega)^d} < 1$ , this is,

$$\Omega_2^\boldsymbol{\theta} := (\mathbf{I} + \boldsymbol{\theta})\Omega_2.$$

We consider the following space of admissible deformations,

$$\Theta_{\text{ad}} := \{\boldsymbol{\theta} \in \mathcal{C}^{1,\infty}(\Omega)^d; \quad \|\boldsymbol{\theta}\|_{W^{1,\infty}(\Omega)^d} < 1, \quad \boldsymbol{\theta} = 0 \text{ in } \Omega_1, \quad \boldsymbol{\theta} = 0 \text{ on } \Gamma \cup \Gamma_D \cup \partial\Omega\}.$$

We first recall the definition of the notion of shape derivative of a shape functional in our context.



**Definition 2.2.** *The shape derivative of a function  $J(\Omega_2)$  is defined as the Fréchet derivative at 0 of the map  $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto J(\Omega_2^\boldsymbol{\theta}) \in \mathbb{R}$ . It is denoted by  $J'(\Omega_2)$  and it is then given by*

$$J(\Omega_2^\boldsymbol{\theta}) = J(\Omega_2) + \langle J'(\Omega_2), \boldsymbol{\theta} \rangle + o(\boldsymbol{\theta}), \text{ with } \lim_{\boldsymbol{\theta} \rightarrow 0} \frac{o(\boldsymbol{\theta})}{\|\boldsymbol{\theta}\|_{W^{1,\infty}(\Omega)^d}} = 0.$$

In the following, we introduce  $\mathbf{T}_\boldsymbol{\theta} \in H^1(\Omega_1, \Gamma) \times H^1(\Omega_2^\boldsymbol{\theta}, \Gamma)$  the perturbed solution, i.e. the solution of approximated convection-diffusion Problem (1.4) defined on  $\Omega_1 \cup \Omega_2^\boldsymbol{\theta}$  instead of  $\Omega_1 \cup \Omega_2$ .

**Proposition 2.3** (Existence and characterization of the shape derivative). *If  $\mathbf{T}_{\text{ext}} \in H^2(\mathbb{R}^d)$ , then there exists an extension  $\tilde{\mathbf{T}}_\boldsymbol{\theta} \in H^1(\mathbb{R}^d) \times H^1(\mathbb{R}^d)$  of  $\mathbf{T}_\boldsymbol{\theta}$  such that the application  $\boldsymbol{\theta} \rightarrow \tilde{\mathbf{T}}_\boldsymbol{\theta}$  from  $\Theta_{\text{ad}}$  to  $L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$  is  $\mathcal{C}^1$  at 0 and the derivative, denoted  $\mathbf{T}'$ , is called shape derivative of  $\mathbf{T}$ . In addition, for  $\boldsymbol{\theta} \in \Theta_{\text{ad}}$  and assuming that  $\mathbf{T}_2$  belongs to  $H^2(\Omega_2)$ , the shape derivative  $\mathbf{T}' \in \mathcal{H}_0$  is characterized by,*

$$\left\{ \begin{array}{l} \text{Find } \mathbf{T}' \in \mathcal{H}_0, \text{ such that } \forall \phi \in \mathcal{H}_0, \\ \int_{\Omega_1 \cup \Omega_2} \kappa \nabla \mathbf{T}' \cdot \nabla \phi \, dx + \int_{\Omega_1} \nabla \mathbf{T}' \cdot \mathbf{u} \phi \, dx + \int_{\Gamma_R} \alpha \mathbf{T}' \phi \, ds \\ \quad + \int_{\Gamma} \left( \epsilon \kappa_m \nabla_\tau \langle \mathbf{T}' \rangle \cdot \nabla_\tau \langle \phi \rangle + \kappa_m H[\mathbf{T}'] \langle \phi \rangle + \frac{\kappa_m}{\epsilon} [\mathbf{T}'][\phi] \right) ds \\ = \int_{\Omega_2} \kappa_2 (\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t) \nabla \mathbf{T} \cdot \nabla \phi - \kappa_2 \operatorname{div}(\boldsymbol{\theta}) \nabla \mathbf{T} \cdot \nabla \phi - \kappa_2 \nabla(\boldsymbol{\theta} \cdot \nabla \mathbf{T}) \cdot \nabla \phi \, dx \\ \quad - \int_{\Gamma_R} (\alpha \operatorname{div}_\tau(\boldsymbol{\theta})(\mathbf{T} - \mathbf{T}_{\text{ext}}) \phi + \alpha \phi \boldsymbol{\theta} \cdot \nabla(\mathbf{T} - \mathbf{T}_{\text{ext}})) \, ds. \end{array} \right. \quad (2.4)$$

Furthermore, its strong form is given by,

$$\left\{ \begin{array}{l} -\kappa_1 \Delta \mathbf{T}'_1 + \nabla \mathbf{T}'_1 \cdot \mathbf{u} = 0 \text{ in } \Omega_1, \\ -\kappa_2 \Delta \mathbf{T}'_2 = 0 \text{ in } \Omega_2, \\ \mathbf{T}'_1 = 0 \text{ on } \Gamma_D, \\ \kappa_1 \frac{\partial \mathbf{T}'_1}{\partial \mathbf{n}} = 0 \text{ on } \Gamma_N, \\ \kappa_2 \frac{\partial \mathbf{T}'_2}{\partial \mathbf{n}} + \alpha \mathbf{T}'_2 = \operatorname{div}_\tau((\boldsymbol{\theta} \cdot \mathbf{n}) \kappa_2 \nabla_\tau \mathbf{T}_2) - \alpha(\boldsymbol{\theta} \cdot \mathbf{n}) \left( \frac{\partial}{\partial \mathbf{n}}(\mathbf{T}_2 - \mathbf{T}_{\text{ext}}) + H(\mathbf{T}_2 - \mathbf{T}_{\text{ext}}) \right) \text{ on } \Gamma_R, \\ \left\langle \kappa \frac{\partial \mathbf{T}'}{\partial \mathbf{n}} \right\rangle = -\frac{\kappa_m}{\epsilon} [\mathbf{T}'] \text{ on } \Gamma, \\ \left[ \kappa \frac{\partial \mathbf{T}'}{\partial \mathbf{n}} \right] = \epsilon \kappa_m \Delta_\tau \langle \mathbf{T}' \rangle - \kappa_m H[\mathbf{T}'] \text{ on } \Gamma. \end{array} \right. \quad (2.5)$$

Finally we can state the result of shape differentiability concerning the objective functional.

**Proposition 2.4** (Shape derivative of the functional). *If  $\mathbf{T}_{\text{ext}} \in H^2(\mathbb{R}^d)$  and  $\mathbf{T}_2 \in H^2(\Omega_2)$ , then the functional  $J$  is differentiable with respect to  $\boldsymbol{\theta} \in \Theta_{\text{ad}}$  and the shape derivative is given by*

$$\begin{aligned} J'(\Omega_2)(\boldsymbol{\theta}) = & \int_{\Gamma_R} \operatorname{div}_\tau(\boldsymbol{\theta}) \alpha^2 (\mathbf{T}_2 - \mathbf{T}_{\text{ext}})^2 - \operatorname{div}_\tau(\boldsymbol{\theta}) \alpha (\mathbf{T}_2 - \mathbf{T}_{\text{ext}}) \mathbf{R}_2 - (2\alpha^2 (\mathbf{T}_2 - \mathbf{T}_{\text{ext}}) - \alpha \mathbf{R}_2) (\nabla \mathbf{T}_{\text{ext}} \cdot \boldsymbol{\theta}) \, ds \\ & + \int_{\Omega_2} \kappa_2 ((\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t) \nabla \mathbf{T}_2) \cdot \nabla \mathbf{R}_2 - \operatorname{div}(\boldsymbol{\theta}) (\kappa \nabla \mathbf{T}_2 \cdot \nabla \mathbf{R}_2) \, dx, \end{aligned} \quad (2.6)$$

where  $\mathbb{T} = (\mathbb{T}_1, \mathbb{T}_2) \in \mathcal{H}_{\mathbb{T}_D}$  is the solution of the convection-diffusion equation (1.4) and where  $\mathbb{R} = (\mathbb{R}_1, \mathbb{R}_2) \in \mathcal{H}_0$  is the solution of the following adjoint equation

$$\left\{ \begin{array}{ll} -\operatorname{div}(\kappa_1 \nabla \mathbb{R}_1 + \mathbb{R}_1 \mathbf{u}) = 0 & \text{in } \Omega_1, \\ -\operatorname{div}(\kappa_2 \nabla \mathbb{R}_2) = 0 & \text{in } \Omega_2, \\ \mathbb{R}_1 = 0 & \text{on } \Gamma_D, \\ \kappa_1 \frac{\partial \mathbb{R}_1}{\partial \mathbf{n}} + \mathbb{R}_1 \mathbf{u} \cdot \mathbf{n} = 0 & \text{on } \Gamma_N, \\ \kappa_2 \frac{\partial \mathbb{R}_2}{\partial \mathbf{n}} + \alpha \mathbb{R}_2 = 2\alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}}) & \text{on } \Gamma_R, \\ \left\langle \kappa \frac{\partial \mathbb{R}}{\partial \mathbf{n}} \right\rangle = -\kappa_m \epsilon^{-1} [\mathbb{R}] - \kappa_m H \langle \mathbb{R} \rangle & \text{on } \Gamma, \\ \left[ \kappa \frac{\partial \mathbb{R}}{\partial \mathbf{n}} \right] = \epsilon \operatorname{div}_\tau(\kappa_m \nabla_\tau \langle \mathbb{R} \rangle) & \text{on } \Gamma. \end{array} \right. \quad (2.7)$$

If furthermore  $\mathbb{R}_2 \in H^2(\Omega_2)$ , then the shape derivative can be expressed on its surface form as

$$J'(\Omega_2)(\boldsymbol{\theta}) = \int_{\Gamma_R} f(\mathbb{T}_2, \mathbb{R}_2)(\boldsymbol{\theta} \cdot \mathbf{n}) \, ds, \quad (2.8)$$

with

$$\begin{aligned} f(\mathbb{T}_2, \mathbb{R}_2) = & \alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}})^2 \left( H - \frac{4\alpha}{\kappa} \right) + \alpha(\mathbb{T}_2 - \mathbb{T}_{\text{ext}}) \mathbb{R}_2 \left( \frac{2\alpha}{\kappa} - H \right) - \kappa \nabla \mathbb{T}_2 \cdot \nabla \mathbb{R}_2 \\ & + \frac{\partial \mathbb{T}_{\text{ext}}}{\partial \mathbf{n}} (\alpha \mathbb{R}_2 - 2\alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}})). \end{aligned}$$

### 2.3 Shape sensitivity analysis with random exterior temperature

Notice that previously, we have assumed to know the exterior parameter  $\mathbb{T}_{\text{ext}}$  precisely. We want now to consider the more realistic case of an imprecise knowledge of this parameter and we then aim to take into account uncertainties on this data  $\mathbb{T}_{\text{ext}}$ . To do that we will assume that we have information about the uncertainties.

Since in this part we are interested on study the random exterior temperature, we will make explicit the dependence on  $\mathbb{T}_{\text{ext}}$  by means of the notation:

$$J(\Omega_2, \mathbb{T}_{\text{ext}}) = \int_{\Gamma_R} \alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}})^2 \, ds,$$

where  $\mathbb{T} = (\mathbb{T}_1, \mathbb{T}_2)$  is the solution of the convection-diffusion problem (1.4) with exterior temperature  $\mathbb{T}_{\text{ext}}$ .

Let  $(\Xi, \mathcal{A}, \mathbb{P})$  be a complete probability space. We consider the case where the exterior temperature is given as a random process in the Bochner space  $L^2(\Xi, H^{1/2}(\Gamma_D))$ . The temperature  $\mathbb{T}(\cdot, \cdot)$

then becomes a random process defined as the unique solution in  $\mathcal{H}_{\Gamma_D}$  to the following system

$$\left\{ \begin{array}{ll} -\operatorname{div}(\kappa_1 \nabla T_1(\cdot, \omega)) + \mathbf{u} \cdot \nabla T_1(\cdot, \omega) = 0 & \text{in } \Omega_1, \\ -\operatorname{div}(\kappa_2 \nabla T_2(\cdot, \omega)) = 0 & \text{in } \Omega_2, \\ T_1(\cdot, \omega) = T_D & \text{on } \Gamma_D, \\ \kappa_1 \frac{\partial T_1(\cdot, \omega)}{\partial \mathbf{n}} = 0 & \text{on } \Gamma_N, \\ \kappa_2 \frac{\partial T_2(\cdot, \omega)}{\partial \mathbf{n}} + \alpha T_2(\cdot, \omega) = \alpha T_{\text{ext}}(\cdot, \omega) & \text{on } \Gamma_R, \\ \left\langle \kappa \frac{\partial T(\cdot, \omega)}{\partial \mathbf{n}} \right\rangle = -\kappa_m \epsilon^{-1} [T(\cdot, \omega)] & \text{on } \Gamma, \\ \left[ \kappa \frac{\partial T(\cdot, \omega)}{\partial \mathbf{n}} \right] = \epsilon \operatorname{div}_\tau(\kappa_m \nabla_\tau \langle T(\cdot, \omega) \rangle) - \kappa_m H[T(\cdot, \omega)] & \text{on } \Gamma. \end{array} \right. \quad (2.9)$$

The objective is now to minimize  $\mathbb{E}[J(\Omega_2, T_{\text{ext}}(x, \cdot))]$  the expectation of the objective functional  $J$ . The functional of interested  $J$  is quadratic in a temperature that depends linearly on the random parameter. This situation fits to the context of the work of Dambrine *et al.* [14]. Note that considering higher order moments can be done by a mere adaptation of the methods (see [15]). The gradient of the objective can be computed thanks to the two points correlation of the random input  $T_{\text{ext}}$ . In order to avoid the needed introduction of tensor calculus for the general case (see [14] for the quadratic case and [12] for the general polynomial case), we restrict ourselves in this work to the particular case where  $T_{\text{ext}}$  is a finite sum

$$T_{\text{ext}}(x, \omega) = T_{\text{ext}}^0(x) + \sum_{k=1}^m \xi_k(\omega) T_{\text{ext}}^k(x), \quad x \in \Omega, \quad \omega \in \Xi, \quad (2.10)$$

where the random variables  $\xi_k$  are assumed independent following centered Gaussian distributions with variance  $\sigma_k^2$ . This case can be dealt with easily but remains representative of the general situation when  $m$  the number of terms goes to  $\infty$ . The expression (2.10) is a so-called truncated Karhunen-Loeve decomposition.

**Theorem 2.5** (Shape derivative of the expectation of  $J$ ). *Let us consider an uncertain exterior temperature expanded as in (2.10). Let us also assume that the random variables  $\xi_k$  have zero expected value and are independent. Then the expectation of  $J$  can be computed as*

$$\mathbb{E}[J(\Omega_2, T_{\text{ext}})] = J(\Omega_2, T_{\text{ext}}^0) + \sum_{k=1}^m \sigma_k^2 J(\Omega_2, T_{\text{ext}}^k) \quad (2.11)$$

and, under regularity assumptions similar to those of Proposition 2.4, its shape derivative is then given by

$$(\mathbb{E}[J])'(\Omega_2, T_{\text{ext}})(\boldsymbol{\theta}) = J'(\Omega_2, T_{\text{ext}}^0)(\boldsymbol{\theta}) + \sum_{k=1}^m \sigma_k^2 J'(\Omega_2, T_{\text{ext}}^k)(\boldsymbol{\theta}). \quad (2.12)$$

**Remark 2.6.** *In the above theorem, we need to define the solution associated to each  $T_{\text{ext}}^0$  and  $T_{\text{ext}}^k$  (in order to define the associated functional). Then we specify that (see the corresponding proof), for each  $k = 1, \dots, m$ ,  $T^k \in \mathcal{H}_0$  solves Equation (1.4) with respectively  $T_{\text{ext}}^k$  and 0 as conditions on  $\Gamma_R$  and  $\Gamma_D$ , and where  $T^0 \in \mathcal{H}_{\Gamma_D}$  solves Equation (1.4) with respectively  $T_{\text{ext}}^0$  and  $T_D$  as conditions on  $\Gamma_R$  and  $\Gamma_D$ .*

### 3 Proofs

#### 3.1 Proof of the well-posedness theorem 2.1

*Proof of Theorem 2.1.* We follow the usual strategy: lift the boundary condition and apply Lax-Milgram theorem in the space  $\mathcal{H}_0$ . The crucial point is to prove that  $a$  is coercive. The presence of an interface condition on  $\Gamma$  is not completely customary. We therefore demonstrate this point.

Let  $S \in \mathcal{H}_0$ . We split  $a(S, S)$  into  $a_1(S, S) + a_2(S, S) + a_3(S, S)$  where

$$\begin{aligned} a_1(S, S) &:= \int_{\Omega_1 \cup \Omega_2} \kappa |\nabla S|^2 dx + \kappa_m \int_{\Gamma} \left( \epsilon |\nabla_{\tau} \langle S \rangle|^2 + \frac{1}{\epsilon} [S]^2 \right) ds + \int_{\Gamma_R} \alpha S^2 ds, \\ a_2(S, S) &:= \int_{\Omega_1} S(\mathbf{u} \cdot \nabla S) dx, \\ a_3(S, S) &:= \kappa_m \int_{\Gamma} H[S] \langle S \rangle ds. \end{aligned}$$

The bilinear form  $a_1$  clearly is coercive,

$$a_1(S, S) \geq \|\kappa^{1/2} \nabla S\|_{0, \Omega_1 \cup \Omega_2}^2 + \epsilon \kappa_m \|\nabla_{\tau} \langle S \rangle\|_{L^2(\Gamma)}^2 + \frac{\kappa_m}{\epsilon} \|[S]\|_{L^2(\Gamma)}^2.$$

Concerning  $a_2$ , we get after integration by parts

$$a_2(S, S) = \int_{\Omega_1} \mathbf{u} \cdot \nabla \left( \frac{S^2}{2} \right) dx = \frac{1}{2} \int_{\Gamma_N} S^2 \mathbf{u} \cdot \mathbf{n} ds.$$

We have used the boundary conditions  $\mathbf{u} = 0$  on  $\Gamma$  and  $S = 0$  on  $\Gamma_D$  and the incompressibility of the fluid  $\operatorname{div}(\mathbf{u}) = 0$  in  $\Omega_1$ . Now since the output normal velocity  $\mathbf{u} \cdot \mathbf{n}$  is positive by the exit condition (2.2), we get  $a_2(S, S) > 0$ . The difficulty lays in the product  $[S] \langle S \rangle$  that has no sign. Using successively Cauchy-Schwarz then Peter-Paul inequalities, one gets

$$\begin{aligned} \left| \int_{\Gamma} H[S] \langle S \rangle ds \right| &= \frac{1}{2} \left| \int_{\Gamma} [S] (H S_1 + H S_2) ds \right| \\ &\leq \frac{1}{2} \|[S]\|_{L^2(\Gamma)}^2 \left( \|H S_1\|_{L^2(\Gamma)}^2 + \|H S_2\|_{L^2(\Gamma)}^2 \right) \\ &\leq \frac{1}{2} \left( \frac{1}{2\epsilon} \|[S]\|_{L^2(\Gamma)}^2 + \frac{\epsilon}{2} \|H S_1\|_{L^2(\Gamma)}^2 + \frac{1}{2\epsilon} \|[S]\|_{L^2(\Gamma)}^2 + \frac{\epsilon}{2} \|H S_2\|_{L^2(\Gamma)}^2 \right) \\ &\leq \frac{1}{2\epsilon} \|[S]\|_{L^2(\Gamma)}^2 + \frac{\epsilon \|H\|_{\infty}^2}{4} \left( \|S_1\|_{L^2(\Gamma)}^2 + \|S_2\|_{L^2(\Gamma)}^2 \right). \end{aligned}$$

Since  $S_1 = 0$  on  $\Gamma_D$ , one infers from the trace theorem and Poincaré inequality for  $S_1$ , the existence of a positive constant  $C > 0$ , such that,  $\|S_1\|_{L^2(\Gamma)}^2 \leq C \|\nabla S_1\|_{L^2(\Omega_1)}^2$ . This is not the case for  $S_2$ . Using the definition of the jump, ones gets

$$\|S_2\|_{L^2(\Gamma)} \leq \|S_1\|_{L^2(\Gamma)} + \|[S]\|_{L^2(\Gamma)} \text{ then } \|S_2\|_{L^2(\Gamma)}^2 \leq 2 \left( \|S_1\|_{L^2(\Gamma)}^2 + \|[S]\|_{L^2(\Gamma)}^2 \right)$$

by the triangle inequality. Finally, we have obtained the bound

$$\left| \int_{\Gamma} H[S] \langle S \rangle ds \right| \leq \frac{1}{2} \left( \frac{1}{\epsilon} + \epsilon \|H\|_{\infty}^2 \right) \|[S]\|_{L^2(\Gamma)}^2 + \frac{3\epsilon C \|H\|_{\infty}^2}{4} \|\nabla S_1\|_{L^2(\Omega_1)}^2.$$

Therefore,

$$\begin{aligned}
a_1(\mathbf{S}, \mathbf{S}) + a_3(\mathbf{S}, \mathbf{S}) &\geq \|\kappa^{1/2} \nabla \mathbf{S}\|_{L^2(\Omega_1 \cup \Omega_2)}^2 - \epsilon \frac{3C\kappa_m \|H\|_\infty^2}{4} \|\nabla \mathbf{S}_1\|_{L^2(\Omega_1)}^2 + \epsilon \kappa_m \|\nabla_\tau \langle \mathbf{S} \rangle\|_{L^2(\Gamma)}^2 \\
&\quad + \frac{\kappa_m}{2} \left( \frac{1}{\epsilon} - \epsilon \|H\|_\infty^2 \right) \|\mathbf{S}\|_{L^2(\Gamma)}^2.
\end{aligned}$$

We impose  $\epsilon < \|H\|_\infty^{-1}$  so that the last term is nonnegative. The second term is absorbed by the correspond term in  $a_1$  if we impose that

$$\kappa_1 - \epsilon \frac{3C\kappa_m \|H\|_\infty^2}{4} \geq \frac{1}{2}\kappa_1 \Leftrightarrow \epsilon \leq \frac{2\kappa_1}{3C\kappa_m \|H\|_\infty^2}.$$

In conclusion  $a$  is coercive if

$$\epsilon < \epsilon_0 := \min \left( \frac{1}{\|H\|_\infty}, \frac{2\kappa_1}{3C\kappa_m \|H\|_\infty^2} \right),$$

which concludes the proof.  $\square$

### 3.2 Shape sensitivity analysis

Before proving the main result of this part (Proposition 2.4), we need some auxiliary results, as the existence of the derivative. As is classical in shape optimization, the first step is to show the existence of the material derivative and then compute it (see, e.g., [23, 1]). For the sake of simplicity, we assume without loss of generality  $\mathbb{T}_D = 0$ .

We recall that, for  $\boldsymbol{\theta} \in \Theta_{\text{ad}}$ ,  $\mathbb{T}_{\boldsymbol{\theta}} \in H^1(\Omega_1, \Gamma) \times H^1(\Omega_2^\boldsymbol{\theta}, \Gamma)$  is the solution of the convection-diffusion Problem (1.4) defined on  $\Omega_1 \cup \Omega_2^\boldsymbol{\theta}$  instead of  $\Omega_1 \cup \Omega_2$ .

**Proposition 3.1** (Existence and characterization of the material derivative of  $\mathbb{T}$ ). *For all  $\boldsymbol{\theta} \in \Theta_{\text{ad}}$ , we define  $\bar{\mathbb{T}}_{\boldsymbol{\theta}} := \mathbb{T}_{\boldsymbol{\theta}} \circ (\mathbf{I} + \boldsymbol{\theta})$ . If  $\mathbb{T}_{\text{ext}} \in H^2(\mathbb{R}^d)$ , then*

$$\boldsymbol{\theta} \in \Theta_{\text{ad}} \rightarrow \bar{\mathbb{T}}_{\boldsymbol{\theta}} \in \mathcal{H}_0$$

*is differentiable in a neighborhood of 0. Furthermore, its derivative at 0, in the direction  $\boldsymbol{\theta}$ , is called the material derivative of  $\mathbb{T}$ , is denoted by  $\dot{\mathbb{T}} \in \mathcal{H}_0$ , and is the solution of the following variational problem*

$$\left\{ \begin{array}{l} \text{Find } \dot{\mathbb{T}} \in \mathcal{H}_0 \text{ such that, for all } \phi \in \mathcal{H}_0, \\ \int_{\Omega_1 \cup \Omega_2} \kappa \nabla \dot{\mathbb{T}} \cdot \nabla \phi \, dx + \int_{\Omega_1} \nabla \dot{\mathbb{T}} \cdot \mathbf{u} \phi \, dx + \int_{\Gamma_R} \alpha \dot{\mathbb{T}} \phi \, ds \\ \quad + \int_{\Gamma} \left( \epsilon \kappa_m \nabla_\tau \langle \dot{\mathbb{T}} \rangle \cdot \nabla_\tau \langle \phi \rangle + \kappa_m H[\dot{\mathbb{T}}] \langle \phi \rangle + \frac{\kappa_m}{\epsilon} [\dot{\mathbb{T}}][\phi] \right) ds \\ = \int_{\Omega_2} \kappa (\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t - \text{div}(\boldsymbol{\theta})I) \nabla \mathbb{T} \cdot \nabla \phi \, dx - \int_{\Gamma_R} (\alpha \text{div}_\tau(\boldsymbol{\theta})(\mathbb{T} - \mathbb{T}_{\text{ext}})\phi - \alpha \nabla \mathbb{T}_{\text{ext}} \cdot \boldsymbol{\theta} \phi) \, ds. \end{array} \right. \quad (3.1)$$

*Proof of Proposition 3.1.* We proceed as described in [23]. Let  $\phi \in \mathcal{H}_0$  and let  $\boldsymbol{\theta} \in \Theta_{\text{ad}}$ . We define  $\phi_{\boldsymbol{\theta}} := \phi \circ (\mathbf{I} + \boldsymbol{\theta})^{-1}$  and we have

$$\int_{\Omega_1 \cup \Omega_2^\boldsymbol{\theta}} \kappa \nabla \mathbb{T}_{\boldsymbol{\theta}} \cdot \nabla \phi_{\boldsymbol{\theta}} \, dx + \int_{\Omega_1} \nabla \mathbb{T}_{\boldsymbol{\theta}} \cdot \mathbf{u} \phi_{\boldsymbol{\theta}} \, dx + \int_{\Gamma_R} \alpha \mathbb{T}_{\boldsymbol{\theta}} \phi_{\boldsymbol{\theta}} \, ds$$

$$+ \int_{\Gamma_{\theta}} (\epsilon \kappa_m \nabla_{\tau_{\theta}} \langle \mathbf{T}_{\theta} \rangle \cdot \nabla_{\tau_{\theta}} \langle \phi_{\theta} \rangle + \kappa_m H_{\theta}[\mathbf{T}_{\theta}] \langle \phi_{\theta} \rangle + \epsilon^{-1} \kappa_m [\mathbf{T}_{\theta}][\phi_{\theta}]) \, ds = \int_{\Gamma_{\mathbb{R}}^{\theta}} \alpha \mathbf{T}_{\text{ext}} \phi_{\theta} \, dx.$$

Changing variables, we get

$$\begin{aligned} & \int_{\Omega_2} \kappa A(\boldsymbol{\theta}) \nabla \bar{\mathbf{T}}_{\boldsymbol{\theta}} \cdot \nabla \phi \, dx + \int_{\Omega_1} (\kappa \nabla \bar{\mathbf{T}}_{\boldsymbol{\theta}} \cdot \nabla \phi + \nabla \bar{\mathbf{T}}_{\boldsymbol{\theta}} \cdot \mathbf{u} \phi) \, dx + \int_{\Gamma_{\mathbb{R}}} \alpha B(\boldsymbol{\theta}) \bar{\mathbf{T}}_{\boldsymbol{\theta}} \phi \, ds \\ & + \int_{\Gamma} (\epsilon \kappa_m \nabla_{\tau} \langle \bar{\mathbf{T}}_{\boldsymbol{\theta}} \rangle \cdot \nabla_{\tau} \langle \phi \rangle + \kappa_m H[\bar{\mathbf{T}}_{\boldsymbol{\theta}}] \langle \phi \rangle + \epsilon^{-1} \kappa_m [\bar{\mathbf{T}}_{\boldsymbol{\theta}}][\phi]) \, ds = \int_{\Gamma_{\mathbb{R}}} \alpha B(\boldsymbol{\theta}) \mathbf{T}_{\text{ext}} \circ (\mathbf{I} + \boldsymbol{\theta}) \phi \, dx, \end{aligned} \quad (3.2)$$

where  $A(\boldsymbol{\theta}) := \det(\mathbf{I} + \nabla \boldsymbol{\theta})(\mathbf{I} + \nabla \boldsymbol{\theta})^{-t}(\mathbf{I} + \nabla \boldsymbol{\theta})$  and  $B(\boldsymbol{\theta}) := \det(\mathbf{I} + \nabla \boldsymbol{\theta})|(\mathbf{I} + \nabla \boldsymbol{\theta})^{-t} \mathbf{n}|_{\mathbb{R}^d}$ . Then, we introduce  $\mathcal{F} : \Theta_{\text{ad}} \times \mathcal{H}_0 \rightarrow (\mathcal{H}_0)'$ , defined for all  $S \in \mathcal{H}_0$  by,

$$\begin{aligned} \langle \mathcal{F}(\boldsymbol{\theta}, \bar{\mathbf{T}}), S \rangle & := \int_{\Omega_2} \kappa A(\boldsymbol{\theta}) \nabla \bar{\mathbf{T}} \cdot \nabla S \, dx + \int_{\Omega_1} (\kappa \nabla \bar{\mathbf{T}} \cdot \nabla S + \nabla \bar{\mathbf{T}} \cdot \mathbf{u} S) \, dx + \int_{\Gamma_{\mathbb{R}}} \alpha B(\boldsymbol{\theta}) \bar{\mathbf{T}} S \, ds \\ & + \int_{\Gamma} \kappa_m \left( \epsilon \nabla_{\tau} \langle \bar{\mathbf{T}} \rangle \cdot \nabla_{\tau} \langle S \rangle + H[\bar{\mathbf{T}}] \langle S \rangle + \frac{1}{\epsilon} [\bar{\mathbf{T}}][S] \right) \, ds - \int_{\Gamma_{\mathbb{R}}} \alpha B(\boldsymbol{\theta}) \mathbf{T}_0 \circ (\mathbf{I} + \boldsymbol{\theta}) S \, ds. \end{aligned}$$

By construction  $\mathcal{F}(0, 0) = 0$ . Similarly to [23, Theorem 5.5.1], we show that  $\mathcal{F}$  is  $\mathcal{C}^1$ . Finally, the operator  $D_{\bar{\mathbf{T}}} \mathcal{F}(0, 0)$  is an isomorphism from  $\mathcal{H}_0$  into  $(\mathcal{H}_0)'$ , since for all  $S, \hat{S} \in \mathcal{H}_0$ ,

$$\begin{aligned} \langle D_{\bar{\mathbf{T}}} \mathcal{F}(0, 0) S, \hat{S} \rangle & = \int_{\Omega_1 \cup \Omega_2} \kappa \nabla S \cdot \nabla \hat{S} \, dx + \int_{\Omega_1} \nabla S \cdot \mathbf{u} \hat{S} \, dx \\ & + \int_{\Gamma_{\mathbb{R}}} \alpha S \hat{S} \, ds + \int_{\Gamma} \left( \epsilon \kappa_m \nabla_{\tau} \langle S \rangle \cdot \nabla_{\tau} \langle \hat{S} \rangle + \kappa_m H[S][\hat{S}] + \frac{\kappa_m}{\epsilon} [S][\hat{S}] \right) \, ds. \end{aligned}$$

In virtue of the implicit function theorem, there exists a  $\mathcal{C}^1$  function  $\boldsymbol{\theta} \in \Theta_{\text{ad}} \rightarrow \bar{\mathbf{T}}(\boldsymbol{\theta}) \in \mathcal{H}_0$  in a neighborhood of 0 such that,  $\mathcal{F}(0, \bar{\mathbf{T}}(\boldsymbol{\theta})) = 0$ . By uniqueness of the solution  $\bar{\mathbf{T}}_{\boldsymbol{\theta}}$ , we deduce  $\bar{\mathbf{T}}_{\boldsymbol{\theta}} = \bar{\mathbf{T}}(\boldsymbol{\theta})$ , then,  $\boldsymbol{\theta} \rightarrow \bar{\mathbf{T}}_{\boldsymbol{\theta}}$  is  $\mathcal{C}^1$ .

To prove that the material derivative  $\dot{\mathbf{T}}$  satisfies (3.1), we proceeded as in [4, Proposition 6.30]. We first recall that

$$A'(0)(\boldsymbol{\theta}) = \text{div}(\boldsymbol{\theta})I - \nabla \boldsymbol{\theta} - (\nabla \boldsymbol{\theta})^t, \quad B'(0)(\boldsymbol{\theta}) = \text{div}_{\tau}(\boldsymbol{\theta}) \quad \text{and} \quad \bar{\mathbf{T}}'(0)(\boldsymbol{\theta}) = \dot{\mathbf{T}}.$$

Then, differentiating (3.2) at  $\boldsymbol{\theta} = 0$ , in the direction  $\boldsymbol{\theta}$  and using the chain rule of those derivatives, we get (3.1).  $\square$

After showing the existence and computing the material derivative, we can do the same for the eulerian derivative, which proof uses the previous results and some integrations by parts.

*Proof of Proposition 2.3.* Let us introduce a linear continuous extension  $E : \mathcal{H}_0 \rightarrow \mathbf{H}^1(\mathbb{R}^d) \times \mathbf{H}^1(\mathbb{R}^d)$ . We define  $\tilde{\mathbf{T}}_{\boldsymbol{\theta}} := E(\bar{\mathbf{T}}_{\boldsymbol{\theta}}) \circ (\mathbf{I} + \boldsymbol{\theta})^{-1}$  and since  $\boldsymbol{\theta} \in \Theta_{\text{ad}} \rightarrow \bar{\mathbf{T}}_{\boldsymbol{\theta}} \in \mathcal{H}_0$  is differentiable in a neighborhood of 0, we obtain the existence of the shape derivative using [23, Lemma 5.3.3].

To get (2.4), we use that  $\mathbf{T}'_2 = \dot{\mathbf{T}}_2 - \boldsymbol{\theta} \cdot \nabla \mathbf{T}_2$  belongs to  $\mathbf{H}^1(\Omega_2)$  since we have assumed that  $\mathbf{T}_2 \in \mathbf{H}^2(\Omega_2)$ , and also that  $\mathbf{T}'_1 = \dot{\mathbf{T}}_1 \in \mathbf{H}^1(\Omega_1)$  and  $\mathbf{T}'_i = \dot{\mathbf{T}}_i \in \mathbf{H}^1(\Gamma)$  for  $i = 1, 2$ . In order to obtain

the strong form for the shape derivative (2.5), we integrate by parts in formula (2.4), this is,

$$\begin{aligned}
& \int_{\Omega_1 \cup \Omega_2} (\kappa \nabla \mathbf{T}' \cdot \nabla \phi + \phi \nabla \mathbf{T}' \cdot \mathbf{u}) \, dx + \int_{\Gamma_R} \alpha \mathbf{T}' \phi \, ds \\
& \quad + \int_{\Gamma} (\epsilon \kappa_m \nabla_{\tau} \langle \mathbf{T}' \rangle \cdot \nabla_{\tau} \langle \phi \rangle + \kappa_m H[\mathbf{T}'] \langle \phi \rangle + \kappa_m \epsilon^{-1} [\mathbf{T}'] [\phi]) \, ds \\
& = \int_{\Omega_2} (\kappa (\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t) \nabla \mathbf{T} \cdot \nabla \phi - \kappa \operatorname{div}(\boldsymbol{\theta}) \nabla \mathbf{T} \cdot \nabla \phi - \kappa \nabla(\boldsymbol{\theta} \cdot \nabla \mathbf{T}) \cdot \nabla \phi) \, dx \\
& \quad - \int_{\Gamma_R} (\alpha \operatorname{div}_{\tau}(\boldsymbol{\theta})(\mathbf{T} - \mathbf{T}_{\text{ext}}) \phi + \alpha \phi \boldsymbol{\theta} \cdot \nabla(\mathbf{T} - \mathbf{T}_{\text{ext}})) \, ds \\
& = \int_{\Omega_2} (\kappa (\nabla \boldsymbol{\theta} - \operatorname{div}(\boldsymbol{\theta}) I) \nabla \mathbf{T} \cdot \nabla \phi - \kappa (\nabla^2 \mathbf{T}) \boldsymbol{\theta} \cdot \nabla \phi) \, dx \\
& \quad - \int_{\Gamma_R} (\alpha \operatorname{div}_{\tau}(\boldsymbol{\theta})(\mathbf{T} - \mathbf{T}_{\text{ext}}) \phi + \alpha \phi \boldsymbol{\theta} \cdot \nabla(\mathbf{T} - \mathbf{T}_{\text{ext}})) \, ds \\
& = \int_{\Omega_2} (\kappa \operatorname{div}((\boldsymbol{\theta} \cdot \nabla \phi) \nabla \mathbf{T} - (\nabla \mathbf{T} \cdot \nabla \phi) \boldsymbol{\theta}) - (\boldsymbol{\theta} \cdot \nabla \phi) \kappa \Delta \mathbf{T}) \, dx \\
& \quad - \int_{\Gamma_R} (\alpha \operatorname{div}_{\tau}(\boldsymbol{\theta})(\mathbf{T} - \mathbf{T}_{\text{ext}}) \phi + \alpha \phi \boldsymbol{\theta} \cdot \nabla(\mathbf{T} - \mathbf{T}_{\text{ext}})) \, ds.
\end{aligned}$$

Since  $\mathbf{T}$  is the solution of the convection-diffusion equation (1.4),  $\kappa_2 \Delta \mathbf{T} = 0$  in  $\Omega_2$  with the boundary condition  $\kappa \frac{\partial \mathbf{T}}{\partial \mathbf{n}} = \alpha(\mathbf{T}_{\text{ext}} - \mathbf{T})$  on  $\Gamma_R$ , then

$$\begin{aligned}
& \int_{\Omega_1 \cup \Omega_2} (\kappa \nabla \mathbf{T}' \cdot \nabla \phi + \phi \nabla \mathbf{T}' \cdot \mathbf{u}) \, dx + \int_{\Gamma_R} \alpha \mathbf{T}' \phi \, ds \\
& \quad + \int_{\Gamma} (\epsilon \kappa_m \nabla_{\tau} \langle \mathbf{T}' \rangle \cdot \langle \phi \rangle + \kappa_m H[\mathbf{T}'] \langle \phi \rangle + \kappa_m \epsilon^{-1} [\mathbf{T}'] [\phi]) \, ds \\
& = \int_{\Omega_2} (\kappa \operatorname{div}((\boldsymbol{\theta} \cdot \nabla \phi) \nabla \mathbf{T} - (\nabla \mathbf{T} \cdot \nabla \phi) \boldsymbol{\theta})) \, dx - \alpha \int_{\Gamma_R} \left( \operatorname{div}_{\tau}((\mathbf{T} - \mathbf{T}_{\text{ext}}) \boldsymbol{\theta}) \phi + (\boldsymbol{\theta} \cdot \mathbf{n}) \phi \frac{\partial}{\partial \mathbf{n}} (\mathbf{T} - \mathbf{T}_{\text{ext}}) \right) \, ds.
\end{aligned}$$

By divergence theorem and the fact that  $\boldsymbol{\theta} = 0$  on  $\Gamma$ ,

$$\begin{aligned}
& \int_{\Omega_1 \cup \Omega_2} (\kappa \nabla \mathbf{T}' \cdot \nabla \phi + \phi \nabla \mathbf{T}' \cdot \mathbf{u}) \, dx + \int_{\Gamma_R} \alpha \mathbf{T}' \phi \, ds \\
& \quad + \int_{\Gamma} (\epsilon \kappa_m \nabla_{\tau} \langle \mathbf{T}' \rangle \cdot \langle \phi \rangle + \kappa_m H[\mathbf{T}'] \langle \phi \rangle + \kappa_m \epsilon^{-1} [\mathbf{T}'] [\phi]) \, ds \\
& = \int_{\Gamma_R} \left( (\boldsymbol{\theta} \cdot \nabla \phi) \kappa \frac{\partial \mathbf{T}}{\partial \mathbf{n}} - \kappa \nabla \mathbf{T} \cdot \nabla \phi - \alpha \operatorname{div}_{\tau}((\mathbf{T} - \mathbf{T}_{\text{ext}}) \boldsymbol{\theta}) \phi - \alpha (\boldsymbol{\theta} \cdot \mathbf{n}) \phi \frac{\partial}{\partial \mathbf{n}} (\mathbf{T} - \mathbf{T}_{\text{ext}}) \right) \, ds.
\end{aligned}$$

Decomposing the gradient as  $\nabla \phi = \nabla_{\tau} \phi + \mathbf{n} \frac{\partial \phi}{\partial \mathbf{n}}$  and using again that  $\mathbf{T}$  verifies the Robin boundary condition at  $\Gamma_R$ , we obtain that

$$\begin{aligned}
& \int_{\Omega_1 \cup \Omega_2} (\kappa \nabla \mathbf{T}' \cdot \nabla \phi + \phi \nabla \mathbf{T}' \cdot \mathbf{u}) \, dx + \int_{\Gamma_R} \alpha \mathbf{T}' \phi \, ds \\
& \quad + \int_{\Gamma} (\epsilon \kappa_m \nabla_{\tau} \langle \mathbf{T}' \rangle \cdot \nabla_{\tau} \langle \phi \rangle + \kappa_m H[\mathbf{T}'] \langle \phi \rangle + \kappa_m \epsilon^{-1} [\mathbf{T}'] [\phi]) \, ds \\
& = \int_{\Gamma_R} \left( -\alpha \operatorname{div}_{\tau}(\phi(\mathbf{T} - \mathbf{T}_{\text{ext}}) \boldsymbol{\theta}) - \kappa \nabla_{\tau} \mathbf{T} \cdot \nabla_{\tau} \phi (\boldsymbol{\theta} \cdot \mathbf{n}) - \alpha \phi (\boldsymbol{\theta} \cdot \mathbf{n}) \frac{\partial}{\partial \mathbf{n}} (\mathbf{T} - \mathbf{T}_{\text{ext}}) \right) \, ds.
\end{aligned}$$

Finally, integrating by parts on the surface  $\Gamma_R$  (see [23, Proposition 5.4.9]) yields to the desired formula.  $\square$

Finally, afterwards the existence of the shape derivative of  $\mathbb{T}$  is assured, the shape derivative derivative can be computed by using the chain rule.

*Proof of Proposition 2.4.* Let  $\mathbb{T}'$  the Eulerian derivative of the convection-diffusion equation (1.4), that verifies (2.4) and let  $\boldsymbol{\theta} \in \Theta_{\text{ad}}$ . By chain rule,

$$J'(\Omega_2)(\boldsymbol{\theta}) = \int_{\Gamma_R} \left( 2\alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}})\mathbb{T}'_2 \, ds + \int_{\Gamma_R} 2\alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}})\nabla(\mathbb{T}_2 - \mathbb{T}_{\text{ext}}) \cdot \boldsymbol{\theta} + \alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}})^2 \operatorname{div}_\tau(\boldsymbol{\theta}) \right) ds. \quad (3.3)$$

Testing with  $\mathbb{R}$  in the eulerian derivative equation (2.5) and  $\mathbb{T}'$  in the adjoint equation (2.7), we get respectively

$$\begin{aligned} & \int_{\Omega_1 \cup \Omega_2} \kappa \nabla \mathbb{T}' \cdot \nabla \mathbb{R} \, dx + \int_{\Omega_1} \nabla \mathbb{T}' \cdot \mathbf{u} \mathbb{R} \, dx + \int_{\Gamma_R} \alpha \mathbb{T}' \mathbb{R} \, ds \\ & \quad + \int_{\Gamma} \left( \epsilon \kappa_m \nabla_\tau \langle \mathbb{R} \rangle \cdot \nabla_\tau \langle \mathbb{T}' \rangle + \kappa_m H \langle \mathbb{R} \rangle [\mathbb{T}'] + \frac{\kappa_m}{\epsilon} [\mathbb{R}][\mathbb{T}'] \right) ds \\ & = \int_{\Omega_2} \kappa (\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t - \operatorname{div}(\boldsymbol{\theta})I) \nabla \mathbb{T} \cdot \nabla \mathbb{R} - \kappa \nabla(\boldsymbol{\theta} \cdot \nabla \mathbb{T}) \cdot \nabla \mathbb{R} \, dx \\ & \quad - \int_{\Gamma_R} \operatorname{div}_\tau(\boldsymbol{\theta}) \alpha (\mathbb{T} - \mathbb{T}_{\text{ext}}) \mathbb{R} - \alpha \nabla(\mathbb{T} - \mathbb{T}_{\text{ext}}) \cdot \boldsymbol{\theta} \mathbb{R} \, ds \quad (3.4) \end{aligned}$$

and

$$\begin{aligned} & \int_{\Omega_1 \cup \Omega_2} \kappa \nabla \mathbb{T}' \cdot \nabla \mathbb{R} \, dx + \int_{\Omega_1} \mathbb{R} \mathbf{u} \cdot \nabla \mathbb{T}' \, dx + \int_{\Gamma_R} \alpha \mathbb{T}' \mathbb{R} \, ds \\ & \quad + \int_{\Gamma} \epsilon \kappa_m \nabla_\tau \langle \mathbb{R} \rangle \cdot \nabla_\tau \langle \mathbb{T}' \rangle + \kappa_m H \langle \mathbb{R} \rangle [\mathbb{T}'] + \frac{\kappa_m}{\epsilon} [\mathbb{R}][\mathbb{T}'] \, ds = \int_{\Gamma_R} 2\alpha^2(\mathbb{T} - \mathbb{T}_{\text{ext}})\mathbb{T}' \, ds. \quad (3.5) \end{aligned}$$

Using (3.4) and (3.5), we get

$$\begin{aligned} \int_{\Gamma_R} 2\alpha^2(\mathbb{T} - \mathbb{T}_{\text{ext}})\mathbb{T}' \, ds & = \int_{\Omega_2} \kappa (\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t - \operatorname{div}(\boldsymbol{\theta})I) \nabla \mathbb{T} \cdot \nabla \mathbb{R} - \kappa \nabla(\boldsymbol{\theta} \cdot \nabla \mathbb{T}) \cdot \nabla \mathbb{R} \, dx \\ & \quad - \int_{\Gamma_R} \operatorname{div}_\tau(\boldsymbol{\theta}) \alpha (\mathbb{T} - \mathbb{T}_{\text{ext}}) \mathbb{R} + \alpha \nabla(\mathbb{T} - \mathbb{T}_{\text{ext}}) \cdot \boldsymbol{\theta} \mathbb{R} \, ds. \quad (3.6) \end{aligned}$$

Plugging (3.6) into (3.3), it yields to

$$\begin{aligned} J'(\Omega_2)(\boldsymbol{\theta}) & = \int_{\Gamma_R} 2\alpha^2(\mathbb{T} - \mathbb{T}_{\text{ext}})\nabla(\mathbb{T} - \mathbb{T}_{\text{ext}}) \cdot \boldsymbol{\theta} + \alpha^2(\mathbb{T} - \mathbb{T}_{\text{ext}})^2 \operatorname{div}_\tau(\boldsymbol{\theta}) \, ds \\ & \quad + \int_{\Omega_2} \kappa (\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t - \operatorname{div}(\boldsymbol{\theta})I) \nabla \mathbb{T} \cdot \nabla \mathbb{R} - \kappa \nabla(\boldsymbol{\theta} \cdot \nabla \mathbb{T}) \cdot \nabla \mathbb{R} \, dx \\ & \quad - \int_{\Gamma_R} \operatorname{div}_\tau(\boldsymbol{\theta}) \alpha (\mathbb{T} - \mathbb{T}_{\text{ext}}) \mathbb{R} + \alpha \nabla(\mathbb{T} - \mathbb{T}_{\text{ext}}) \cdot \boldsymbol{\theta} \mathbb{R} \, ds. \end{aligned}$$

Using that  $\kappa_2 \frac{\partial \mathbb{R}_2}{\partial \mathbf{n}} = 2\alpha^2(\mathbb{T}_2 - \mathbb{T}_{\text{ext}}) - \alpha \mathbb{R}_2$  on  $\Gamma_R$ , we get

$$\begin{aligned} J'(\Omega_2)(\boldsymbol{\theta}) & = \int_{\Gamma_R} \alpha^2(\mathbb{T} - \mathbb{T}_{\text{ext}})^2 \operatorname{div}_\tau(\boldsymbol{\theta}) + \kappa \frac{\partial \mathbb{R}}{\partial \mathbf{n}} \nabla \mathbb{T} \cdot \boldsymbol{\theta} - (2\alpha^2(\mathbb{T} - \mathbb{T}_{\text{ext}}) - \alpha \mathbb{R}) \nabla \mathbb{T}_{\text{ext}} \cdot \boldsymbol{\theta} \, ds \\ & \quad + \int_{\Omega_2} \kappa (\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t - \operatorname{div}(\boldsymbol{\theta})I) \nabla \mathbb{T} \cdot \nabla \mathbb{R} - \kappa \nabla(\boldsymbol{\theta} \cdot \nabla \mathbb{T}) \cdot \nabla \mathbb{R} \, dx - \int_{\Gamma_R} \operatorname{div}_\tau(\boldsymbol{\theta}) \alpha (\mathbb{T} - \mathbb{T}_{\text{ext}}) \mathbb{R} \, ds. \end{aligned}$$



Since  $R$  solves the adjoint problem (2.7),

$$\int_{\Omega_2} \nabla(\boldsymbol{\theta} \cdot \nabla T_2) \cdot \nabla R_2 \, dx + \int_{\Gamma_R} \kappa_2 \frac{\partial R_2}{\partial \mathbf{n}} \nabla T_2 \cdot \boldsymbol{\theta} \, ds = 0,$$

( $\boldsymbol{\theta} = 0$  in  $\Omega_1$ ), obtaining (2.6).

To prove the surface expression (2.8), since now we have more regularity, we can integrate by parts, yielding to the terms  $\boldsymbol{\theta} \cdot \mathbf{n}$ . By chain rule,

$$J'(\Omega_2)(\boldsymbol{\theta}) = \int_{\Gamma_R} 2\alpha^2(T_2 - T_{\text{ext}})T_2' \, ds + \int_{\Gamma_R} \alpha^2 \left( \frac{\partial}{\partial \mathbf{n}}(T_2 - T_{\text{ext}})^2 + H(T_2 - T_{\text{ext}})^2 \right) (\boldsymbol{\theta} \cdot \mathbf{n}) \, ds. \quad (3.7)$$

Testing the eulerian equation (2.5) with  $R$  and the adjoint equation (2.7) with  $T'$ , we have respectively

$$\begin{aligned} & \int_{\Omega_1 \cup \Omega_2} \kappa \nabla T' \cdot \nabla R \, dx + \int_{\Omega_1} \nabla T' \cdot \mathbf{u} R \, dx + \int_{\Gamma_R} \alpha T' R \, ds \\ & \quad + \int_{\Gamma} \epsilon \kappa_m \nabla_\tau \langle R \rangle \cdot \nabla_\tau \langle T' \rangle + \kappa_m H \langle R \rangle [T'] + \frac{\kappa_m}{\epsilon} [R][T'] \, ds \\ & = - \int_{\Gamma_R} \left( \kappa \nabla_\tau T \cdot \nabla_\tau R + \alpha R \left( \frac{\partial}{\partial \mathbf{n}}(T - T_{\text{ext}}) + H(T - T_{\text{ext}}) \right) \right) (\boldsymbol{\theta} \cdot \mathbf{n}) \, ds \quad (3.8) \end{aligned}$$

and

$$\begin{aligned} & \int_{\Omega_1 \cup \Omega_2} \kappa \nabla T' \cdot \nabla R \, dx + \int_{\Omega_1} R \mathbf{u} \cdot \nabla T' \, dx + \int_{\Gamma_R} \alpha T' R \, ds \\ & \quad + \int_{\Gamma} \epsilon \kappa_m \nabla_\tau \langle R \rangle \cdot \nabla_\tau \langle T' \rangle + \kappa_m H \langle R \rangle [T'] + \frac{\kappa_m}{\epsilon} [R][T'] \, ds = \int_{\Gamma_R} 2\alpha^2(T - T_{\text{ext}})T' \, ds. \quad (3.9) \end{aligned}$$

Using (3.8) and (3.9), we get

$$\int_{\Gamma_R} 2\alpha^2(T - T_{\text{ext}})T' \, ds = - \int_{\Gamma_R} \left( \kappa \nabla_\tau T \cdot \nabla_\tau R + \alpha R \left( \frac{\partial}{\partial \mathbf{n}}(T - T_{\text{ext}}) + H(T - T_{\text{ext}}) \right) \right) (\boldsymbol{\theta} \cdot \mathbf{n}) \, ds. \quad (3.10)$$

Then, (3.7) becomes

$$\begin{aligned} J'(\Omega_2)(\boldsymbol{\theta}) & = \int_{\Gamma_R} \left( \alpha^2 \frac{\partial}{\partial \mathbf{n}}(T - T_{\text{ext}})^2 + \alpha^2 H(T - T_{\text{ext}})^2 - \kappa \nabla_\tau T \cdot \nabla_\tau R \right. \\ & \quad \left. - \alpha R \left( \frac{\partial}{\partial \mathbf{n}}(T - T_{\text{ext}}) - H(T - T_{\text{ext}}) \right) \right) (\boldsymbol{\theta} \cdot \mathbf{n}) \, ds \\ & = \int_{\Gamma_R} \left( 2\alpha^2(T - T_{\text{ext}}) \frac{\partial T}{\partial \mathbf{n}} + \alpha^2 H(T - T_{\text{ext}})^2 - \alpha R \frac{\partial T}{\partial \mathbf{n}} - \alpha H R (T - T_{\text{ext}}) \right. \\ & \quad \left. - \kappa \nabla_\tau T \cdot \nabla_\tau R - \frac{\partial T_{\text{ext}}}{\partial \mathbf{n}} (2\alpha^2(T - T_{\text{ext}}) - \alpha R) \right) (\boldsymbol{\theta} \cdot \mathbf{n}) \, ds. \end{aligned}$$

Using the boundary conditions  $\kappa_2 \frac{\partial T_2}{\partial \mathbf{n}} = \alpha(T_{\text{ext}} - T_2)$  and  $\kappa_2 \frac{\partial R_2}{\partial \mathbf{n}} = 2\alpha(T_2 - T_{\text{ext}}) - \alpha R_2$  on  $\Gamma_R$  and that  $\nabla_\tau T_2 \cdot \nabla_\tau R_2 = \nabla T_2 \cdot \nabla R_2 - \frac{\partial T_2}{\partial \mathbf{n}} \frac{\partial R_2}{\partial \mathbf{n}}$ , we obtain (2.8).  $\square$

**Remark 3.2.** We also expose an alternative method using the Eulerian derivative in Appendix A.

### 3.3 Shape sensitivity analysis with random exterior temperature

*Proof of Proposition 2.5.* Let  $\omega \in \Xi$  be fixed. Recall that  $\mathbb{T}_{\text{ext}}(x, \omega) = \mathbb{T}_{\text{ext}}^0(x) + \sum_{k=1}^m \xi_k(\omega) \mathbb{T}_{\text{ext}}^k(x)$ , for  $x \in \Omega$ . Then, by linearity,

$$\mathbb{T}(\cdot, \omega) = \mathbb{T}^0(\cdot) + \sum_{k=1}^m \xi_k(\omega) \mathbb{T}^k(\cdot)$$

is the unique solution in  $\mathcal{H}_{\Gamma_D}$  of (2.9) where, for each  $k = 1, \dots, m$ ,  $\mathbb{T}^k \in \mathcal{H}_0$  solves Equation (1.4) with respectively  $\mathbb{T}_{\text{ext}}^k$  and 0 as conditions on  $\Gamma_R$  and  $\Gamma_D$ , and where  $\mathbb{T}^0 \in \mathcal{H}_{\Gamma_D}$  solves Equation (1.4) with respectively  $\mathbb{T}_{\text{ext}}^0$  and  $\mathbb{T}_D$  as conditions on  $\Gamma_R$  and  $\Gamma_D$ .

Now we will show (2.11). Using that  $J$  is quadratic with respect to the temperature gap at the boundary, we have

$$\begin{aligned} \mathbb{E}[J](\Omega_2, \mathbb{T}_{\text{ext}}) &= \mathbb{E}[J(\Omega_2, \mathbb{T}_{\text{ext}}^0 + \sum_{k=1}^m \xi_k \mathbb{T}_{\text{ext}}^k)] = \mathbb{E} \left[ \int_{\Gamma_R} \alpha^2 \left( (\mathbb{T}^0 - \mathbb{T}_{\text{ext}}^0 + \sum_{k=1}^m \xi_k (\mathbb{T}^k - \mathbb{T}_{\text{ext}}^k)) \right)^2 \right] \\ &= \int_{\Gamma_R} \alpha^2 (\mathbb{T}^0 - \mathbb{T}_{\text{ext}}^0)^2 + 2 \sum_{k=1}^m \mathbb{E}[\xi_k] \int_{\Gamma_R} (\mathbb{T}^0 - \mathbb{T}_{\text{ext}}^0) (\mathbb{T}^k - \mathbb{T}_{\text{ext}}^k) \\ &\quad + \sum_{k,l=1}^m \mathbb{E}[\xi_k \xi_l] \int_{\Gamma} (\mathbb{T}^l - \mathbb{T}_{\text{ext}}^l) (\mathbb{T}^k - \mathbb{T}_{\text{ext}}^k). \end{aligned}$$

Since the random variables  $\xi_k$  are independent and centered, many terms cancel and one gets

$$\mathbb{E}[J](\Omega_2, \mathbb{T}_{\text{ext}}) = J(\Omega_2, \mathbb{T}_{\text{ext}}^0) + \int_{\Xi} \sum_{k=1}^m \xi_k^2 J(\Omega_2, \mathbb{T}_{\text{ext}}^k) \mathbb{P}(d\omega) = J(\Omega_2, \mathbb{T}_{\text{ext}}^0) + \sum_{k=1}^m \sigma_k^2 J(\Omega_2, \mathbb{T}_{\text{ext}}^k).$$

The expression of the shape derivative (2.12) follows by linearity of the shape derivative.  $\square$

## 4 Numerical methods used to solve the involved problems

### 4.1 Numerical resolution with FEM

We highlight that the approximated convection-diffusion (1.4) and the adjoint equations (2.7) can not be implemented directly due to the use of the Broken Sobolev spaces such as  $\mathcal{H}_0$ . Allaire *et al* proposed a method in [2] to approximate this kind of equations in order to use any finite element software with continuous spaces. However this method involves to duplicate the degrees of freedom, which we do not want for our 3D simulations. Indeed, it becomes too expensive in our context. Domain decomposition method can be used as well, adapting [25] for example. However, it is not clear how many iterations it can take to converge to no mismatch at the interface, in particular in 3D geometries with a large quantity of vertices at the interface (and we require to solve it a lot of times in the shape optimization procedure). Furthermore, the factor  $\frac{1}{\epsilon}$  can lead to poor conditioning of the linear systems and then slow resolution. Finally, in our shape optimization context, we have to compute the shape derivative which is an integral over the interface  $\Gamma$  (which changes at every step of the shape optimization algorithm) and it is then crucial to have precise approximations of this integral. For all these reasons, we solve these equations directly using the dedicated Nitsche method we have introduced in our previous work [10]. The main advantages is the efficiency and the robustness with respect to the small parameter  $\epsilon$ .

Concerning the Navier-Stokes equations (1.3), they can be solved with any finite element software. We rely on FreeFem++ (see [22]) for this purpose. Since  $\Omega_1$  is fixed, the Navier-Stokes equations (1.3) have to be solved just once. However, it is necessary to interpolate the solution in every step of the shape optimization algorithm, since the mesh that describes  $\Omega_1$  will change slightly: indeed the remeshing step MMG concerns the level set function that describes the boundary  $\Gamma_R$  but then naturally affects the whole mesh.

All the equations involved are solved in parallel by means of FreeFEM++ and PETSc (see [5, 6]), up to the non-standard equations (1.4) and (2.7) which involve the discretization of the Sobolev Broken Spaces and are then solved with an optimized sequential version in C++.

#### 4.1.1 Nitsche extended finite element method of a Ventcel transmission problem with discontinuities at the interface

For the sake of simplicity, in this part, we suppose  $T_D = 0$ . In the case of the convection-diffusion problem (2.3), we decompose  $a$  into  $a = b + c$  where

$$\begin{aligned} b(\mathbf{T}, \mathbf{S}) &:= \int_{\Omega_1 \cup \Omega_2} \kappa \nabla \mathbf{T} \cdot \nabla \mathbf{S} \, dx + \int_{\Omega_1} \mathbf{S} \mathbf{u} \cdot \nabla \mathbf{T} \, dx \\ &\quad + \int_{\Gamma_R} \alpha \mathbf{T} \mathbf{S} \, ds + \int_{\Gamma} \epsilon \kappa_m \nabla_\tau \langle \mathbf{T} \rangle \cdot \nabla_\tau \langle \mathbf{S} \rangle + \kappa_m H[\mathbf{T}] \langle \mathbf{S} \rangle \, ds, \\ c(\mathbf{T}, \mathbf{S}) &:= \frac{\kappa_m}{\epsilon} \int_{\Gamma} [\mathbf{T}][\mathbf{S}] \, ds. \end{aligned}$$

The term  $c(\mathbf{T}, \mathbf{S})$  produces poor conditioning when  $\epsilon$  is small. To deal with this, we consider the Nitsche approach previously used in [10] to stabilize our matrix with respect to  $\epsilon$ , improving the conditioning of the matrix. We first introduce some notations to briefly explain this method.

Let  $\mathcal{T}_h$  be a regular simplicial mesh of  $\Omega$  and let  $\mathcal{F}_h$  be the set of faces of  $\mathcal{T}_h$ ,  $\mathcal{F}_{h,\Gamma}$  the set of faces situated on  $\Gamma$  and  $\mathcal{T}_{h,\Gamma}$  the set of elements which have one face on  $\Gamma$ . Let  $h_F$  be the diameter of the face  $F \in \mathcal{F}_{h,\Gamma}$ . We consider the polynomial spaces

$$\mathbb{P}_h^1 := \{\mathbf{S}_h \in \mathcal{C}(\Omega_1 \cup \Omega_2); \mathbf{S}_h|_K \in \mathbb{P}^1, \forall K \in \mathcal{T}_h\} \quad \text{and} \quad \mathbb{P}_{h,0}^1 := \mathbb{P}_h^1 \cap \mathcal{H}_0.$$

Then, we define the following mesh-depending bilinear form, for any  $\mathbf{T}_h, \mathbf{S}_h \in \mathbb{P}_{h,0}^1$ ,

$$a_h(\mathbf{T}_h, \mathbf{S}_h) := a(\mathbf{T}_h, \mathbf{S}_h) - \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{\gamma \epsilon h_F}{\epsilon + \gamma \kappa_m h_F} \left( \left\langle \kappa \frac{\partial \mathbf{T}_h}{\partial \mathbf{n}} \right\rangle + \frac{\kappa_m}{\epsilon} [\mathbf{T}_h], \left\langle \kappa \frac{\partial \mathbf{S}_h}{\partial \mathbf{n}} \right\rangle + \frac{\kappa_m}{\epsilon} [\mathbf{S}_h] \right)_{L^2(F)}.$$

Hence

$$a_h(\mathbf{T}_h, \mathbf{S}_h) = b(\mathbf{T}_h, \mathbf{S}_h) + c_h(\mathbf{T}_h, \mathbf{S}_h),$$

with

$$\begin{aligned} c_h(\mathbf{T}_h, \mathbf{S}_h) &:= \sum_{F \in \mathcal{F}_{h,\Gamma}} \int_F \frac{\kappa_m}{\epsilon + \gamma \kappa_m h_F} [\mathbf{T}_h][\mathbf{S}_h] - \frac{\gamma \epsilon h_F}{\epsilon + \gamma \kappa_m h_F} \left\langle \kappa \frac{\partial \mathbf{T}_h}{\partial \mathbf{n}} \right\rangle \left\langle \kappa \frac{\partial \mathbf{S}_h}{\partial \mathbf{n}} \right\rangle \\ &\quad - \frac{\gamma \kappa_m h_F}{\epsilon + \gamma \kappa_m h_F} \left( \left\langle \kappa \frac{\partial \mathbf{T}_h}{\partial \mathbf{n}} \right\rangle [\mathbf{S}_h] + \left\langle \kappa \frac{\partial \mathbf{S}_h}{\partial \mathbf{n}} \right\rangle [\mathbf{T}_h] \right) \, ds, \end{aligned}$$

where  $\gamma > 0$  is a stabilization parameter, that it is small enough in order to guarantee the coercivity of  $a_h$ . Let us remark, that in the decomposition of the new bilinear form  $a_h$ , the bilinear form  $b$  continues to appear; what it changes is the bilinear form  $c_h$  instead of  $c$ , which associated matrix

has a better conditioning due to the stabilization. Then we consider the following Nitsche problem to approximate the equation (2.3) is

$$\begin{cases} \text{Find } \mathbb{T}_h \in \mathbb{P}_{h,0}^1 \text{ such that} \\ a_h(\mathbb{T}_h, \mathbb{S}_h) = l(\mathbb{S}_h), \quad \forall \mathbb{S}_h \in \mathbb{P}_{h,0}^1, \end{cases} \quad (4.1)$$

that estimates the continuous solution  $\mathbb{T}$  of the convection-diffusion equation (1.4) in the energy sense as it is stated in the next result (the proof is a mere adaptation of [10, Theorem 4.6]).

**Theorem 4.1** (Error estimate in energy norm). *Let  $\mathbb{T} \in \mathcal{H}_0 \cap (\mathbb{H}^2(\Omega_1, \Gamma) \times \mathbb{H}^2(\Omega_2, \Gamma))$  the solution of the continuous convection-diffusion equation (1.4) and  $\mathbb{T}_h$  the solution of the (discrete) Nitsche problem (4.1). For  $\gamma$  sufficiently small, there exists a constant  $C > 0$  independent of  $h$  and  $\epsilon$  such that:*

$$\|\|\mathbb{T} - \mathbb{T}_h\|\|_h \leq Ch \left( \|\kappa^{1/2} \mathbb{T}\|_{\mathbb{H}^2(\Omega_1 \cup \Omega_2)}^2 + \|(\kappa_m \epsilon)^{1/2} \langle \mathbb{T} \rangle\|_{\mathbb{H}^2(\Gamma)}^2 + \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{\kappa_m h_F}{\gamma} \|[\mathbb{T}]\|_{\mathbb{H}^2(F)}^2 \right)^{1/2}, \quad (4.2)$$

where  $\|\|\cdot\|\| := \left( \|\cdot\|_{\mathcal{H}_0} + \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{1}{\epsilon + \gamma h_F} \|[\cdot]\|_{L^2(F)}^2 \right)^{1/2}$  is a mesh-dependent norm on  $\mathbb{P}_h^1$ .

We proceed in a similar way concerning the adjoint equation (2.7). Let  $\mathbb{R}, \mathbb{S} \in \mathcal{H}_0$ . We denote

$$\begin{aligned} \tilde{b}(\mathbb{R}, \mathbb{S}) &:= \int_{\Omega_1 \cup \Omega_2} \kappa \nabla \mathbb{R} \cdot \nabla \mathbb{S} \, dx + \int_{\Omega_1} \mathbf{R} \mathbf{u} \cdot \nabla \mathbb{S} \, dx \\ &\quad + \int_{\Gamma_R} \alpha \mathbb{R} \mathbb{S} \, ds + \int_{\Gamma} \epsilon \kappa_m \nabla_{\tau} \langle \mathbb{R} \rangle \cdot \nabla_{\tau} \langle \mathbb{S} \rangle + \kappa_m H \langle \mathbb{R} \rangle [\mathbb{S}] \, ds, \\ \tilde{c}(\mathbb{R}, \mathbb{S}) &:= \int_{\Gamma} \frac{\kappa_m}{\epsilon} [\mathbb{R}][\mathbb{S}] \, ds \end{aligned}$$

in such a way that  $\tilde{a}(\mathbb{R}, \mathbb{S}) := \tilde{b}(\mathbb{R}, \mathbb{S}) + \tilde{c}(\mathbb{R}, \mathbb{S})$  is the bilinear form associated to the adjoint problem (2.7) with right-hand side  $\tilde{l}(\mathbb{S}) := \int_{\Gamma_N} 2\alpha^2 (\mathbb{T} - \mathbb{T}_0) \mathbb{S} \, ds$ . As previously, the matrix associated to the term  $\tilde{c}$  has poor conditioning. To stabilize it, we define

$$\begin{aligned} \tilde{a}_h(\mathbb{R}, \mathbb{S}) &:= \tilde{a}(\mathbb{R}, \mathbb{S}) \\ &\quad - \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{\gamma \epsilon h_F}{\epsilon + \gamma \kappa_m h_F} \left( \left\langle \kappa \frac{\partial \mathbb{R}}{\partial \mathbf{n}} \right\rangle + \frac{\kappa_m}{\epsilon} [\mathbb{R}] + \kappa_m H \langle \mathbb{R} \rangle, \left\langle \kappa \frac{\partial \mathbb{S}}{\partial \mathbf{n}} \right\rangle + \frac{\kappa_m}{\epsilon} [\mathbb{S}] + \kappa_m H \langle \mathbb{S} \rangle \right)_{L^2(F)}. \end{aligned}$$

Therefore, we obtain  $\tilde{a}_h(\mathbb{R}, \mathbb{S}) = \tilde{b}(\mathbb{R}, \mathbb{S}) + c_h(\mathbb{R}, \mathbb{S}) - d_h(\mathbb{R}, \mathbb{S})$ , where

$$\begin{aligned} d_h(\mathbb{R}, \mathbb{S}) &:= \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{\gamma \kappa_m \epsilon h_F}{\epsilon + \gamma \kappa_m h_F} \int_F H \langle \mathbb{S} \rangle \left( \left\langle \kappa \frac{\partial \mathbb{R}}{\partial \mathbf{n}} \right\rangle + \frac{\kappa_m}{\epsilon} [\mathbb{R}] \right) \\ &\quad + H \langle \mathbb{R} \rangle \left( \left\langle \kappa \frac{\partial \mathbb{S}}{\partial \mathbf{n}} \right\rangle + \frac{\kappa_m}{\epsilon} [\mathbb{S}] \right) + \kappa_m H^2 \langle \mathbb{R} \rangle \langle \mathbb{S} \rangle \, ds. \end{aligned}$$

Then the Nitsche problem considered to approximate the adjoint equation (2.7) is

$$\begin{cases} \text{Find } \mathbb{R}_h \in \mathbb{P}_{h,0}^1 \text{ such that} \\ \tilde{a}_h(\mathbb{R}_h, \mathbb{S}_h) = \tilde{l}(\mathbb{S}_h), \quad \forall \mathbb{S}_h \in \mathbb{P}_{h,0}^1. \end{cases} \quad (4.3)$$

The error estimation is similar to the one given in Theorem 4.1.

### 4.1.2 Implementation of the discrete Sobolev Broken space

Starting from  $\mathcal{T}_h$ , we have to truncate this mesh to get  $\mathcal{T}_h^1$  and  $\mathcal{T}_h^2$  (meshes of  $\Omega_1$  and  $\Omega_2$ ), creating a bijection between the vertices on  $\Gamma$  of both meshes, in order to discretize integrals on  $\Gamma$  like  $\int_{\Gamma} \mathbb{T}_1 \mathbb{T}_2 ds$ . Once we have that, we can assemble the matrix  $A_i$  associated to each domain independently without considering the integrals on  $\Gamma$  (discontinuous terms). Then, the matrix  $A$  has structure of matrix by blocks, that is

$$A = \begin{pmatrix} A_1 & B \\ C & A_2 \end{pmatrix},$$

where  $B, C$  are the matrix obtained from discretizing the integrals on  $\Gamma$ . In this way, we have to solve the system (without considering the Dirichlet boundary conditions),

$$\begin{pmatrix} A_1 & B \\ C & A_2 \end{pmatrix} \begin{pmatrix} \mathbb{T}_{h,1} \\ \mathbb{T}_{h,2} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}.$$

Figure 4 shows the sparsity of the matrix system. Notice that this block structure can be useful from a numerical point of view, for example to use an appropriate preconditioner. However, we have not yet investigated this for the moment.

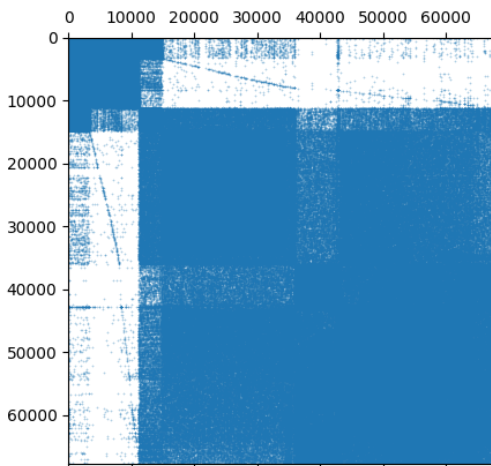


Figure 4: Stiffness matrix associated to the convection-diffusion equation (2.3) .

## 4.2 Optimization framework: level set and null space methods

In the context of shape optimization, the level set evolution method was introduced by Allaire *et al.* in [3]. The idea consists in considering a fixed domain  $D$  that contains  $\Omega$  and such that the fixed boundaries  $\Gamma_D$  and  $\Gamma_N$  belong to  $\partial D$ . In practice,  $D$  is a box. This allows to describe  $\Omega$  by means of a level set function  $\phi : D \rightarrow \mathbb{R}$  as follows

$$\begin{cases} x \in \Omega & \iff \phi(x) < 0 \\ x \in \Gamma_R & \iff \phi(x) = 0 \\ x \in D \setminus \bar{\Omega} & \iff \phi(x) > 0. \end{cases}$$

In particular this allows us to track the boundary  $\Gamma_R$  that we aim to optimize. Then, the mesh is done following the level set function, which implies that there is not cut element at the boundary  $\Gamma_R$ . After initialization, at the step  $n$  of the shape optimization process, we compute the level set  $\phi^n$  by solving the following equation,

$$\begin{cases} \frac{\partial \phi^n}{\partial t} + \boldsymbol{\theta} \cdot \nabla \phi^n = 0, & 0 < t < \tau, x \in D \\ \phi^n(0, x) = \phi^{n-1}(x), & x \in D, \end{cases} \quad (4.4)$$

for some  $\tau > 0$ , where  $\boldsymbol{\theta}$  is an appropriate velocity field. Numerically speaking, the equation (4.4) can be computed by ADVECT (see [9]) and the remeshing step by MMG (see [16]). Notice that in our case, we have two level set functions,  $\phi_1$  and  $\phi_2$  that describe  $\Omega_1$  and  $\Omega_2$ , respectively. Since  $\Omega_1$  is fixed, we will just have to update  $\phi_2$  for the remeshing.

The velocity field  $\boldsymbol{\theta}$  that we will use belongs to  $H^1(D)^d$ , such that  $\boldsymbol{\theta} = 0$  on  $\partial D$  and  $\boldsymbol{\theta} = 0$  in  $\bar{\Omega}_1$ . It is obtained by solving the following extension-regularization problem,

$$\int_D h^2 \nabla \boldsymbol{\theta} : \nabla \psi + \boldsymbol{\theta} \psi \, dx = \langle J'(\Gamma_R), \psi \rangle, \quad \forall \psi \in \{\psi \in H^1(D)^d; \psi = 0 \text{ on } \partial D \text{ and } \psi = 0 \text{ in } \bar{\Omega}_1\}.$$

It is important to remark, that by construction,  $\boldsymbol{\theta}$  is a descent direction.

Finally, as constrained optimization algorithm, we use the *null space algorithm* introduced in [20] under the implementation of Feppon [18]. This method first decreases the violation of the constraint in order to be feasible, then minimizes the objective function. It is particularly well suited when we start from shapes that does not satisfy the constraints and when numerous constraints are considered.

## 5 Numerical examples

We consider the thermal insulation in dimension three. We consider the inlet velocity  $\mathbf{u}_D$  as a parabolic profile with maximum speed at the  $\Gamma_D$  centered  $(0, y_c, z_c)$ , equal to 1: in other words,  $\mathbf{u}_D := ((r^2 - (y - y_c)^2 - (z - z_c)^2)/r^2, 0, 0)$ , where  $r$  is the radius of  $\Omega_1$  which is fixed to 0.1 in the simulations below. Moreover, we consider  $T_D \equiv 40$  and  $\epsilon = 1 \cdot 10^{-3}$  in the following examples, and except for the last example, we consider  $D = [0, 1] \times [0, 1] \times [0, 1]$ . Finally, except for the random outer temperature example of subsection 5.1.2, we take  $T_{\text{ext}} = 0$ . Let us conclude these preliminaries by highlighting two points.

- *On the Robin coefficient  $\alpha$ .* From [29], we know that for  $\alpha$  small (with respect to  $\kappa_2$ ), the functional decreases removing insulation material, meanwhile for  $\alpha$  large enough the functional decreases adding insulation material, that is more intuitive. Hence we will consider this latter case and we summarize the values of the parameters chosen in the following Table 1.

$\kappa_1$	$1.5 \cdot 10^{-7}$	$m^2 s^{-1}$
$\kappa_2$	$10^{-7}$	$m^2 s^{-1}$
$\kappa_m$	$1.1 \cdot 10^{-4}$	$m^2 s^{-1}$
$\alpha$	$2 \cdot 10^{-5}$	$m s^{-1}$
$\nu$	$10^{-2}$	$m^2 s^{-1}$

Table 1: Values of the parameters

- *On the no recirculation at the outlet assumption (2.2).* In the four following examples, we numerically check that the hypothesis  $\mathbf{u} \cdot \mathbf{n} \geq 0$  on  $\Gamma_N$  is well satisfied.

All the presented simulations were performed on a personal laptop with an AMD Ryzen 9 4900hs @3.0 GHz, with 40 GB RAM.

**Remark 5.1.** *We have previously assumed that  $T_D \in H_{00}^{1/2}(\Gamma_R)$  which is not the case here. However we chose a constant inlet temperature to simplify the simulations and the previous results can be adapted to this case.*

## 5.1 First example: cylinder case

The first example is the cylindric case. We have to mention the work [24] where it was showed, in another context close to our own, that a cylinder is not the optimal solution to minimize the fluid dissipation. We consider here a fixed cylinder  $\Omega_1$  of radius  $r = 0.1$ , of axis  $(Ox)$  and with  $(y_c, z_c) = (0.5, 0.5)$ . The target volume  $V_0$  is the difference between the volume of a cylinder of radius 0.2 and the volume of another cylinder of radius 0.1. It will be chosen similarly in the following examples (changing the cylinder by the respective considered pipes).

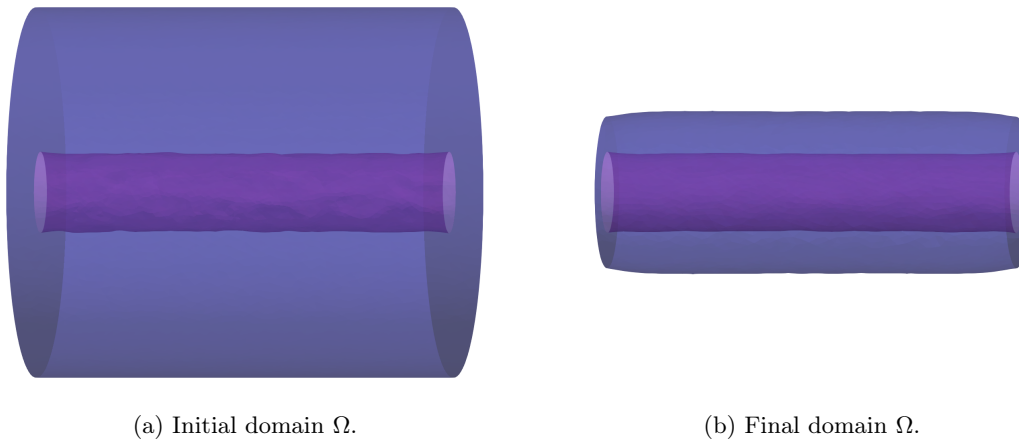


Figure 5: First example - initial and final domains in the deterministic case.

### 5.1.1 Deterministic case

The initial geometry is depicted on Figure 5a. The meshes considered vary from 160000 to 180000 vertices and 900000 to 1000000 tetrahedrons. The optimal design is shown in Figure 5b.

On the one hand, we observe that we do not obtain two concentric cylinders, similarly to what happens in the case of [24]: at the extremes there is less material which can be explained by the model we have chosen, in particular the boundary conditions chosen on this part. On the other hand, as expected, the objective functional  $J$  increases (see Figure 6) until the solution satisfies the volume constraint and then is optimize (it is well-known and natural that if the volume is larger the insulation is better).

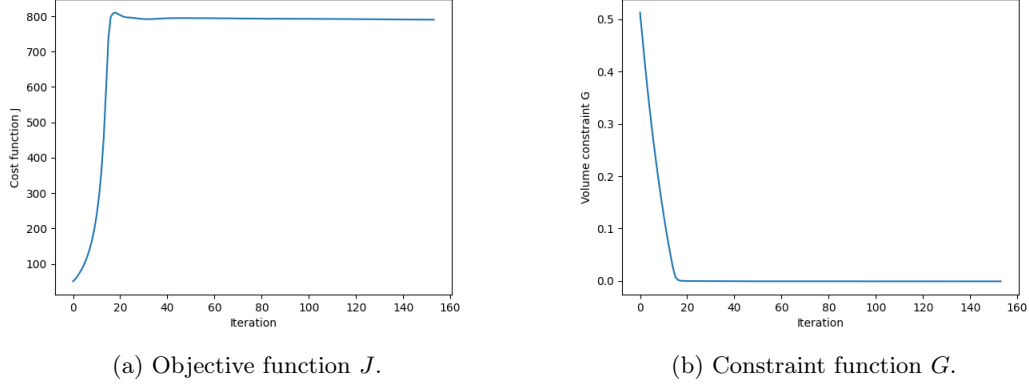


Figure 6: First example - convergence history in the deterministic case.

### 5.1.2 With random outside temperature

We now illustrate, on the previous example, the consideration of a random exterior temperature of the form (following the notations introduced in (2.10))

$$T_{\text{ext}} = T_{\text{ext}}^0 + \xi_1(\omega)T_{\text{ext}}^1(x, y, z) + \xi_2(\omega)T_{\text{ext}}^2(x, y, z),$$

where  $T_{\text{ext}}^0 = 0$ ,  $T_{\text{ext}}^1 = 20x$  and  $T_{\text{ext}}^2 = 10z$ , the random variables  $\xi_1, \xi_2$  are statistically independent, with zero expectation and variance  $\sigma_1^2 = \text{Var}(\xi_1) = 0.3$  and  $\sigma_2^2 = \text{Var}(\xi_2) = 0.7$ . Figure 7 summarizes the obtained result, which is very similar to the deterministic case 5. This can be explained as the deterministic component is the predominant in the formulas of Theorem 2.5 for the chosen values of the outside temperature, for two reasons, first, since the random part, is multiplied by the variance  $\sigma_i^2 < 1$ ,  $i = 1, 2$  and second, since the difference of the values between the outside temperature and inlet Dirichlet temperature is larger for the deterministic case (recall that there are three solutions of the temperature, the deterministic temperature has  $T^0 = 40$  on  $\Gamma_D$  and  $T_{\text{ext}}^0 = 0$  on  $\Gamma_R$  as data, meanwhile the random temperatures have  $T^1 = 0$  on  $\Gamma_D$ ,  $T_{\text{ext}}^1 = 20z$  on  $\Gamma_R$  and  $T^2 = 0$  on  $\Gamma_D$ ,  $T_{\text{ext}}^2 = 10x$  on  $\Gamma_R$ ). The convergence is depicted by Figure 8, where we can actually see that the gap between the deterministic and random case is small with respect to the values of  $J$ ; the insulation in the random case is slightly larger as expected since it has the random contribution.

## 5.2 Second example: perpendicular tubes

In this example,  $\Omega_1$  is a pipe of radius  $r = 0.1$  with two right-angled bends. The Dirichlet and Neumann boundaries are, respectively,

$$\begin{aligned} \Gamma_D &= \{(0., y, z) \in D; (y - 0.5)^2 + (z - 0.75)^2 = r^2\}, \\ \Gamma_N &= \{(1., y, z) \in D; (y - 0.5)^2 + (z - 0.25)^2 = r^2\}. \end{aligned}$$

The initial geometry is depicted on Figure 9a. The meshes considered vary from 75000 to 100000 vertices and 450000 to 615000 tetrahedrons.

The optimal design is shown in Figure 9b. Moreover, in Figure 10 are displayed the isosurfaces of the temperature at the beginning and the last iteration: we see that the initial temperature is lower on  $\Gamma_R$  than the final temperature, which is reasonable since there is more insulator in the



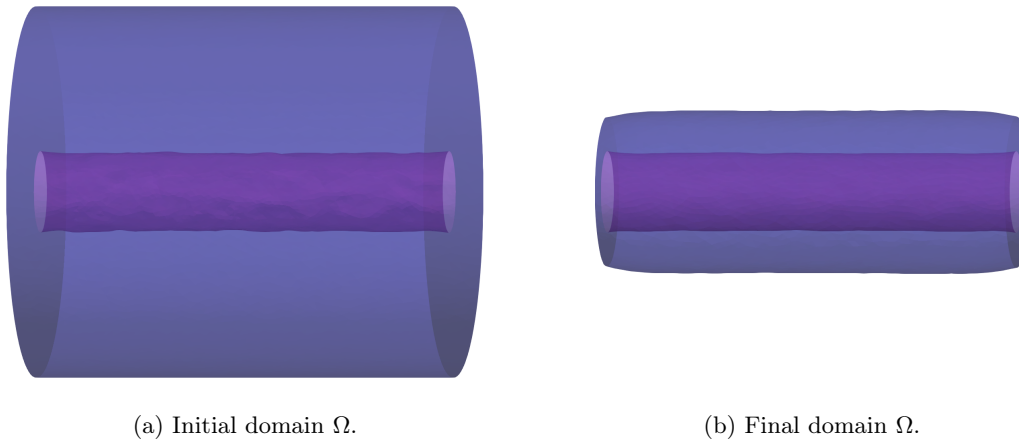


Figure 7: First example - initial and final domains with random temperature.

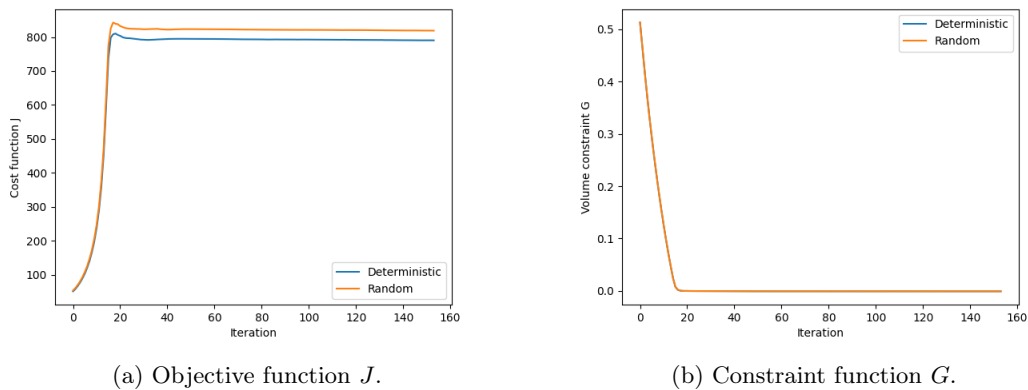


Figure 8: First example - convergence history with random temperature.

beginning (we do not satisfy the volume constraint). In the optimal domain, the solution satisfies the volume constraint and also keeps better the temperature inside the pipe: this is validated in Figure 11 that shows the convergence history which illustrates that in the first 20 iterations the algorithm tries to satisfy the constraint, decreasing the volume but increasing the objective function  $J$  until that the constraint is satisfied, and then the objective function decreases.

### 5.3 Third example: tubes with angle of inclination

As a third example, we consider a slight variation to the second one, now with an angle of inclination. In this example, the angle formed by the tube at the bottom and at the middle is of  $\frac{11}{6}\pi$ . The results are similar to the previous case as depicted in Figures 12 and 13.

### 5.4 Fourth example: Z pipe

We conclude these numerical experiments with a Z pipe geometry as  $\Omega_1$ . Here we consider  $D = [0, 2] \times [0, 1] \times [0, 1]$ . Figure 14 shows that as in the previous example, the material in the

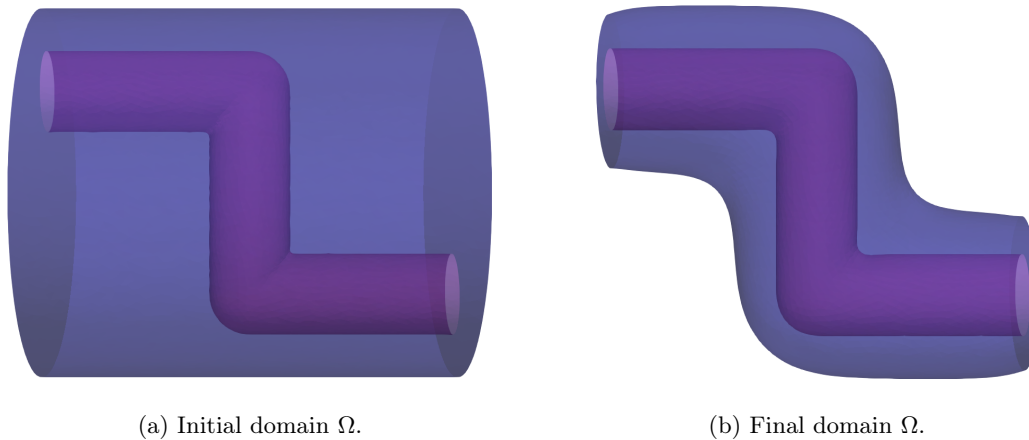


Figure 9: Second example - initial and final domains.

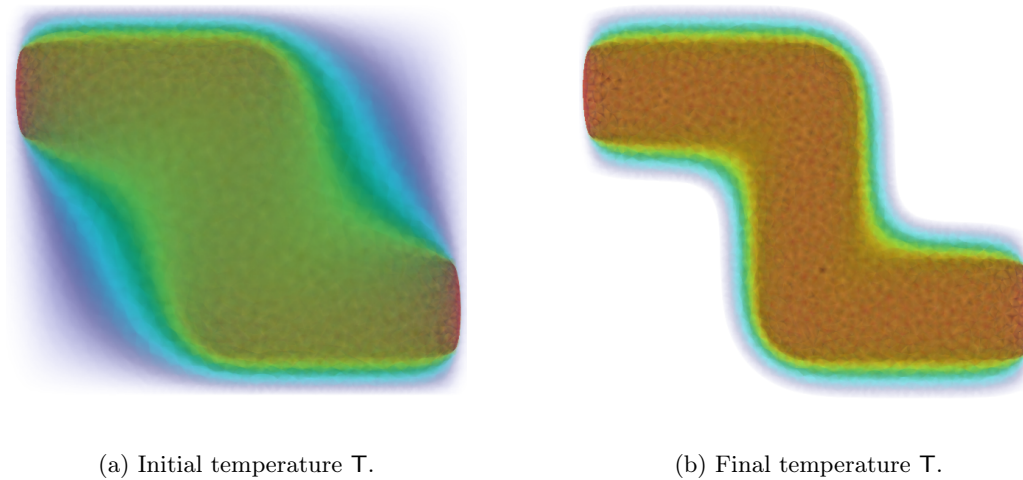


Figure 10: Second example - solution  $T$  in the initial and final domains (red means hotter, blue colder, white is almost zero).

zones far from the pipe is removed. Convergence history is depicted in 15, where we can notice that more iterations are needed to converge (nearly sixty iterations) due to the fact that the shape is larger (in the  $z$  axis).

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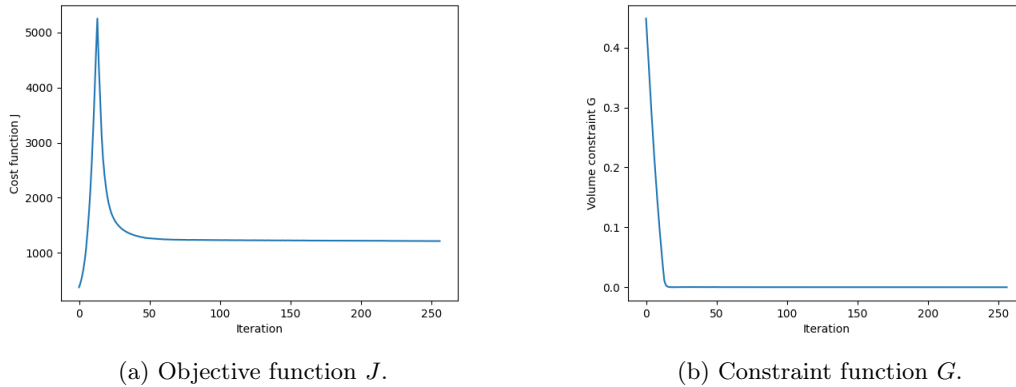


Figure 11: Second example - convergence history.

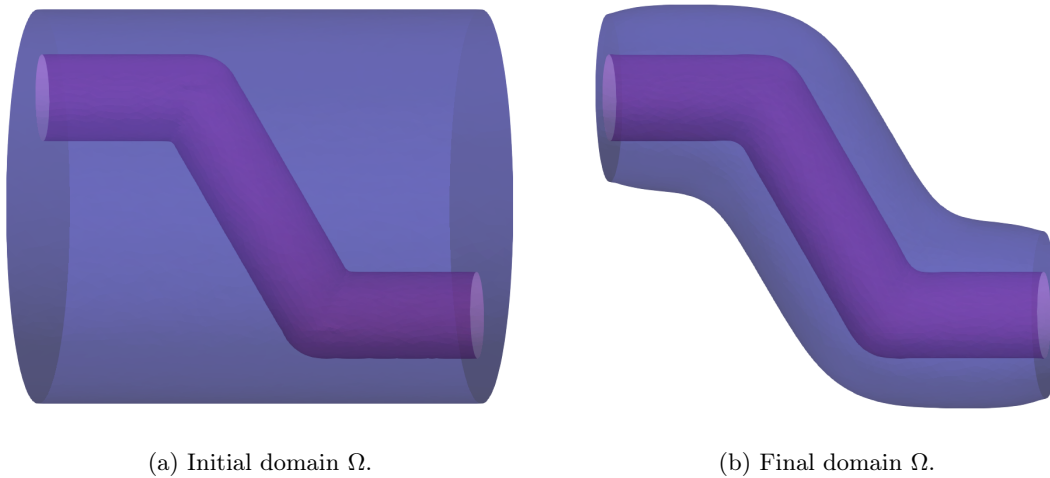


Figure 12: Third example - initial and final domains.

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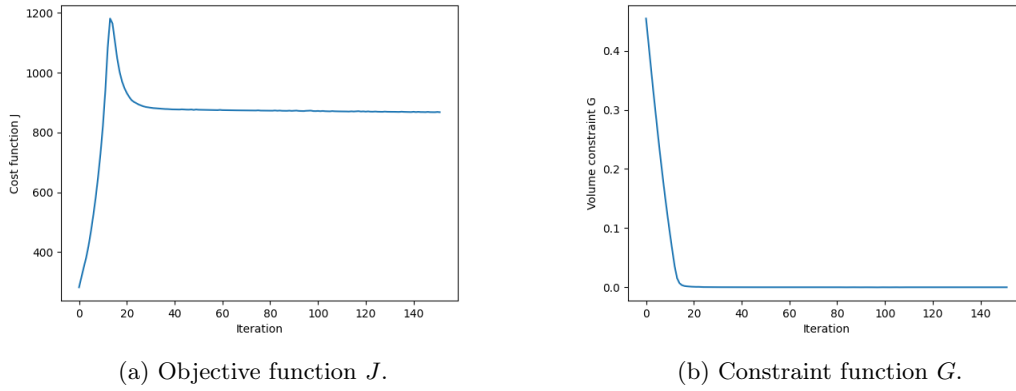


Figure 13: Third example - convergence history.

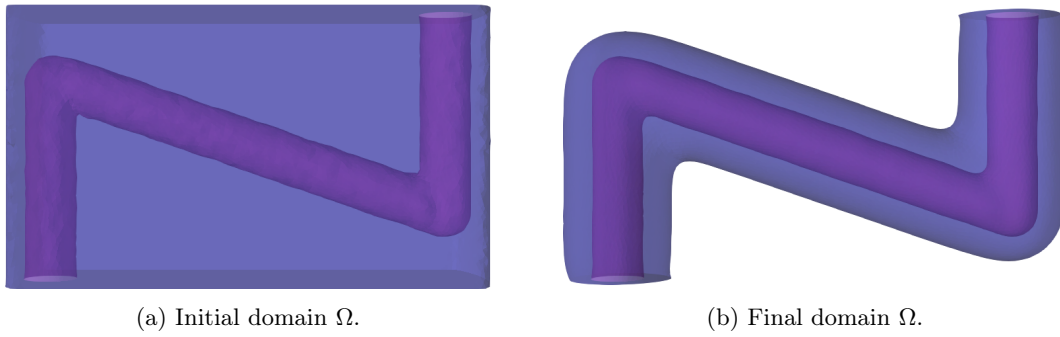


Figure 14: Fourth example - initial and final domains (with  $\pi/2$  rotation).

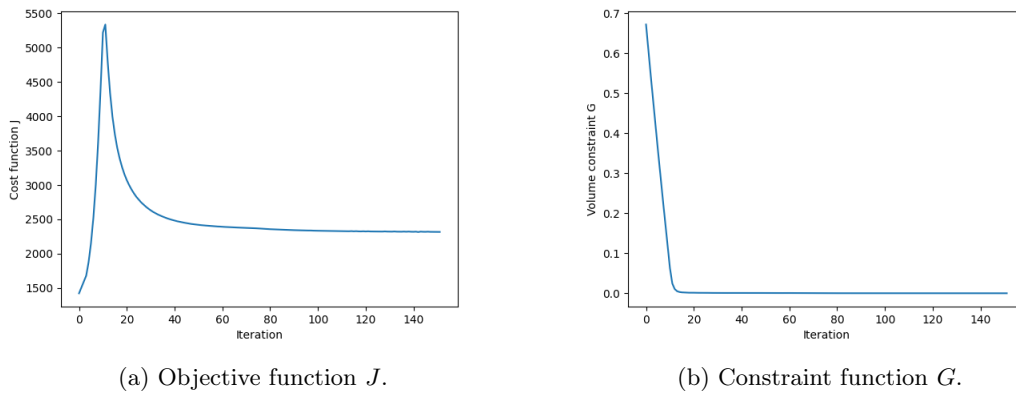


Figure 15: Fourth example - convergence history.

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## A Shape derivatives using a fully Lagrangian approach

In the present article, we focus on a specific objective functional  $J$  measuring the heart loss given in (1.5). In this appendix, we give some results in order to consider another objective functional which will imply to do some computations (the chain rule part) which can be annoying. In [19] was developed a framework to compute the shape derivatives of general functionals for a multi-physics problem, that requires only to compute again some partial derivatives.

We keep the same notation than before (see Section 2.2) and consider a general functional  $J$  that depends on  $\Omega_2$  and on the solution  $\mathbf{T}$  of the convection-diffusion problem (1.4). We first recall the concept of *transported functional* given in the following definition.

**Definition A.1.** *The transported functional of  $J$  is the functional  $\mathcal{J}$  such that for all  $\boldsymbol{\theta} \in \Theta_{\text{ad}}$  and all  $\hat{\mathbf{T}} \in H^1(\Omega_1, \Gamma) \times H^1(\Omega_2, \Gamma)$ ,*

$$\mathcal{J}(\boldsymbol{\theta}, \hat{\mathbf{T}}) := J(\Omega_2^\boldsymbol{\theta}, \hat{\mathbf{T}} \circ (\mathbf{I} + \boldsymbol{\theta})^{-1}),$$

where  $\Omega_2^\boldsymbol{\theta} = (\mathbf{I} + \boldsymbol{\theta})\Omega_2$ .

We suppose that  $J$  has continuous partial derivatives at  $(\boldsymbol{\theta}, \hat{\mathbf{T}}) = (0, \mathbf{T}(\Omega_2))$ . To keep notations as simple as possible, we will omit the evaluations of the partial derivatives at  $(\boldsymbol{\theta}, \hat{\mathbf{T}}) = (0, \mathbf{T}(\Omega_2))$ . We introduce the solution  $\mathbf{R} \in \mathcal{H}_0$  of the following adjoint problem

$$\left\{ \begin{array}{l} \text{Find } \mathbf{R} \in \mathcal{H}_0, \text{ such that, for all } \mathbf{S} \in \mathcal{H}_0, \\ \int_{\Omega_1 \cup \Omega_2} \kappa \nabla \mathbf{R} \cdot \nabla \mathbf{S} \, dx + \int_{\Omega_1} \mathbf{R} u \cdot \nabla \mathbf{S} \, dx + \int_{\Gamma_{\mathbf{R}}} \alpha \mathbf{R} \mathbf{S} \, ds \\ + \int_{\Gamma} \epsilon \kappa_m \nabla_\tau \langle \mathbf{R} \rangle \cdot \nabla_\tau \langle \mathbf{S} \rangle + \kappa_m H \langle \mathbf{R} \rangle [\mathbf{S}] + \epsilon^{-1} \kappa_m [\mathbf{R}] [\mathbf{S}] \, ds = \frac{\partial \mathcal{J}}{\partial \hat{\mathbf{T}}}(\mathbf{S}). \end{array} \right. \quad (\text{A.1})$$

**Remark A.2.** *In the particular case of the insulation functional (1.5),*

$$\frac{\partial \mathcal{J}}{\partial \hat{\mathbf{T}}}(\mathbf{S}) = \int_{\Gamma_{\mathbf{R}}} 2\alpha^2 (\mathbf{T}_2 - \mathbf{T}_0) \mathbf{S}_2 \, ds.$$

Then we can give a formula to compute the shape derivative general for any functional, requiring just to compute the partial derivative  $\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta})$ .

**Proposition A.3** (Volume shape derivative). *If  $\mathsf{T}_0 \in \mathsf{H}^2(\mathbb{R}^d)$  and  $J$  is differentiable with respect to the shape, then the volume shape derivative is given by*

$$J'(\Omega_2)(\boldsymbol{\theta}) = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) + \int_{\Omega_2} \kappa_2((\nabla \boldsymbol{\theta} + \nabla \boldsymbol{\theta}^t) \nabla \mathsf{T}_2) \cdot \nabla \mathsf{R}_2 - \operatorname{div}(\boldsymbol{\theta})(\kappa_2 \nabla \mathsf{T}_2 \cdot \nabla \mathsf{R}_2) \, dx \\ - \int_{\Gamma_{\mathsf{R}}} \operatorname{div}_{\tau}(\boldsymbol{\theta}) \alpha (\mathsf{T}_2 - \mathsf{T}_0) \mathsf{R}_2 - \alpha \nabla \mathsf{T}_0 \cdot \boldsymbol{\theta} \mathsf{R}_2 \, ds,$$

where  $\mathsf{T}$  solves the convection-diffusion equation (1.4) and  $\mathsf{R}$  solves the adjoint equation (A.1).

*Proof.* Let  $\dot{\mathsf{T}}$  the Lagrangian derivative of  $\mathsf{T}$  given in (3.1). We obtain the result by using the chain rule

$$J'(\Omega_2)(\boldsymbol{\theta}) = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) + \frac{\partial \mathcal{J}}{\partial \mathsf{T}}(\dot{\mathsf{T}})$$

and then proceeding as in the proof of 2.4.  $\square$

**Remark A.4.** *In the particular case of the insulation functional (1.5),*

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = \int_{\Gamma_{\mathsf{R}}} \operatorname{div}_{\tau}(\boldsymbol{\theta}) \alpha^2 (\mathsf{T}_2 - \mathsf{T}_0)^2 - 2\alpha^2 (\mathsf{T}_2 - \mathsf{T}_0) (\nabla \mathsf{T}_0 \cdot \boldsymbol{\theta}) \, ds.$$

We can also get a surface expression, which is an integral over the free boundary, that in this case is  $\Gamma_{\mathsf{R}}$ , and depending only on the normal component of the perturbation field. The result is obtained by integrating by parts the previous formula and using the structure theorem.

**Proposition A.5** (Surface shape derivative). *If  $\mathsf{T}_0 \in \mathsf{H}^2(\mathbb{R}^d)$ ,  $J$  is differentiable with respect to the shape, and  $\mathsf{T}_2, \mathsf{R}_2 \in \mathsf{H}^2(\Omega_2)$ , then the shape derivative is given by*

$$J'(\Omega_2)(\boldsymbol{\theta}) = \frac{\partial \overline{\mathcal{J}}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) + \int_{\Gamma_{\mathsf{R}}} \left( \kappa_2 \frac{\partial \mathsf{T}_2}{\partial \mathbf{n}} \frac{\partial \mathsf{R}_2}{\partial \mathbf{n}} - \kappa_2 \nabla_{\tau} \mathsf{T}_2 \cdot \nabla_{\tau} \mathsf{R}_2 - H \alpha (\mathsf{T}_2 - \mathsf{T}_0) \mathsf{R}_2 + \alpha \frac{\partial \mathsf{T}_0}{\partial \mathbf{n}} \mathsf{R}_2 \right) (\boldsymbol{\theta} \cdot \mathbf{n}) \, ds, \quad (\text{A.2})$$

where  $\frac{\partial \overline{\mathcal{J}}}{\partial \boldsymbol{\theta}}$  is the part of  $\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}$  that depends only on  $\boldsymbol{\theta} \cdot \mathbf{n}$ .

**Remark A.6.** *In the particular case of the insulation functional (1.5),*

$$\frac{\partial \overline{\mathcal{J}}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = \int_{\Gamma_{\mathsf{R}}} \left( H \alpha^2 (\mathsf{T}_2 - \mathsf{T}_0)^2 - 2\alpha^2 (\mathsf{T}_2 - \mathsf{T}_0) \frac{\partial \mathsf{T}_0}{\partial \mathbf{n}} \right) (\boldsymbol{\theta} \cdot \mathbf{n}) \, ds.$$

Indeed, changing variables in  $\Omega_2^{\boldsymbol{\theta}} = (I + \boldsymbol{\theta})\Omega_2$  (analogous to the proof of Proposition 2.3), we obtain

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = \int_{\Gamma_{\mathsf{R}}} \operatorname{div}_{\tau}(\boldsymbol{\theta}) \alpha^2 (\mathsf{T}_2 - \mathsf{T}_0)^2 - 2\alpha^2 (\mathsf{T}_2 - \mathsf{T}_0) (\nabla \mathsf{T}_0 \cdot \boldsymbol{\theta}) \, ds.$$

We conclude by integrating by parts and taking the normal component.