Shape optimization with Ventcel transmission condition: application to the design of a heat exchanger

Fabien Caubet[*], Carlos Conca[†], Marc Dambrine[‡], Rodrigo Zelada[§]

April 14, 2025

Abstract

This paper aims to optimize the shape of a fluid-to-fluid heat exchanger in order to maximize heat exchange under constraints of energy dissipation and volume. The novelty consists in taking into account the thin layer separating the two fluids by using Ventcel-type second-order transmission conditions. The physical model is then a weakly coupled problem between the steady-state Navier-Stokes equations for the dynamics of the two fluids dynamics and the convection-diffusion equation for the heat. We provide a shape sensitivity analysis and characterize the shape derivatives involved. Finally, we demonstrate the feasibility and effectiveness of the proposed method through 3D numerical simulations.

Keywords: Shape optimization; Fluid-to-fluid heat exchanger; Ventcel transmission conditions; Navier-Stokes equations; Heat equation.

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

1 Introduction

Shape optimization is a valuable tool in industrial contexts, with applications ranging from design to production. The problems considered frequently involve multiphysics and complex geometries, which can present significant challenges. Numerical resolution of these problems can be costly and limit the application of shape optimization. Consequently, reducing the cost of optimization is paramount, and one approach is to consider asymptotic models that take into account small physical or geometric parameters.

This work represents a progress in this direction: it consists in optimizing the geometry of a tube in a heat exchanger, taking advantage of the property that the wall separating a heat transfer fluid from a fluid to be heated is thin. The flow of two coupled fluids with different temperatures must also be considered. To this end, we will employ an approximate model derived from asymptotic analysis with respect to the small parameter represented by this thickness.

One of the original features of this work lies in the optimization of a surface where the quantity of interest, the temperature, is discontinuous. Non-standard transmission conditions are satisfied on this surface at the end of the asymptotic analysis. This problem is original and poses significant technical challenges, particularly in justifying the sensitivity analysis and implementing an optimization method.

[*]Université de Pau et des Pays de l'Adour, E2S UPPA, CNRS, LMAP, UMR 5142, 64000 Pau, France. fabien.caubet@univ-pau.fr

[†]cconca@dim.uchile.cl

[‡]marc.dambrine@univ-pau.fr

[§]rodrigo.zelada-mancini@univ-pau.fr

Our contributions are twofold: first, a theoretical sensitivity analysis in relation to the transmission surface, and second, a numerical analysis with the implementation of a method of optimization of this surface that is both efficient and robust in relation to this small parameter.

Organisation of the paper. The paper is organised as follows. Section 2 is devoted to the introduction of the model problem, the optimization problem we focus on and the functional framework. In Section 3, the shape sensitivity is performed: we prove the existence of the shape derivatives and compute them to obtain an expression that can be used to perform numerical simulations. In Section 4, we recall the classical numerical methods required for the shape optimization algorithm and we discuss the numerical difficulties in solving the problem under consideration. Finally, in Section 5, we perform 3D numerical simulations that highlight the efficiency of the proposed method.

2 Formulation of the optimal heat exchanger design approximated problem

2.1 Problem setting

A heat exchanger between two liquids is a system where two-fluids, one a heat transfer fluid and the other to be heated, are separated by a solid wall. This solid wall is often very thin compared to the size of the system. How to theoretically and numerically address the influence of this solid interface is a major challenge both for formulating the model as a shape optimization problem and for its subsequent solution. In this paper, we propose to address this difficulty using second-order Ventcel-type transmission conditions (see [11] concerning the zero-order approximation, and see [10] concerning a heat insulation problem). Accordingly, we will work with a domain composed of two-fluids, where the effect of the solid part appears in the transmission conditions at the interface.

The geometric setting. Let Ω be an open bounded connected domain of $\mathbb{R}^d$ ($d = 2, 3$), divided into two open bounded subdomains Ω_1, Ω_2 which are separated by an interface $\Gamma = \partial\Omega_1 \cap \partial\Omega_2$ that we assume to have non-zero measure in $\mathbb{R}^{d-1}$ and to be $\mathcal{C}^1$. On part of the boundary of each subdomain Ω_i, $i = 1, 2$, Dirichlet and Neumann boundary conditions are imposed, on $\Gamma_{\mathrm{D},i}$ and $\Gamma_{\mathrm{N},i}$ respectively, which in fact correspond to the inlet and outlet of each fluid. We also assume that the inlets are well separated: $\Gamma_{\mathrm{D},1} \cap \Gamma_{\mathrm{D},2} = \emptyset$. The complementary of the boundary of each subdomain is an exterior wall denoted $\Gamma_{\mathrm{e},i}$, and we thus have $\partial\Omega_i = \Gamma_{\mathrm{D},i} \cup \Gamma \cup \Gamma_{\mathrm{N},i} \cup \Gamma_{\mathrm{e},i}$. Moreover, we assume that $\partial\Gamma \subset \partial\Omega$. Finally, we assume that the pipe containing the hot fluid exits the heat exchanger orthogonally to it so that the tangential plane to $\Gamma_{\mathrm{e},2}$ is orthogonal to the tangential plane to Γ on $\partial\Gamma$. Figure 1 illustrates our configuration.

The physical models. We consider a weak coupling by neglecting the influence of temperature on the flow and the fluid expansion. On the one hand, the motion of the fluids is described by the incompressible Navier-Stokes equations. On the other hand, the temperature field is modeled by the convection-diffusion equation. This simplified model is already used in the literature, for example in the work of Feppon *et al.* [16].

Concerning the fluids, we denote by $\boldsymbol{u}_i$ the velocity and p_i the pressure in the domain Ω_i, $i = 1, 2$. Let $\nu_i, \rho_i > 0$ be the kinematic viscosity and the mass density, respectively, that for the sake of simplicity, we consider constants. The boundary $\Gamma_{\mathrm{D},i}$ represents the inlet of the fluid, so a given inlet velocity $\boldsymbol{u}_{\mathrm{D},i}$ is given there. On the outlet boundary $\Gamma_{\mathrm{N},i}$, a homogeneous Neumann

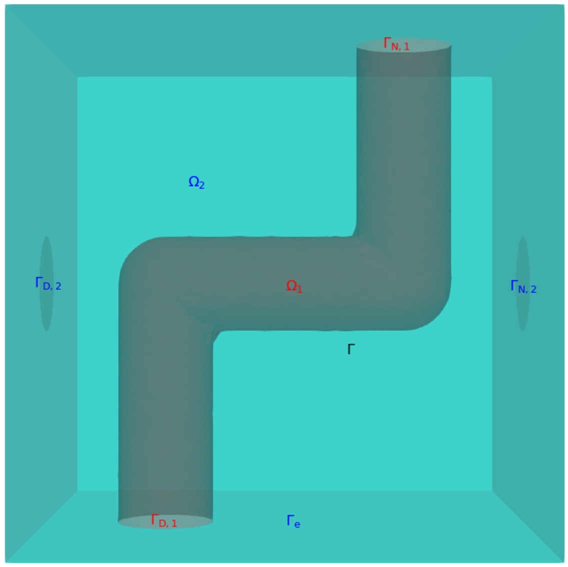


Figure 1: The configuration of the 3D heat exchanger problem where $\Gamma_{\mathrm{e}} = \Gamma_{\mathrm{e},2}$, $\Gamma_{\mathrm{e},1} = \emptyset$.

boundary condition is imposed. Furthermore, Γ and $\Gamma_{\mathrm{e},i}$ are respectively the wall between the fluids and the exterior walls and a non-slip boundary condition is therefore imposed on these boundaries. To summarize, for each $i = 1, 2$, the fluid flow is described by the following equations:

$$\begin{cases} -\nu_i \Delta \boldsymbol{u}_i + (\nabla \boldsymbol{u}_i)\boldsymbol{u}_i + \dfrac{1}{\rho_i}\nabla p_i &= 0 \qquad \text{in } \Omega_i, \\ \operatorname{div}(\boldsymbol{u}_i) &= 0 \qquad \text{in } \Omega_i, \\ \boldsymbol{u}_i &= \boldsymbol{u}_{\mathrm{D},i} \quad \text{on } \Gamma_{\mathrm{D},i}, \\ \sigma(\boldsymbol{u}_i, p_i)\boldsymbol{n} &= 0 \qquad \text{on } \Gamma_{\mathrm{N},i}, \\ \boldsymbol{u}_i &= 0 \qquad \text{on } \Gamma \cup \Gamma_{\mathrm{e},i}, \end{cases} \tag{2.1}$$

where $\boldsymbol{u}_{\mathrm{D},i} \in \mathrm{H}^{1/2}_{00}(\Gamma_{\mathrm{D},i})^d = \{\boldsymbol{v}|_{\Gamma_{\mathrm{D},i}}, \boldsymbol{v} \in \mathrm{H}^1(\Omega_i)^d, \boldsymbol{v}|_{\partial\Omega_i \setminus \overline{\Gamma_{\mathrm{D},i}}} = 0\}$ are the velocities of the fluids at the inlet, where $\boldsymbol{n}$ denotes the exterior unit normal, and where $\sigma(\boldsymbol{u}, p)$ is the fluid stress tensor defined by

$$\sigma(\boldsymbol{u}, p) = 2\nu\varepsilon(\boldsymbol{u}) - \frac{p}{\rho}\mathrm{I},$$

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

In the sequel, for a piece-wise smooth function ϕ defined on Ω, we denote by $\phi_i = \phi|_{\Omega_i}$ its restriction to Ω_i, and we define the jump and mean of ϕ at the interface Γ by $[\cdot]$ and $\langle\cdot\rangle$, respectively, as follows:

$$[\phi] = \phi_1 - \phi_2 \qquad \text{and} \qquad \langle\phi\rangle = \frac{\phi_1 + \phi_2}{2}.$$

Then, in terms of temperature, which we denote as T, a given temperature is imposed at the entry of the fluids and a homogeneous Neumann boundary condition at the outlet, meanwhile at the interface there is an effective transmission condition associated to the solid. Then, the associated thermal diffusivity κ_1, κ_2 and κ_s (κ_s is the thermal diffusivity of the solid) are assumed to be constant positive numbers. After asymptotic analysis when the thickness $\eta > 0$ of the solid wall separating the fluids tends to 0, we obtain the following asymptotic model to order 1 in η:

$$\begin{cases} -\operatorname{div}(\kappa_i \nabla \mathsf{T}_i) + \boldsymbol{u}_i \cdot \nabla \mathsf{T}_i &= 0 & \text{in } \Omega_i, i = 1, 2, \\ \mathsf{T}_i &= \mathsf{T}_{\mathrm{D},i} & \text{on } \Gamma_{\mathrm{D},i}, i = 1, 2, \\ \kappa_i \dfrac{\partial \mathsf{T}_i}{\partial \boldsymbol{n}} &= 0 & \text{on } \Gamma_{\mathrm{N},i} \cup \Gamma_{\mathrm{e},i}, i = 1, 2, \\ \left\langle \kappa \dfrac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right\rangle &= -\dfrac{\kappa_s}{\eta} [\mathsf{T}] & \text{on } \Gamma, \\ \left[\kappa \dfrac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right] &= \eta \operatorname{div}_\tau(\kappa_s \nabla_\tau \langle \mathsf{T} \rangle) - \kappa_s H[\mathsf{T}] & \text{on } \Gamma, , \\ \kappa_i \dfrac{\partial \mathsf{T}_i}{\partial \boldsymbol{n}} &= 0 & \text{on } \partial\Gamma, i = 1, 2, \end{cases} \tag{2.2}$$

where $\mathsf{T}_{\mathrm{D},i} \in \mathrm{H}^{1/2}(\Gamma_{\mathrm{D},i})$ are the given input temperatures and where $\boldsymbol{u}_i$ is the solution of the Navier-Stokes equations (2.1). Here, H denotes the mean curvature of Γ, div_τ is the tangential divergence and ∇_τ is the tangential gradient. Here and in the following, $\boldsymbol{n}$ is the unit normal to Γ exterior to Ω_1, that is, $\boldsymbol{n} = \boldsymbol{n}_1 = -\boldsymbol{n}_2$.

The shape optimization problem. We want to optimize the shape of the pipe connecting the inlet to the outlet of Ω_1 in order to maximize the heat exchanged between the fluids under two constraints: firstly, the volume of the pipe is prescribed, and secondly, the pressure drop seen from the angle of the energy dissipated by the fluid must remain below a prescribed threshold. To work with a minimization problem, we define the negative heat exchanged W as

$$W(\Gamma) = \int_{\Omega_1} \boldsymbol{u}_1 \cdot \nabla \mathsf{T}_1 \,\mathrm{d}x - \int_{\Omega_2} \boldsymbol{u}_2 \cdot \nabla \mathsf{T}_2 \,\mathrm{d}x, \tag{2.3}$$

where $\boldsymbol{u}_i$ and T_i, $i = 1, 2$, denote the respective solutions of the above problems (2.1) and (2.2). We consider three constraints: firstly the energy dissipation D_i, with a given threshold $D_{0,i} > 0$ in the fluid labelled by i, defined as

$$D_i(\Gamma) = \int_{\Omega_i} 2\nu_i |\varepsilon(\boldsymbol{u}_i)|^2 \,\mathrm{d}x - D_{0,i}, \qquad i = 1, 2, \tag{2.4}$$

and secondly the gap between the volume occupied by the hot fluid and a target volume $V_0 > 0$ given by

$$V(\Gamma) = \int_{\Omega_1} 1 \,\mathrm{d}x - V_0. \tag{2.5}$$

The problem that we will consider in this article is the following:

$$\inf_\Gamma W(\Gamma) \quad \text{such that} \quad D_i(\Gamma) \le 0,\ i = 1, 2, \quad \text{and} \quad V(\Gamma) = 0. \tag{2.6}$$

2.2 Functional setting

To keep the notation as light as possible, we define

$$\Gamma_{\mathrm{D}} = \Gamma_{\mathrm{D},1} \cup \Gamma_{\mathrm{D},2} \qquad \text{and} \qquad \mathsf{T}_{\mathrm{D}} = \mathsf{T}_{\mathrm{D},1} \mathbb{1}_{\Gamma_{\mathrm{D},1}} + \mathsf{T}_{\mathrm{D},2} \mathbb{1}_{\Gamma_{\mathrm{D},2}},$$

where $\mathbb{1}$ denotes the indicator function. We consider the following affine spaces associated to the non-homogeneous Dirichlet boundary data $\boldsymbol{u}_{\mathrm{D},i} \in \mathrm{H}^{1/2}_{00}(\Gamma_{\mathrm{D},i})^d$ and $\mathsf{T}_{\mathrm{D},i} \in \mathrm{H}^{1/2}(\Gamma_{\mathrm{D},i})$:

$$\mathcal{V}_{\boldsymbol{u}_{\mathrm{D},i}}(\Omega_i) = \{\boldsymbol{w} \in \mathrm{H}^1(\Omega_i)^d; \quad \boldsymbol{w} = \boldsymbol{u}_{\mathrm{D},i} \text{ on } \Gamma_{\mathrm{D},i} \text{ and } \boldsymbol{w} = 0 \text{ on } \Gamma \cup \Gamma_{\mathrm{e},i}\},$$

and

$$\mathcal{H}_{\mathsf{T}_\mathrm{D}}(\Omega_1,\Omega_2) = \{\phi = (\phi_1,\phi_2) \in \mathcal{H}^1(\Omega_1,\Omega_2);\ \phi = \mathsf{T}_\mathrm{D} \text{ on } \Gamma_\mathrm{D}\},$$

where

$$\mathcal{H}^k(\Omega_1,\Omega_2) = \{\phi = (\phi_1,\phi_2) \in \mathrm{H}^k(\Omega_1)\times \mathrm{H}^k(\Omega_2);\ \langle\phi\rangle \in \mathrm{H}^k(\Gamma)\},\quad k\in\mathbb{N}^*.$$

The spaces $\mathcal{V}_0(\Omega_i)$ and $\mathcal{H}_0(\Omega_1,\Omega_2)$ are Hilbert spaces when they are equipped with the respective norms $\|\boldsymbol{w}\|_{\mathcal{V}_0(\Omega_i)} = \|\boldsymbol{w}\|_{\mathrm{H}^1(\Omega_i)^d}$ and

$$\|\phi\|_{\mathcal{H}_0(\Omega_1,\Omega_2)} = \left(\sum_{i=1}^2 \|\nabla\phi_i\|^2_{\mathrm{L}^2(\Omega_i)^d} + \|\nabla_\tau\langle\phi\rangle\|^2_{\mathrm{L}^2(\Gamma)^d} + \|[\phi]\|^2_{\mathrm{L}^2(\Gamma)}\right)^{1/2}.$$

The space $\mathcal{H}_0(\Omega_1,\Omega_2)$ is sometimes called broken Sobolev space. In the following, we also denote

$$\mathrm{H}^k(\Omega_i,\Gamma) = \{\phi\in\mathrm{H}^k(\Omega_i);\ \phi|_\Gamma \in \mathrm{H}^k(\Gamma)\},\quad k\in\mathbb{N}^*.$$

Remark 2.1. *Note that the norm $\|\cdot\|_{\mathcal{H}_0(\Omega_1,\Omega_2)}$ is equivalent to the norm*

$$\|\cdot\|_{\mathcal{H}^1(\Omega_1,\Omega_2)} = \left(\sum_{i=1}^2 \|\nabla\cdot\|^2_{\mathrm{L}^2(\Omega_i)^d} + \|\nabla_\tau\langle\cdot\rangle\|^2_{\mathrm{L}^2(\Gamma)^d}\right)^{1/2},$$

in $\mathcal{H}_0(\Omega_1,\Omega_2)$, thanks to trace and Poincare's inequalities.

Firstly, the Navier-Stokes equations (2.1) have the following variational formulation:

$$\begin{gathered}\textit{Find } (\boldsymbol{u}_i,p_i)\in\mathcal{V}_{\boldsymbol{u}_{\mathrm{D},i}}(\Omega_i)\times\mathrm{L}^2(\Omega_i) \textit{ such that for all } (\boldsymbol{w},r)\in\mathcal{V}_0(\Omega_i)\times\mathrm{L}^2(\Omega_i),\\ \int_{\Omega_i}\left(2\nu_i\varepsilon(\boldsymbol{u}_i):\varepsilon(\boldsymbol{w}) + (\nabla\boldsymbol{u}_i)\boldsymbol{u}_i\cdot\boldsymbol{w} - \frac{p_i}{\rho_i}\operatorname{div}(\boldsymbol{w}) - \frac{r}{\rho_i}\operatorname{div}(\boldsymbol{u}_i)\right)\mathrm{d}x = 0.\end{gathered}\tag{2.7}$$

If the viscosity ν_i is large enough, this problem is well-posed, this is, there exists a unique weak solution $(\boldsymbol{u}_i,p_i)\in\mathcal{V}_{\boldsymbol{u}_{\mathrm{D},i}}(\Omega_i)\times\mathrm{L}^2(\Omega_i)$ (see for example [26] for details). As we are interested in questions of optimal design rather than the existence of solutions to this type of problem, we place ourselves in this context and assume that we have a unique solution to these Navier-Stokes equations.

Secondly, for the temperature, the corresponding variational formulation of the approximated convection-diffusion equation (2.2) is given by:

$$\begin{gathered}\textit{Find } \mathsf{T}=(\mathsf{T}_1,\mathsf{T}_2)\in\mathcal{H}_{\mathsf{T}_\mathrm{D}}(\Omega_1,\Omega_2) \textit{ such that for all } \phi=(\phi_1,\phi_2)\in\mathcal{H}_0(\Omega_1,\Omega_2),\\ \sum_{i=1}^2\int_{\Omega_i}(\kappa_i\nabla\mathsf{T}_i\cdot\nabla\phi_i + \boldsymbol{u}_i\cdot\nabla\mathsf{T}_i\phi_i)\,\mathrm{d}x + \int_\Gamma\left(\eta\kappa_\mathrm{s}\nabla_\tau\langle\mathsf{T}\rangle\cdot\nabla_\tau\langle\phi\rangle + \kappa_\mathrm{s}H[\mathsf{T}]\langle\phi\rangle + \frac{\kappa_\mathrm{s}}{\eta}[\mathsf{T}][\phi]\right)\mathrm{d}s = 0.\end{gathered}\tag{2.8}$$

This problem is non-standard. Its well-posedness was proved in our previous work [10, Theorem 2.1] under the following additional hypothesis: the fluids leave the domain at the outlet:

$$\boldsymbol{u}_i\cdot\boldsymbol{n}\geq 0 \text{ on } \Gamma_{\mathrm{N},i},\ i=1,2.\tag{2.9}$$

Remark 2.2. *The assumption $\boldsymbol{u}_{\mathrm{D},i}\in\mathrm{H}^{1/2}_{00}(\Gamma_{\mathrm{D},i})^d$ permits to ensure that the Dirichlet data belongs to $\mathrm{H}^{1/2}(\Gamma_{\mathrm{D},i}\cup\Gamma)^d$ since we have $\boldsymbol{u}_i = 0$ on Γ and $\boldsymbol{u}_i=\boldsymbol{u}_{\mathrm{D},i}$ on $\Gamma_{\mathrm{D},i}$. Notice that, in particular, $\overline{\Gamma}\cap\overline{\Gamma}_{\mathrm{D},1}\neq\emptyset$.*

Remark 2.3. *Let us emphasize a point regarding the way to derive the previous variational formulation. Let* T *the strong solution of* (2.2) *that we suppose* $\mathcal{H}^2(\Omega_1, \Omega_2)$ *and* $\phi \in \mathcal{H}_0(\Omega_1, \Omega_2)$. *Using Green's formula on* Γ, *we get:*

$$\int_\Gamma -(\Delta_\tau \langle \mathsf{T} \rangle) \langle \phi \rangle \; \mathrm{d}s = \int_\Gamma \nabla_\tau \langle \mathsf{T} \rangle \cdot \langle \phi \rangle \; \mathrm{d}s - \int_{\partial\Gamma} \langle \phi \rangle \nabla_\tau \langle \mathsf{T} \rangle \cdot \bar{\boldsymbol{\tau}} \mathrm{d}l,$$

where $\bar{\boldsymbol{\tau}}$ *is the unit tangent vector to* Γ *normal to* $\partial\Gamma$, *and* $\mathrm{d}l$ *is the* $(d-2)$ *dimensional measure along* $\partial\Gamma$. *In our situation,* $\bar{\boldsymbol{\tau}}$ *corresponds to the normal to* Γ_{D} *on* $\overline{\Gamma} \cap \overline{\Gamma_{\mathrm{D}}}$ *and the normal to* Γ_{N} *on* $\overline{\Gamma} \cap \overline{\Gamma_{\mathrm{N}}}$. *Then*

$$\int_{\partial\Gamma} \langle \phi \rangle \nabla_\tau \langle \mathsf{T} \rangle \cdot \bar{\boldsymbol{\tau}} \mathrm{d}l = 0$$

since $\nabla_\tau \langle \mathsf{T} \rangle \cdot \bar{\boldsymbol{\tau}} = \frac{\partial \langle \mathsf{T} \rangle}{\partial \boldsymbol{n}} = \left\langle \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right\rangle$ *and since* $\frac{\partial \mathsf{T}_i}{\partial \boldsymbol{n}} = 0$ *on* $\partial\Gamma$, $i = 1, 2$.

3 Shape sensitivity analysis

We perform a shape sensitivity analysis relying on boundary variations. One novelty in our work is the computation of the shape derivative of the non-standard equation (2.2) dealing with the temperature field. The difficulty comes from the fact that these surface derivatives are involved in a jump condition on an interface and are coupled with coefficient discontinuities. Since [1], we know that in the case of sensitivity with respect to a conductivity discontinuity interface, only the material derivative (not the shape derivative) exists in the variational space where the solution of the state problem lives. Therefore, we have to first study material derivatives and then pass to shape derivatives that will be used for numerical computations.

Admissible deformations. Only the interface Γ is subject to variations. For a positive real number $\delta > 0$, and for $i = 1, 2$, we define

$$\Omega^\delta_{\mathrm{D},i} = \{x \in \Omega_i; \; d(x, \Gamma_{\mathrm{D}}) < \delta\}.$$

We assume δ small enough to have $\overline{\Omega^\delta_{\mathrm{D},1}} \cap \overline{\Omega^\delta_{\mathrm{D},2}} = \emptyset$. The set of admissible deformations Θ_{ad} is defined as

$$\Theta_{\mathrm{ad}} = \{\boldsymbol{\theta} \in \mathcal{C}^2(\Omega)^d \cap \mathrm{W}^{2,\infty}(\Omega)^d; \; \|\boldsymbol{\theta}\|_{\mathrm{W}^{2,\infty}(\Omega)^d} < 1, \; \boldsymbol{\theta} = 0 \text{ on } \partial\Omega, \; \boldsymbol{\theta} = 0 \text{ in } \Omega^\delta_{\mathrm{D},i}, i = 1, 2\},$$

and we consider small perturbations of the interface Γ, for $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}}$:

$$\Gamma^{\boldsymbol{\theta}} = (\boldsymbol{I} + \boldsymbol{\theta})\Gamma \qquad \text{and} \qquad \Omega_i^{\boldsymbol{\theta}} = (\boldsymbol{I} + \boldsymbol{\theta})\Omega_i, \quad i = 1, 2,$$

where $\boldsymbol{I}$ is the identity mapping from $\mathrm{W}^{2,\infty}$ into $\mathrm{W}^{2,\infty}$. Such deformations leave the Ω domain and the vicinity of the inlet and outlet invariant, but allow the shape of the interface between the hot and cold fluids to be modified.

Assumptions and notations. To compute the shape derivatives for this equation, we assume Γ at least $\mathcal{C}^3$. We use the following overcharged notations. Let A be a matrix, A^{-1}, A^t and A^{-t} are respectively its inverse, its transpose and the inverse of its transpose. Let d_{Ω_1} be the signed distance function to the domain Ω_1. We set

$$\boldsymbol{n} = \nabla d_{\Omega_1} \quad \text{ and } \quad H = \Delta d_{\Omega_1} \text{ in a neighborhood of } \Gamma. \tag{3.1}$$

These functions are defined in the volume and not only on the surface Γ. On the surface Γ, they coincide respectively with the outer unit normal vector and of the mean curvature of Γ. Notice that derivation with respect to a shape of terms involving a Laplace-Beltrami operator gives rise to derivatives of curvature, which we can conveniently be expressed using these two functions. In particular, writing $\frac{\partial H}{\partial \boldsymbol{n}}$ makes sense with these definitions, even if it can be confusing at first sight.

In the following, we introduce $(\boldsymbol{u}_{\boldsymbol{\theta},i}, p_{\boldsymbol{\theta},i}) \in \mathcal{V}_{\boldsymbol{u}_{\mathrm{D,i}}}(\Omega_i^{\boldsymbol{\theta}}) \times \mathrm{L}^2(\Omega_i^{\boldsymbol{\theta}})$ and $\mathsf{T}_{\boldsymbol{\theta}} \in \mathcal{H}_{\mathsf{T}_{\mathrm{D}}}(\Omega_1^{\boldsymbol{\theta}}, \Omega_2^{\boldsymbol{\theta}})$ the perturbed solutions, *i.e.* the solution of the Navier-Stokes equations defined in $\Omega_i^{\boldsymbol{\theta}}$ (instead of Ω_i) and the approximated convection-diffusion equations (2.2) defined in $\Omega_1^{\boldsymbol{\theta}} \cup \Omega_2^{\boldsymbol{\theta}}$ (instead of $\Omega_1 \cup \Omega_2$).

3.1 Shape sensitivity of the velocity and pressure

The shape calculus is well known for the solutions of the Stokes and Navier-Stokes equations: the interested reader can refer to [6] for first order derivatives and [12, 9] for second-order derivatives. Let us recall the expression of the material and shape derivatives of velocity and pressure.

Proposition 3.1 (Shape derivative of the Navier-Stokes equations). *For each $i = 1, 2$, the material derivative $(\dot{\boldsymbol{u}}_i, \dot{p}_i) \in \mathcal{V}_0(\Omega_i) \times \mathrm{L}^2(\Omega_i)$ of the solution $(\boldsymbol{u}_i, p_i) \in \mathcal{V}_{\boldsymbol{u}_{\mathrm{D}},i}(\Omega_i) \times \mathrm{L}^2(\Omega_i)$ of the Navier-Stokes equations* (2.1) *exists and solves the following problem:* Find $(\dot{\boldsymbol{u}}_i, \dot{p}_i) \in \mathcal{V}_0(\Omega_i) \times \mathrm{L}^2(\Omega_i)$ such that for all $(\boldsymbol{w}_i, \phi_i) \in \mathcal{V}_0(\Omega_i) \times \mathrm{L}^2(\Omega_i)$,

$$\int_{\Omega_i} \left(2\nu_i \varepsilon(\dot{\boldsymbol{u}}_i) : \varepsilon(\boldsymbol{w}_i) + (\nabla \dot{\boldsymbol{u}}_i)\boldsymbol{u}_i \cdot \boldsymbol{w}_i + (\nabla \boldsymbol{u}_i)\dot{\boldsymbol{u}}_i \cdot \boldsymbol{w}_i - \frac{\dot{p}_i}{\rho_i} \operatorname{div}(\boldsymbol{w}_i) - \frac{\phi_i}{\rho_i} \operatorname{div}(\dot{\boldsymbol{u}}_i) \right) \mathrm{d}x$$
$$= \int_{\Omega_i} - \operatorname{div}(\boldsymbol{\theta})(\sigma(\boldsymbol{u}_i, p_i) : \nabla \boldsymbol{w}_i + (\nabla \boldsymbol{u}_i)\boldsymbol{u}_i \cdot \boldsymbol{w}_i) \, \mathrm{d}x$$
$$+ \int_{\Omega_i} (\sigma(\boldsymbol{u}_i, p_i) : (\nabla \boldsymbol{w}_i \nabla \boldsymbol{\theta}) + \sigma(\boldsymbol{w}_i, \phi_i) : (\nabla \boldsymbol{u}_i \nabla \boldsymbol{\theta}) + (\nabla \boldsymbol{u}_i \nabla \boldsymbol{\theta})\boldsymbol{u}_i \cdot \boldsymbol{w}_i) \, \mathrm{d}x. \quad (3.2)$$

Furthermore, assuming that $(\boldsymbol{u}_i, p_i)$ belongs to $\mathrm{H}^2(\Omega_i)^d \times \mathrm{H}^1(\Omega_i)$, it is differentiable with respect to the domain and the shape derivatives $(\boldsymbol{u}_i', p_i') \in \mathrm{H}^1(\Omega_i)^d \times \mathrm{L}^2(\Omega_i)$ are characterized by

$$\begin{cases} -\nu_i \Delta \boldsymbol{u}_i' + (\nabla \boldsymbol{u}_i)\boldsymbol{u}_i' + (\nabla \boldsymbol{u}_i')\boldsymbol{u}_i + \dfrac{1}{\rho_i}\nabla p_i' = 0 & \text{in } \Omega_i, \\ \operatorname{div}(\boldsymbol{u}_i') = 0 & \text{in } \Omega_i, \\ \boldsymbol{u}' = 0 & \text{on } \Gamma_{\mathrm{D},i} \cup \Gamma_{\mathrm{e},i}, \\ \sigma(\boldsymbol{u}_i', p_i')\boldsymbol{n} = 0 & \text{on } \Gamma_{\mathrm{N},i}, \\ \boldsymbol{u}_i' = -\dfrac{\partial \boldsymbol{u}_i}{\partial \boldsymbol{n}}(\boldsymbol{\theta} \cdot \boldsymbol{n}) & \text{on } \Gamma. \end{cases} \quad (3.3)$$

3.2 Sensitivity of the temperature

3.2.1 Material derivative

We follow the usual procedure given in the book [21]: transport on a fixed domain, obtain the differentiability by applying the implicit function theorem and then derive the material derivative.

Notice that, in the class Θ_{ad} of deformations, the domain $\Omega_{\mathrm{D},i}^{\delta}$ is untouched by the deformation. Then, we consider a lifting F of the Dirichlet data T_{D}, independent of the deformation field $\boldsymbol{\theta}$, such that

$$F \in \mathrm{H}^1(\Omega), \quad F = \mathsf{T}_{\mathrm{D}} \text{ on } \Gamma_{\mathrm{D}} \quad \text{and} \quad F = 0 \text{ in } \Omega \backslash (\Omega_{\mathrm{D},1}^{\delta} \cup \Omega_{\mathrm{D},2}^{\delta}). \quad (3.4)$$

Such a lifting exists by considering, for instance, considering the solutions of the two following problems, for $i = 1, 2$,

$$\begin{cases} -\Delta F_i &= 0 & \text{in } \Omega_i^\delta, \\ F_i &= \mathsf{T}_{\mathrm{D},i} & \text{on } \Gamma_{\mathrm{D},i}, \\ F_i &= 0 & \text{on } \partial\Omega_i^\delta \setminus \partial\Omega, \\ \dfrac{\partial F_i}{\partial \boldsymbol{n}} &= 0 & \text{on } \partial\Omega_i^\delta \cap (\partial\Omega \setminus \Gamma_{\mathrm{D,i}}^\delta), \end{cases}$$

where $\Omega_i^\delta = \{x \in \Omega;\ d(x, \Gamma_{\mathrm{D},i}) < \delta\}$ is a subset of Ω that contains $\Omega_{\mathrm{D,i}}^\delta$. Then extending F_i by 0 to Ω, which extension we continue calling F_i and we define $F := F_1 + F_2$.

Finally, for $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}}$, we recall that $\mathsf{T}_{\boldsymbol{\theta}}$ is the solution of (2.8) in $\mathcal{H}_{\mathsf{T}_\mathrm{D}}(\Omega_1^{\boldsymbol{\theta}}, \Omega_2^{\boldsymbol{\theta}})$ and we introduce its correction by the lifting F of the Dirichlet boundary conditions:

$$\mathsf{R}_{\boldsymbol{\theta}} = \mathsf{T}_{\boldsymbol{\theta}} - F \in \mathcal{H}_0(\Omega_1^{\boldsymbol{\theta}}, \Omega_2^{\boldsymbol{\theta}}).$$

Proposition 3.2 (Material derivative of the approximated convection-diffusion equation)**.** *The applications*

$$\boldsymbol{\theta} \in \Theta_{\mathrm{ad}} \mapsto \overline{\mathsf{R}}_{\boldsymbol{\theta}} = \mathsf{R}_{\boldsymbol{\theta}} \circ (\boldsymbol{I} + \boldsymbol{\theta}) \in \mathcal{H}_0(\Omega_1, \Omega_2) \ \ \textit{and} \ \ \boldsymbol{\theta} \in \Theta_{\mathrm{ad}} \mapsto \overline{\mathsf{T}}_{\boldsymbol{\theta}} = \mathsf{T}_{\boldsymbol{\theta}} \circ (\boldsymbol{I} + \boldsymbol{\theta}) \in \mathcal{H}^1(\Omega_1, \Omega_2)$$

are $\mathcal{C}^1$ in a neighborhood of 0*. Furthermore, the derivative of the last mapping at 0, in the direction $\boldsymbol{\theta}$ is called the material derivative of $\mathsf{T} \in \mathcal{H}_{\mathsf{T}_\mathrm{D}}(\Omega_1, \Omega_2)$, is denoted by $\dot{\mathsf{T}}$, and is the solution of the following variational problem:*

Find $\dot{\mathsf{T}} \in \mathcal{H}_0(\Omega_1, \Omega_2)$ such that for all $\phi \in \mathcal{H}_0(\Omega_1, \Omega_2)$,

$$\sum_{i=1}^{2} \int_{\Omega_i} \Big(\kappa_i \nabla \dot{\mathsf{T}}_i \cdot \nabla \phi_i + \Big(\boldsymbol{u}_i \cdot \nabla \dot{\mathsf{T}}_i + \dot{\boldsymbol{u}}_i \cdot \nabla \mathsf{T}_i\Big)\,\phi_i\Big)\,\mathrm{d}x$$
$$+ \int_\Gamma \Big(\eta\kappa_s \nabla_\tau \Big\langle \dot{\mathsf{T}} \Big\rangle \cdot \nabla_\tau \langle\phi\rangle + \kappa_s H [\dot{\mathsf{T}}]\,\langle\phi\rangle + \frac{\kappa_s}{\eta}[\dot{\mathsf{T}}][\phi]\Big)\,\mathrm{d}s$$
$$= \sum_{i=1}^{2} \int_{\Omega_i} \big(\kappa_i \left(\nabla\boldsymbol{\theta} + \nabla\boldsymbol{\theta}^t - \mathrm{div}(\boldsymbol{\theta})\mathrm{I}\right) \nabla \mathsf{T}_i \cdot \nabla\phi_i + (((\nabla\boldsymbol{\theta})\,\boldsymbol{u}_i - \mathrm{div}(\boldsymbol{\theta})\boldsymbol{u}_i) \cdot \nabla \mathsf{T}_i)\,\phi_i\big)\,\mathrm{d}x$$
$$+ \int_\Gamma \eta\kappa_s \left(\left(\nabla_\tau\boldsymbol{\theta} + \nabla_\tau\boldsymbol{\theta}^t - \mathrm{div}_\tau(\boldsymbol{\theta})\mathrm{I}\right) \nabla_\tau \langle\mathsf{T}\rangle\right) \cdot \nabla_\tau \langle\phi\rangle\,\mathrm{d}s$$
$$- \int_\Gamma (\kappa_s H\,\mathrm{div}_\tau(\boldsymbol{\theta})[\mathsf{T}]\,\langle\phi\rangle - \kappa_s \Delta_\tau(\boldsymbol{\theta}\cdot\boldsymbol{n})[\mathsf{T}]\,\langle\phi\rangle + \kappa_s \nabla H \cdot \theta[\mathsf{T}]\langle\phi\rangle)\,\mathrm{d}s$$
$$- \int_\Gamma \frac{\kappa_s}{\eta}\,\mathrm{div}_\tau(\boldsymbol{\theta})[\mathsf{T}][\phi]\,\mathrm{d}s. \quad (3.5)$$

Proof. Step 1: transport on a fixed domain with a fixed interface. Let $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}}$. We define the transported solution of the Navier-Stokes equations (2.1) $\overline{\boldsymbol{u}}_{\boldsymbol{\theta},i} := \boldsymbol{u}_{\boldsymbol{\theta},i} \circ (\boldsymbol{I} + \boldsymbol{\theta}) \in \mathcal{V}_{\boldsymbol{u}_{\mathrm{D,i}}}(\Omega_i)$. Given $\phi \in \mathcal{H}_0(\Omega_1, \Omega_2)$, we define $\phi_{\boldsymbol{\theta}} = \phi \circ (\boldsymbol{I} + \boldsymbol{\theta})^{-1} \in \mathcal{H}_0(\Omega_1^{\boldsymbol{\theta}}, \Omega_2^{\boldsymbol{\theta}})$. One starts from the weak formulation of the convection-diffusion equation (2.8) on the perturbed domain:

$$\sum_{i=1}^{2} \int_{\Omega_i^{\boldsymbol{\theta}}} (\kappa_i \nabla \mathsf{T}_{\boldsymbol{\theta},i} \cdot \nabla\phi_{\boldsymbol{\theta},i} + \boldsymbol{u}_{\boldsymbol{\theta},i} \cdot \nabla \mathsf{T}_{\boldsymbol{\theta},i}\phi_{\boldsymbol{\theta},i})\,\mathrm{d}x$$
$$+ \int_{\Gamma^{\boldsymbol{\theta}}} \Big(\eta\kappa_s \nabla_{\tau_{\boldsymbol{\theta}}} \langle\mathsf{T}_{\boldsymbol{\theta}}\rangle \cdot \nabla_{\tau_{\boldsymbol{\theta}}} \langle\phi_{\boldsymbol{\theta}}\rangle + \kappa_s H_{\boldsymbol{\theta}} [\mathsf{T}_{\boldsymbol{\theta}}]\,\langle\phi_{\boldsymbol{\theta}}\rangle + \frac{\kappa_s}{\eta}[\mathsf{T}_{\boldsymbol{\theta}}][\phi_{\boldsymbol{\theta}}]\Big)\,\mathrm{d}s = 0,$$

and $\mathsf{R}_{\boldsymbol{\theta}}$ satisfies,

$$\sum_{i=1}^{2}\int_{\Omega_i^{\boldsymbol{\theta}}}(\kappa_i\nabla\mathsf{R}_{\boldsymbol{\theta},i}\cdot\nabla\phi_{\boldsymbol{\theta},i}+\boldsymbol{u}_{\boldsymbol{\theta},i}\cdot\nabla\mathsf{R}_{\boldsymbol{\theta},i}\phi_{\boldsymbol{\theta},i})\,\mathrm{d}x$$
$$+\int_{\Gamma^{\boldsymbol{\theta}}}\left(\eta\kappa_s\nabla_{\tau_{\boldsymbol{\theta}}}\langle\mathsf{R}_{\boldsymbol{\theta}}\rangle\cdot\nabla_{\tau_{\boldsymbol{\theta}}}\langle\phi_{\boldsymbol{\theta}}\rangle+\kappa_s H_{\boldsymbol{\theta}}[\mathsf{R}_{\boldsymbol{\theta}}]\langle\phi_{\boldsymbol{\theta}}\rangle+\frac{\kappa_s}{\eta}[\mathsf{R}_{\boldsymbol{\theta}}][\phi_{\boldsymbol{\theta}}]\right)\mathrm{d}s$$
$$=-\sum_{i=1}^{2}\int_{\Omega_{\mathrm{D},i}^{\delta}}(\kappa_i\nabla F\cdot\nabla\phi_i+\boldsymbol{u}_{\boldsymbol{\theta},i}\cdot\nabla F\phi_i)\,\mathrm{d}x-\int_{\Gamma\cap\partial\Omega_{\mathrm{D},1}^{\delta}}\eta\kappa_s\nabla_\tau F\cdot\nabla_\tau\langle\phi\rangle\,\mathrm{d}s,$$

where we have used that the lifting F is independent of $\boldsymbol{\theta}$, satisfies $[F]=0$ on $\Gamma^{\boldsymbol{\theta}}$, $F=0$ in $\Omega\backslash(\Omega_{\mathrm{D},1}^{\delta}\cup\Omega_{\mathrm{D},2}^{\delta})$ and that the deformation field $\boldsymbol{\theta}\in\Theta$ verifies, $\boldsymbol{\theta}=0$ in $\Omega_{\mathrm{D},1}^{\delta}\cup\Omega_{\mathrm{D},2}^{\delta}$.

After a change of variables to the reference configuration, one gets:

$$\sum_{i=1}^{2}\int_{\Omega_i}\left(\kappa_i A(\boldsymbol{\theta})\nabla\overline{\mathsf{R}}_{\boldsymbol{\theta},i}\cdot\nabla\phi_i+B(\boldsymbol{\theta})\overline{\boldsymbol{u}}_{\boldsymbol{\theta},i}\cdot\nabla\overline{\mathsf{R}}_{\boldsymbol{\theta},i}\phi_i\right)\,\mathrm{d}x$$
$$+\int_{\Gamma}\eta\kappa_s C(\boldsymbol{\theta})\left((\mathrm{I}+\nabla\boldsymbol{\theta})^{-1}(\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\left\langle\overline{\mathsf{R}}_{\boldsymbol{\theta}}\right\rangle\right)\cdot\nabla\langle\phi\rangle\,\mathrm{d}s$$
$$-\int_{\Gamma}\eta\kappa_s C(\boldsymbol{\theta})\left((\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\langle\overline{\mathsf{R}}_{\boldsymbol{\theta}}\rangle\cdot\boldsymbol{n}_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})\right)\left((\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\langle\phi\rangle\cdot\boldsymbol{n}_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})\right)\,\mathrm{d}s$$
$$+\int_{\Gamma}\left(\kappa_s C(\boldsymbol{\theta})H_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})[\overline{\mathsf{R}}_{\boldsymbol{\theta}}]\langle\phi\rangle+\frac{\kappa_s}{\eta}C(\boldsymbol{\theta})[\overline{\mathsf{R}}_{\boldsymbol{\theta}}][\phi]\right)\mathrm{d}s$$
$$+\sum_{i=1}^{2}\int_{\Omega_{\mathrm{D},i}^{\delta}}(\kappa_i\nabla F\cdot\nabla\phi_i+\boldsymbol{u}_{\boldsymbol{\theta},i}\cdot\nabla F\phi_i)\,\mathrm{d}x+\int_{\Gamma\cap\partial\Omega_{\mathrm{D},1}^{\delta}}\eta\kappa_s\nabla_\tau F\cdot\nabla_\tau\langle\phi\rangle\,\mathrm{d}s=0, \quad (3.6)$$

where

$$\begin{aligned}A(\boldsymbol{\theta}) &= |\det(\mathrm{I}+\nabla\boldsymbol{\theta})|\;(\mathrm{I}+\nabla\boldsymbol{\theta})^{-1}(\mathrm{I}+\nabla\boldsymbol{\theta})^{-t},\\ B(\boldsymbol{\theta}) &= |\det(\mathrm{I}+\nabla\boldsymbol{\theta})|\;(\mathrm{I}+\nabla\boldsymbol{\theta})^{-1},\\ C(\boldsymbol{\theta}) &= |\det(\mathrm{I}+\nabla\boldsymbol{\theta})|\;|(\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\boldsymbol{n}|_{\mathbb{R}^d},\end{aligned}$$

where $|\cdot|_{\mathbb{R}^d}$ is the usual Eucledian norm in $\mathbb{R}^d$.

Step 2: going for the implicit function theorem. Define $\mathcal{F}:\Theta_{\mathrm{ad}}\times\mathcal{H}_0(\Omega_1,\Omega_2)\mapsto(\mathcal{H}_0(\Omega_1,\Omega_2))'$ by: for all $\phi\in\mathcal{H}_0(\Omega_1,\Omega_2)$,

$$\langle\mathcal{F}(\boldsymbol{\theta},\psi),\phi\rangle=\sum_{i=1}^{2}\int_{\Omega_i}(\kappa_i A(\boldsymbol{\theta})\nabla\psi_i\cdot\nabla\phi_i+B(\boldsymbol{\theta})\overline{\boldsymbol{u}}_{\boldsymbol{\theta},i}\cdot\nabla\psi_i\phi_i)\,\mathrm{d}x$$
$$+\int_{\Gamma}\eta\kappa_s C(\boldsymbol{\theta})\Big(\left((\mathrm{I}+\nabla\boldsymbol{\theta})^{-1}(\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\langle\psi\rangle\right)\cdot\nabla\langle\phi\rangle$$
$$-\left((\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\langle\psi\rangle\cdot\boldsymbol{n}_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})\right)\left((\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\langle\phi\rangle\cdot\boldsymbol{n}_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})\right)\Big)\mathrm{d}s$$
$$+\int_{\Gamma}\left(\kappa_s C(\boldsymbol{\theta})H_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})[\psi]\langle\phi\rangle+\frac{\kappa_s}{\eta}C(\boldsymbol{\theta})[\psi][\phi]\right)\mathrm{d}s$$
$$+\sum_{i=1}^{2}\int_{\Omega_{\mathrm{D},i}^{\delta}}(\kappa_i\nabla F\cdot\nabla\phi_i+\boldsymbol{u}_{\boldsymbol{\theta},i}\cdot\nabla F\phi_i)\,\mathrm{d}x+\int_{\Gamma\cap\partial\Omega_{\mathrm{D},1}^{\delta}}\eta\kappa_s\nabla_\tau F\cdot\nabla_\tau\langle\phi\rangle\,\mathrm{d}s.$$

Let us check the assumptions of the implicit function theorem.

- By construction

$$\mathcal{F}(0, \mathsf{T} - F) = 0,$$

where T is the solution of the convection-diffusion problem (2.8) (with $\boldsymbol{\theta} = 0$).

- We now study the regularity of $\mathcal{F}$. Let us first recall that $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto \boldsymbol{n_\theta} \circ (\boldsymbol{I} + \boldsymbol{\theta}) \in \mathcal{C}^1(\Gamma)^d$ and $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto \boldsymbol{H_\theta} \circ (\boldsymbol{I} + \boldsymbol{\theta}) \in \mathcal{C}^0(\Gamma)$ are $\mathcal{C}^1$ (see , [21, Proposition 5.4.14, Lemma 5.4.15]). Also, $\theta \in \Theta_{\text{ad}} \mapsto \overline{\boldsymbol{u}}_{\boldsymbol{\theta},i} \in \mathcal{V}_0(\Omega_i)$ is $\mathcal{C}^1$ in a neighborhood of 0 as proven in [9] and $\overline{\boldsymbol{u}}_{\boldsymbol{\theta},i} = \boldsymbol{u}_{\boldsymbol{\theta},i}$ in $\Omega^\delta_{\text{D,i}}$. Moreover, from [21, Theorem 5.5.1], $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto A(\boldsymbol{\theta}) \in \mathrm{L}^\infty(\Omega, \mathcal{M}_d)$, $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto B(\boldsymbol{\theta}) \in \mathrm{L}^\infty(\Omega, \mathcal{M}_d)$, $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto C(\boldsymbol{\theta}) \in \mathcal{C}^1(\Gamma)$ are $\mathcal{C}^\infty$, where $\mathcal{M}_d$ is the space of $d \times d$ square matrices. Finally, for every $\boldsymbol{\theta^*} \in \Theta_{\text{ad}}$, the mapping

$$\mathcal{F}(\boldsymbol{\theta}^*, \cdot) : \mathcal{H}_0(\Omega_1, \Omega_2) \mapsto (\mathcal{H}_0(\Omega_1, \Omega_2))'$$

is linear continuous and then $\mathcal{C}^\infty$. By chain rule, we conclude that $\mathcal{F}$ is $\mathcal{C}^1$ in a neighborhood of 0.

- Finally, we check that the operator $\mathrm{D}_\psi \mathcal{F}(0, \mathsf{T} - F)$ is an isomorphism from $\mathcal{H}_0(\Omega_1, \Omega_2)$ into $(\mathcal{H}_0(\Omega_1, \Omega_2))'$. Indeed for all $S, \hat{S} \in \mathcal{H}_0(\Omega_1, \Omega_2)$, we compute

$$\langle \mathrm{D}_\psi \mathcal{F}(0, \mathsf{T} - F) S, \hat{S} \rangle = \sum_{i=1}^{2} \int_{\Omega_i} \left(\kappa_i \nabla S_i \cdot \nabla \hat{S}_i + \nabla S_i \cdot \boldsymbol{u}_i \hat{S}_i \right) \mathrm{d}x + \int_\Gamma \left(\eta \kappa_s \nabla_\tau \langle S \rangle \cdot \nabla_\tau \langle \hat{S} \rangle + \kappa_s H [S][\hat{S}] + \frac{\kappa_s}{\eta} [S][\hat{S}] \right) \mathrm{d}s.$$

This leads to a well-posed problem when the right hand side of the variational problem belongs to $(\mathcal{H}_0(\Omega_1, \Omega_2))'$, thanks to the Lax-Milgram theorem. The proof is analogous to the well-posedness of problem (2.8). Indeed, let us consider $\ell \in (\mathcal{H}_0(\Omega_1, \Omega_2))'$. The coercivity of the bilinear form at the left hand-side was already proved in [10, Theorem 2.1]. The only difference is that we do not have necessarily the integral structure at the right hand-side, but the continuity is straightforward since $\ell \in (\mathcal{H}_0(\Omega_1, \Omega_2))'$. By virtue of the Lax-Milgram theorem, there exists a unique $S_\ell \in \mathcal{H}_0(\Omega_1, \Omega_2)$ such that for all $\hat{S} \in \mathcal{H}_0(\Omega_1, \Omega_2)$,

$$\sum_{i=1}^{2} \int_{\Omega_i} \left(\kappa_i \nabla S_i \cdot \nabla \hat{S}_i + \nabla S_i \cdot \boldsymbol{u}_i \hat{S}_i \right) \mathrm{d}x + \int_\Gamma \left(\eta \kappa_s \nabla_\tau \langle S \rangle \cdot \nabla_\tau \langle \hat{S} \rangle + \kappa_s H [S][\hat{S}] + \frac{\kappa_s}{\eta} [S][\hat{S}] \right) \mathrm{d}s = \left\langle \ell, \hat{S} \right\rangle_{(\mathcal{H}_0(\Omega_1, \Omega_2))', \mathcal{H}_0(\Omega_1, \Omega_2)}.$$

By virtue of the implicit function theorem, there exists a $\mathcal{C}^1$ function

$$\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto \psi(\boldsymbol{\theta}) \in \mathcal{H}_0(\Omega_1, \Omega_2)$$

in a neighborhood of 0 such that, $\mathcal{F}(\boldsymbol{\theta}, \psi(\boldsymbol{\theta})) = 0$. By uniqueness of the solution $\mathsf{R}_{\boldsymbol{\theta}} \in \mathcal{H}_0(\Omega_1^{\boldsymbol{\theta}}, \Omega_2^{\boldsymbol{\theta}})$ and from (3.6), we deduce that $\overline{\mathsf{R}}_{\boldsymbol{\theta}} = \psi(\boldsymbol{\theta})$, then, $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto \overline{\mathsf{R}}_{\boldsymbol{\theta}} \in \mathcal{H}_0(\Omega_1, \Omega_2)$ is $\mathcal{C}^1$ in a neighborhood of 0. Since F is independent of θ, we also obtain that $\boldsymbol{\theta} \in \Theta_{\text{ad}} \mapsto \overline{\mathsf{T}}_{\boldsymbol{\theta}} \in \mathcal{H}^1(\Omega_1, \Omega_2)$ is $\mathcal{C}^1$ in a neighborhood of 0.

Step 3: characterization of the material derivative. To prove that the material derivative satisfies (3.5), we proceeded as in [2, Proposition 6.30]. First, we write the variational problem that solves $\mathsf{T}_{\boldsymbol{\theta}}$ after having performed the pull-back on the reference domain:

$$\sum_{i=1}^{2} \int_{\Omega_i} \left(\kappa_i A(\boldsymbol{\theta}) \nabla \overline{\mathsf{T}}_{\boldsymbol{\theta},i} \cdot \nabla \phi_i + B(\boldsymbol{\theta}) \overline{\boldsymbol{u}}_{\boldsymbol{\theta},i} \cdot \nabla \overline{\mathsf{T}}_{\boldsymbol{\theta},i} \phi_i \right) \mathrm{d}x$$

$$
+\int_\Gamma \eta\kappa_s C(\boldsymbol{\theta})\Big(\big((\mathrm{I}+\nabla\boldsymbol{\theta})^{-1}(\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\left\langle \overline{\mathsf{T}}_{\boldsymbol{\theta}}\right\rangle\big)\cdot\nabla\left\langle\phi\right\rangle
$$

$$
-\big((\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\langle\overline{\mathsf{T}}_{\boldsymbol{\theta}}\rangle\cdot\boldsymbol{n}_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})\big)\big((\mathrm{I}+\nabla\boldsymbol{\theta})^{-t}\nabla\langle\phi\rangle\cdot\boldsymbol{n}_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})\big)\Big)\,\mathrm{d}s
$$

$$
+\int_\Gamma\Big(\kappa_s C(\boldsymbol{\theta})H_{\boldsymbol{\theta}}\circ(\boldsymbol{I}+\boldsymbol{\theta})[\overline{\mathsf{T}}_{\boldsymbol{\theta}}]\left\langle\phi\right\rangle+\frac{\kappa_s}{\eta}C(\boldsymbol{\theta})[\overline{\mathsf{T}}_{\boldsymbol{\theta}}][\phi]\Big)\,\mathrm{d}s=0. \tag{3.7}
$$

Then, differentiating (3.7) at $\boldsymbol{\theta}=0$ in the direction $\boldsymbol{\theta}$ and using the following derivatives:

$$
\begin{aligned}
\mathrm{D}A(0)(\boldsymbol{\theta}) &= \mathrm{div}(\boldsymbol{\theta})\mathrm{I}-\nabla\boldsymbol{\theta}-(\nabla\boldsymbol{\theta})^t,\\
\mathrm{D}B(0)(\boldsymbol{\theta}) &= \mathrm{div}(\boldsymbol{\theta})\mathrm{I}-\nabla\boldsymbol{\theta},\\
\mathrm{D}C(0)(\boldsymbol{\theta}) &= \mathrm{div}_\tau(\boldsymbol{\theta}),\\
\dot{\boldsymbol{n}} &= -\nabla_\tau(\boldsymbol{\theta}\cdot\boldsymbol{n})+(\nabla\boldsymbol{n})\boldsymbol{\theta},\\
\dot{H} &= -\Delta_\tau(\boldsymbol{\theta}\cdot\boldsymbol{n})+\nabla H\cdot\boldsymbol{\theta},
\end{aligned}
$$

where $\dot{\boldsymbol{n}}$ and $\dot{H}$ are the material derivative of the extension of the normal and mean curvature. Finally, we get (3.5) by means of chain rule.

□

3.2.2 Shape derivative of the temperature

We now characterize the shape derivative of the temperature. We begin by proving the following lemma, which is useful for the following proof.

Lemma 3.3. *Let $\boldsymbol{\theta}\in\Theta_{\mathrm{ad}}$. Given $u,\phi\in\mathrm{H}^2(\Gamma)$, we have*

$$
-\int_\Gamma\big((\mathrm{div}_\tau(\boldsymbol{\theta})\mathrm{I}-\nabla_\tau\boldsymbol{\theta}-\nabla_\tau\boldsymbol{\theta}^t)\nabla_\tau u\cdot\nabla_\tau\phi+\nabla_\tau(\boldsymbol{\theta}\cdot\nabla_\tau u)\cdot\nabla_\tau\phi-\Delta_\tau u(\boldsymbol{\theta}\cdot\nabla_\tau\phi)\big)\,\mathrm{d}s
$$

$$
=\int_\Gamma\mathrm{div}_\tau\left(H(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau u-2(\boldsymbol{\theta}\cdot\boldsymbol{n})(\nabla_\tau\boldsymbol{n})\nabla_\tau u\right)\phi\,\mathrm{d}s.
$$

Proof. The proof is based on integration by parts on the boundary together with the decomposition of the deformation vector: $\boldsymbol{\theta}=\boldsymbol{\theta}_\tau+(\boldsymbol{\theta}\cdot\boldsymbol{n})\boldsymbol{n}$ on Γ. A key point is that, by definition both $\boldsymbol{\theta}=0$ and $\partial_{\boldsymbol{n}}\boldsymbol{\theta}=0$ on $\partial\Gamma$. As a consequence the boundary terms on $\partial\Gamma$ disappear. We have the relations:

$$
\begin{aligned}
\int_\Gamma\mathrm{div}_\tau(\boldsymbol{\theta})\nabla_\tau u\cdot\nabla_\tau\phi\,\mathrm{d}s &= \int_\Gamma\left(H(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau u\cdot\nabla_\tau\phi-\nabla_\tau(\nabla_\tau u\cdot\nabla_\tau\phi)\cdot\boldsymbol{\theta}\right)\,\mathrm{d}s\\
&=\int_\Gamma\big(H(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau u\cdot\nabla_\tau\phi-(\nabla(\nabla_\tau u)^t\nabla_\tau\phi)\cdot\boldsymbol{\theta}_\tau-(\nabla(\nabla_\tau\phi)^t\nabla_\tau u)\cdot\boldsymbol{\theta}_\tau\big)\,\mathrm{d}s,
\end{aligned}
$$

$$
\begin{aligned}
\int_\Gamma(\nabla_\tau\boldsymbol{\theta}\nabla_\tau u)\cdot\nabla_\tau\phi\,\mathrm{d}s &= \int_\Gamma\left((\nabla\boldsymbol{\theta}_\tau\nabla_\tau u)\cdot\nabla_\tau\phi+(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla\boldsymbol{n}\nabla_\tau u\cdot\nabla_\tau\phi\right)\,\mathrm{d}s\\
&=\int_\Gamma\left((\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau\boldsymbol{n}\nabla_\tau u+\nabla\boldsymbol{\theta}_\tau\nabla_\tau u\right)\cdot\nabla_\tau\phi\,\mathrm{d}s,
\end{aligned}
$$

$$
\int_\Gamma(\nabla_\tau\boldsymbol{\theta}^t\nabla_\tau u)\cdot\nabla_\tau\phi\,\mathrm{d}s=\int_\Gamma\big((\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau\boldsymbol{n}\nabla_\tau u+(\nabla\boldsymbol{\theta}_\tau)^t\nabla_\tau u\big)\cdot\nabla_\tau\phi\,\mathrm{d}s,
$$

$$
\int_\Gamma-\Delta_\tau u(\boldsymbol{\theta}\cdot\nabla_\tau\phi)\,\mathrm{d}s=\int_\Gamma\nabla_\tau u\cdot\nabla(\boldsymbol{\theta}_\tau\cdot\nabla_\tau\phi)\,\mathrm{d}s,
$$

$$
\int_\Gamma\nabla_\tau(\boldsymbol{\theta}\cdot\nabla_\tau u)\cdot\nabla_\tau\phi\,\mathrm{d}s=\int_\Gamma\nabla(\boldsymbol{\theta}_\tau\cdot\nabla_\tau u)\cdot\nabla_\tau\phi\,\mathrm{d}s=\int_\Gamma\big(\nabla_\tau\boldsymbol{\theta}^t\nabla_\tau u+\nabla(\nabla_\tau u)^t\boldsymbol{\theta}_\tau\big)\cdot\nabla_\tau\phi\,\mathrm{d}s.
$$

Summing up the above equations, we get

$$\int_\Gamma (\mathrm{div}_\tau(\boldsymbol{\theta})\mathrm{I} - \nabla_\tau\boldsymbol{\theta} - \nabla_\tau\boldsymbol{\theta}^t)\nabla_\tau u\cdot\nabla_\tau\phi + \nabla_\tau(\boldsymbol{\theta}\cdot\nabla_\tau u)\cdot\nabla_\tau\phi - \Delta_\tau u(\boldsymbol{\theta}\cdot\nabla_\tau\phi)\,\mathrm{d}s$$
$$= \int_\Gamma \left(H(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau u\cdot\nabla_\tau\phi - (\nabla(\nabla_\tau u)^t\nabla_\tau\phi)\cdot\boldsymbol{\theta}_\tau + (\nabla(\nabla_\tau\phi)^t\nabla_\tau u)\cdot\boldsymbol{\theta}_\tau\right)\,\mathrm{d}s$$
$$- \int_\Gamma 2(\boldsymbol{\theta}\cdot\boldsymbol{n})(\nabla_\tau\boldsymbol{n}\nabla_\tau u)\cdot\nabla_\tau\phi + (\nabla\boldsymbol{\theta}_\tau + \nabla\boldsymbol{\theta}_\tau^t)\nabla_\tau u\cdot\nabla_\tau\phi\,\mathrm{d}s$$
$$+ \int_\Gamma \nabla_\tau u\cdot\left((\nabla\boldsymbol{\theta})^t\nabla_\tau\phi + \nabla(\nabla_\tau\phi)^t\boldsymbol{\theta}_\tau\right)\,\mathrm{d}s + \int_\Gamma \left(\nabla\boldsymbol{\theta}_\tau\nabla_\tau u + \nabla(\nabla_\tau u^t)\boldsymbol{\theta}_\tau\right)\cdot\nabla_\tau\phi\,\mathrm{d}s$$
$$= \int_\Gamma (H(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau u - 2(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau\boldsymbol{n}\nabla_\tau u)\cdot\nabla_\tau\phi\,\mathrm{d}s$$
$$= \int_\Gamma \mathrm{div}_\tau\left(H(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau u - 2(\boldsymbol{\theta}\cdot\boldsymbol{n})(\nabla_\tau\boldsymbol{n})\nabla_\tau u\right)\phi\,\mathrm{d}s.$$

□

Proposition 3.4 (Shape derivative of the temperature)**.** *For each $i = 1,2$, there exists an extension $\tilde{\mathsf{T}}_{\boldsymbol{\theta},i} \in \mathrm{H}^1(\Omega)$ of $\mathsf{T}_{\boldsymbol{\theta},i}$ such that application $\boldsymbol{\theta}\in\Theta_{\mathrm{ad}} \mapsto \tilde{\mathsf{T}}_{\boldsymbol{\theta},i} \in \mathrm{L}^2(\Omega)$ is $\mathcal{C}^1$ at 0 and the derivative, denoted T_i', is called the shape derivative of T_i. Moreover, if in addition $\mathsf{T}\in\mathrm{H}^2(\Omega_1,\Gamma)\times\mathrm{H}^2(\Omega_2,\Gamma)$ and $\boldsymbol{u}_i\in\mathrm{H}^2(\Omega_i)^d$, then the shape derivative*
$\mathsf{T}' = (\mathsf{T}_1',\mathsf{T}_2') \in \mathcal{H}_0(\Omega_1,\Omega_2)$ is characterized by,

$$\begin{cases} -\mathrm{div}(\kappa_i\nabla\mathsf{T}_i') + \boldsymbol{u}_i\cdot\nabla\mathsf{T}_i' &= -\boldsymbol{u}_i'\cdot\nabla\mathsf{T}_i \quad \text{in } \Omega_i, i=1,2,\\ \mathsf{T}_i' &= 0 \quad \text{on } \Gamma_{\mathrm{D},i}, i=1,2,\\ \kappa_i\dfrac{\partial\mathsf{T}_i'}{\partial\boldsymbol{n}} &= 0 \quad \text{on } \Gamma_{\mathrm{N},i}\cup\Gamma_{\mathrm{e},i}, i=1,2,\\ \left\langle\kappa\dfrac{\partial\mathsf{T}'}{\partial\boldsymbol{n}}\right\rangle &= -\dfrac{\kappa_s}{\eta}[\mathsf{T}'] + \xi_1(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n}) \quad \text{on } \Gamma,\\ \left[\kappa\dfrac{\partial\mathsf{T}'}{\partial\boldsymbol{n}}\right] &= \eta\,\mathrm{div}_\tau(\kappa_s\nabla_\tau\langle\mathsf{T}'\rangle) - \kappa_s H[\mathsf{T}'] + \xi_2(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n}) \quad \text{on } \Gamma,\\ \kappa_i\dfrac{\partial\mathsf{T}_i'}{\partial\boldsymbol{n}} &= 0 \quad \text{on } \partial\Gamma, i=1,2, \end{cases} \tag{3.8}$$

with

$$\xi_1(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n}) = \mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n})\langle\kappa\nabla_\tau\mathsf{T}\rangle) - \frac{\kappa_s}{\eta}\left(H[\mathsf{T}] + \left[\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right]\right)(\boldsymbol{\theta}\cdot\boldsymbol{n}),$$
$$\xi_2(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n}) = \mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n})[\kappa\nabla_\tau\mathsf{T}]) - \kappa_s\left(H^2[\mathsf{T}] + H\left[\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right] + \frac{\partial H}{\partial\boldsymbol{n}}[\mathsf{T}]\right)(\boldsymbol{\theta}\cdot\boldsymbol{n}) + \kappa_s[\mathsf{T}]\Delta_\tau(\boldsymbol{\theta}\cdot\boldsymbol{n})$$
$$+ \eta\kappa_s\,\mathrm{div}_\tau(H(\boldsymbol{\theta}\cdot\boldsymbol{n})\nabla_\tau\langle\mathsf{T}\rangle - 2(\boldsymbol{\theta}\cdot\boldsymbol{n})(\nabla_\tau\boldsymbol{n})\nabla_\tau\langle\mathsf{T}\rangle) + \eta\kappa_s\Delta_\tau\left((\boldsymbol{\theta}\cdot\boldsymbol{n})\left\langle\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right\rangle\right).$$

Proof. Let us introduce two linear continuous extensions $E_i : \mathrm{H}^1(\Omega_i)\mapsto\mathrm{H}^1(\Omega)$, $i=1,2$. We define $\tilde{\mathsf{T}}_{\boldsymbol{\theta},i} = E_i(\overline{\mathsf{T}}_{\boldsymbol{\theta},i})\circ(\boldsymbol{I}+\boldsymbol{\theta})^{-1}\in\mathrm{H}^1(\Omega)$ and since $\boldsymbol{\theta}\in\Theta_{\mathrm{ad}}\mapsto\overline{T}_{\boldsymbol{\theta},i}\in\mathrm{H}^1(\Omega_i)$ is $\mathcal{C}^1$ in a neighborhood of 0, by chain rule, we get that $\boldsymbol{\theta}\in\Theta_{\mathrm{ad}}\mapsto E_i(\overline{T}_{\boldsymbol{\theta},i})\in\mathrm{H}^1(\Omega)$ is $\mathcal{C}^1$ in a neighborhood of 0. By using [21, Lemma 5.3.3], we deduce that $\boldsymbol{\theta}\in\Theta_{\mathrm{ad}}\mapsto E_i(\overline{\mathsf{T}}_{\boldsymbol{\theta},i})\circ(\boldsymbol{I}+\boldsymbol{\theta})^{-1}\in\mathrm{L}^2(\Omega)$ is $\mathcal{C}^1$ in a neighborhood of 0.

If in addition, T_i is $\mathrm{H}^2(\Omega_i,\Gamma)$, then using the relationship between the material and the shape derivative $\mathsf{T}_i' = \dot{\mathsf{T}}_i - \nabla \mathsf{T}_i \cdot \boldsymbol{\theta}, i = 1,2$ and $\langle \mathsf{T} \rangle' = \langle \dot{\mathsf{T}} \rangle - \nabla \langle \mathsf{T} \rangle \cdot \boldsymbol{\theta}$, yield that T' belongs to $\mathcal{H}_0(\Omega_1,\Omega_2)$. Similarly for the velocity, we have that $\boldsymbol{u}_i' = \dot{\boldsymbol{u}}_i - (\nabla \boldsymbol{u}_i)\boldsymbol{\theta}$, $i = 1,2$. Then, for any $\phi \in \mathcal{H}_0(\Omega_1,\Omega_2)$, we split the expression:

$$\sum_{i=1}^{2} \int_{\Omega_i} \left(\kappa_i \nabla \mathsf{T}_i' \cdot \nabla \phi_i + (\boldsymbol{u}_i \cdot \nabla \mathsf{T}_i' + \boldsymbol{u}_i' \cdot \nabla \mathsf{T}_i)\, \phi_i\right) \mathrm{d}x \\ + \int_{\Gamma} \left(\eta \kappa_s \nabla_\tau \langle \mathsf{T}' \rangle \cdot \nabla_\tau \langle \phi \rangle + \kappa_s H [\mathsf{T}'] \langle \phi \rangle + \frac{\kappa_s}{\eta} [\mathsf{T}'][\phi] \right) \mathrm{d}s = I_1 + I_2 + I_3 + I_4,$$

where

$$\begin{aligned}
I_1 &= \sum_{i=1}^{2} \int_{\Omega_i} \Big(\kappa_i \left(\nabla \boldsymbol{\theta} - \operatorname{div}(\boldsymbol{\theta}) \nabla \mathsf{T}_i - (\nabla^2 \mathsf{T}_i)\boldsymbol{\theta}\right) \cdot \nabla \phi_i \\
&\qquad - \left(\operatorname{div}(\boldsymbol{\theta}) \boldsymbol{u}_i \cdot \nabla \mathsf{T}_i + (\nabla^2 \mathsf{T}_i)\boldsymbol{u}_i \cdot \boldsymbol{\theta} + (\nabla \boldsymbol{u}_i)\boldsymbol{\theta} \cdot \nabla \mathsf{T}_i\right) \phi_i \Big) \mathrm{d}x, \\
I_2 &= -\frac{\kappa_s}{\eta} \int_\Gamma \left(\operatorname{div}_\tau(\boldsymbol{\theta})[\mathsf{T}][\phi] + \boldsymbol{\theta} \cdot [\nabla \mathsf{T}][\phi]\right) \mathrm{d}s, \\
I_3 &= -\kappa_s \int_\Gamma \left(H \operatorname{div}_\tau(\boldsymbol{\theta})[\mathsf{T}] \langle \phi \rangle - \Delta_\tau(\boldsymbol{\theta} \cdot \boldsymbol{n})[\mathsf{T}] \langle \phi \rangle + (\nabla H \cdot \boldsymbol{\theta})[\mathsf{T}] \langle \phi \rangle + H[\nabla \mathsf{T}] \cdot \boldsymbol{\theta} \langle \phi \rangle\right) \mathrm{d}s, \\
I_4 &= \eta \kappa_s \int_\Gamma \left((\nabla_\tau \boldsymbol{\theta} + \nabla_\tau \boldsymbol{\theta}^t - \operatorname{div}_\tau(\boldsymbol{\theta})\mathrm{I}) \nabla_\tau \langle \mathsf{T} \rangle) \cdot \nabla_\tau \langle \phi \rangle - \nabla_\tau (\nabla \langle \mathsf{T} \rangle \cdot \boldsymbol{\theta}) \cdot \nabla_\tau \langle \phi \rangle \right) \mathrm{d}s.
\end{aligned}$$

We treat each term separately. Let us first focus on I_1. Using the identity

$$\operatorname{div}((\boldsymbol{\theta} \cdot \nabla \phi_i) \nabla \mathsf{T}_i - (\nabla \mathsf{T}_i \cdot \nabla \phi_i)\boldsymbol{\theta}) = (\boldsymbol{\theta} \cdot \nabla \phi_i)\Delta \mathsf{T}_i + (\nabla \boldsymbol{\theta})\nabla \mathsf{T}_i \cdot \nabla \phi_i - \operatorname{div}(\boldsymbol{\theta})\nabla \mathsf{T}_i \cdot \nabla \phi_i - \boldsymbol{\theta} \cdot (\nabla^2 \mathsf{T}_i)\nabla \phi_i$$

and that the solution of the convection-diffusion equation (2.2) satisfies $\kappa_i \Delta \mathsf{T}_i = \nabla \mathsf{T}_i \cdot \boldsymbol{u}_i$ in Ω_i, we obtain

$$\begin{aligned}
I_1 &= \sum_{i=1}^{2} \int_{\Omega_i} \Big(\kappa_i \operatorname{div}\left((\boldsymbol{\theta} \cdot \nabla \phi_i)\nabla \mathsf{T}_i - (\nabla \mathsf{T}_i \cdot \nabla \phi_i)\boldsymbol{\theta}\right) - \boldsymbol{u}_i \cdot \nabla \mathsf{T}_i (\boldsymbol{\theta} \cdot \nabla \phi_i) \\
&\qquad - \left(\operatorname{div}(\boldsymbol{\theta}) \boldsymbol{u}_i \cdot \nabla \mathsf{T}_i + (\nabla^2 \mathsf{T}_i)\boldsymbol{u}_i \cdot \boldsymbol{\theta} + (\nabla \boldsymbol{u}_i)\boldsymbol{\theta} \cdot \nabla \mathsf{T}_i\right) \phi_i \Big) \mathrm{d}x \\
&= \sum_{i=1}^{2} \int_{\Omega_i} \left(\kappa_i \operatorname{div}((\boldsymbol{\theta} \cdot \nabla \phi_i)\nabla \mathsf{T}_i - (\nabla \mathsf{T}_i \cdot \nabla \phi_i)\boldsymbol{\theta}) - \operatorname{div}(\phi_i (\nabla \mathsf{T}_i \cdot \boldsymbol{u}_i)\boldsymbol{\theta}) \right) \mathrm{d}x.
\end{aligned}$$

Then, by the divergence theorem, we get

$$I_1 = \int_\Gamma \left(\left[\kappa \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} (\boldsymbol{\theta} \cdot \nabla \phi) - \kappa (\nabla \mathsf{T} \cdot \nabla \phi)(\boldsymbol{\theta} \cdot \boldsymbol{n}) \right] - [\phi (\nabla \mathsf{T} \cdot \boldsymbol{u})]\, (\boldsymbol{\theta} \cdot \boldsymbol{n}) \right) \mathrm{d}s,$$

and using that $\boldsymbol{u}_i = 0$ on Γ and the gradient decomposition $\nabla \phi = \nabla_\tau \phi + \frac{\partial \phi}{\partial \boldsymbol{n}} \boldsymbol{n}$,

$$I_1 = \int_\Gamma \left[\kappa \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} (\boldsymbol{\theta} \cdot \nabla_\tau \phi) - (\boldsymbol{\theta} \cdot \boldsymbol{n}) \kappa \nabla_\tau \mathsf{T} \cdot \nabla_\tau \phi \right] \mathrm{d}s.$$

Moreover, integrating by parts on Γ and using the identity $[ab] = [a] \langle b \rangle + \langle a \rangle [b]$, we have

$$\begin{aligned}
\int_\Gamma [\kappa \nabla_\tau \mathsf{T} \cdot \nabla_\tau \phi](\boldsymbol{\theta} \cdot \boldsymbol{n})\, \mathrm{d}s &= -\int_\Gamma [\operatorname{div}_\tau\left((\boldsymbol{\theta} \cdot \boldsymbol{n}) \kappa \nabla_\tau \mathsf{T}\right) \phi]\, \mathrm{d}s \\
&= -\int_\Gamma \left(\operatorname{div}_\tau((\boldsymbol{\theta} \cdot \boldsymbol{n}) \langle \kappa \nabla_\tau \mathsf{T} \rangle)[\phi] + \operatorname{div}_\tau((\boldsymbol{\theta} \cdot \boldsymbol{n})[\kappa \nabla_\tau \mathsf{T}] \langle \phi \rangle)\right) \mathrm{d}s.
\end{aligned}$$

Thus, integrating by parts appropriately on Γ and using the boundary conditions

$$\left\langle \kappa \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right\rangle = -\frac{\kappa_s}{\eta}[\mathsf{T}] \text{ and } \left[\kappa \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}}\right] = \eta\kappa_s \Delta_\tau \langle \mathsf{T} \rangle - \kappa_s H[\mathsf{T}] \text{ on } \Gamma,$$

we treat the first term

$$\begin{aligned}
I_1 &= \int_\Gamma \left(\left[\kappa \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}}\right] \boldsymbol{\theta} \cdot \nabla_\tau \langle \phi \rangle + \left\langle \kappa \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right\rangle \boldsymbol{\theta} \cdot \nabla_\tau [\phi] \right) \mathrm{d}s \\
&\quad + \int_\Gamma \Big(\mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n}) \langle \kappa \nabla_\tau \mathsf{T} \rangle)[\phi] + \mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n})[\kappa \nabla_\tau \mathsf{T}]) \langle \phi \rangle \Big) \mathrm{d}s \\
&= \int_\Gamma \left((\eta\kappa_s \nabla_\tau \langle \mathsf{T} \rangle - \kappa_s H[\mathsf{T}]) \nabla_\tau \langle \phi \rangle \cdot \boldsymbol{\theta} - \frac{\kappa_s}{\eta} \nabla_\tau [\phi] \cdot \boldsymbol{\theta} \right) \mathrm{d}s \\
&\quad + \int_\Gamma \left(\mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n}) \langle \kappa \nabla_\tau \mathsf{T} \rangle)[\phi] + \mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n})[\kappa \nabla_\tau \mathsf{T}]) \langle \phi \rangle \right) \mathrm{d}s \\
&= \int_\Gamma \left(\mathrm{div}_\tau(\kappa_s H[\mathsf{T}]\boldsymbol{\theta}) \langle \phi \rangle - \kappa_s H^2 [\mathsf{T}](\boldsymbol{\theta}\cdot\boldsymbol{n}) \langle \phi \rangle + \frac{\kappa_s}{\eta} \mathrm{div}_\tau([\mathsf{T}]\boldsymbol{\theta})[\phi] - \frac{\kappa_s}{\eta} H[\mathsf{T}](\boldsymbol{\theta}\cdot\boldsymbol{n})[\phi] \right) \mathrm{d}s \\
&\quad + \int_\Gamma \Big(\mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n}) \langle \kappa \nabla_\tau \mathsf{T} \rangle)[\phi] + \mathrm{div}_\tau((\boldsymbol{\theta}\cdot\boldsymbol{n})[\kappa \nabla_\tau \mathsf{T}]) \langle \phi \rangle + \eta\kappa_s \Delta_\tau \langle \mathsf{T} \rangle \nabla_\tau \langle \phi \rangle \cdot \boldsymbol{\theta} \Big) \mathrm{d}s.
\end{aligned}$$

For I_2 and I_3, we decompose the gradient, which yields to

$$\begin{aligned}
I_2 &= -\frac{\kappa_s}{\eta} \int_\Gamma \left(\mathrm{div}_\tau(\boldsymbol{\theta})[\mathsf{T}][\phi] + (\boldsymbol{\theta}\cdot\boldsymbol{n}) \left[\frac{\partial \mathsf{T}}{\partial \boldsymbol{n}}\right] [\phi] + (\boldsymbol{\theta} \cdot [\nabla_\tau \mathsf{T}])[\phi] \right) \mathrm{d}s \\
&= -\frac{\kappa_s}{\eta} \int_\Gamma \left(\mathrm{div}_\tau([\mathsf{T}]\boldsymbol{\theta})[\phi] + \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} (\boldsymbol{\theta}\cdot\boldsymbol{n}) \right) \mathrm{d}s
\end{aligned}$$

and

$$\begin{aligned}
I_3 &= -\kappa_s \int_\Gamma \Bigg(H\, \mathrm{div}_\tau(\boldsymbol{\theta})[\mathsf{T}]\langle \phi \rangle + H\boldsymbol{\theta} \cdot [\nabla_\tau \mathsf{T}] \langle \phi \rangle + H(\boldsymbol{\theta}\cdot\boldsymbol{n}) \left[\frac{\partial \mathsf{T}}{\partial \boldsymbol{n}}\right] \langle \phi \rangle \\
&\qquad + \left(-\Delta_\tau(\boldsymbol{\theta}\cdot\boldsymbol{n}) + \frac{\partial H}{\partial \boldsymbol{n}}(\boldsymbol{\theta}\cdot\boldsymbol{n}) + \boldsymbol{\theta}\cdot\nabla_\tau H \right) [\mathsf{T}] \langle \phi \rangle \Bigg) \mathrm{d}s \\
&= -\kappa_s \int_\Gamma \left(H\, \mathrm{div}_\tau([\mathsf{T}]\boldsymbol{\theta}) + H \left[\frac{\partial \mathsf{T}}{\partial \boldsymbol{n}}\right] (\boldsymbol{\theta}\cdot\boldsymbol{n}) - \Delta_\tau(\boldsymbol{\theta}\cdot\boldsymbol{n})[\mathsf{T}] + \frac{\partial H}{\partial \boldsymbol{n}}(\boldsymbol{\theta}\cdot\boldsymbol{n})[\mathsf{T}] + \boldsymbol{\theta}\cdot\nabla_\tau H[\mathsf{T}] \right) \langle \phi \rangle \, \mathrm{d}s \\
&= -\kappa_s \int_\Gamma \left(\mathrm{div}_\tau(H[\mathsf{T}]\boldsymbol{\theta}) + H \left[\frac{\partial \mathsf{T}}{\partial \boldsymbol{n}}\right] (\boldsymbol{\theta}\cdot\boldsymbol{n}) - \Delta_\tau(\boldsymbol{\theta}\cdot\boldsymbol{n})[\mathsf{T}] + \frac{\partial H}{\partial \boldsymbol{n}}(\boldsymbol{\theta}\cdot\boldsymbol{n})[\mathsf{T}] \right) \langle \phi \rangle \, \mathrm{d}s.
\end{aligned}$$

Finally, for I_4, thanks to Lemma 3.3, we have

$$\begin{aligned}
I_4 &= \eta\kappa_s \int_\Gamma \Big(\big(\nabla_\tau \boldsymbol{\theta} + \nabla_\tau \boldsymbol{\theta}^t - \mathrm{div}_\tau(\boldsymbol{\theta}) \mathrm{I}) \nabla_\tau \langle \mathsf{T} \rangle - \nabla_\tau \left(\boldsymbol{\theta} \cdot \nabla_\tau \langle \mathsf{T} \rangle \right) \big) \cdot \nabla_\tau \langle \phi \rangle \Big) \mathrm{d}s \\
&\quad - \eta\kappa_s \int_\Gamma \nabla_\tau \left((\boldsymbol{\theta}\cdot\boldsymbol{n}) \left\langle \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right\rangle \right) \cdot \nabla_\tau \langle \phi \rangle \, \mathrm{d}s \\
&= \eta\kappa_s \int_\Gamma \Big(\mathrm{div}_\tau \left(H(\boldsymbol{\theta}\cdot\boldsymbol{n}) \nabla_\tau \langle \mathsf{T} \rangle - 2(\boldsymbol{\theta}\cdot\boldsymbol{n})(\nabla_\tau \boldsymbol{n}) \nabla_\tau \langle \mathsf{T} \rangle \right) \langle \phi \rangle - \Delta_\tau \langle \mathsf{T} \rangle (\boldsymbol{\theta} \cdot \nabla_\tau \langle \phi \rangle) \Big) \mathrm{d}s \\
&\quad - \eta\kappa_s \int_\Gamma \nabla_\tau \left((\boldsymbol{\theta}\cdot\boldsymbol{n}) \left\langle \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right\rangle \right) \cdot \nabla_\tau \langle \phi \rangle \, \mathrm{d}s \\
&= \eta\kappa_s \int_\Gamma \Big(\mathrm{div}_\tau \left(H(\boldsymbol{\theta}\cdot\boldsymbol{n}) \nabla_\tau \langle \mathsf{T} \rangle - 2(\boldsymbol{\theta}\cdot\boldsymbol{n})(\nabla_\tau \boldsymbol{n}) \nabla_\tau \langle \mathsf{T} \rangle \right) \langle \phi \rangle - \Delta_\tau \langle \mathsf{T} \rangle (\boldsymbol{\theta} \cdot \nabla_\tau \langle \phi \rangle) \Big) \mathrm{d}s \\
&\quad + \eta\kappa_s \int_\Gamma \Delta_\tau \left((\boldsymbol{\theta}\cdot\boldsymbol{n}) \left\langle \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \right\rangle \right) \langle \phi \rangle \, \mathrm{d}s.
\end{aligned}$$

We conclude by adding I_1, I_2, I_3 and I_4. □

3.3 Shape derivative of the objective functionals

The volume. We recall that the shape derivative of the volume V is given, for all $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}}$ by

$$V'(\Gamma)(\boldsymbol{\theta}) = \int_{\Gamma} \boldsymbol{\theta} \cdot \boldsymbol{n} \, \mathrm{d}s. \tag{3.9}$$

The dissipated energy. We obtain the expression of the shape derivative of the dissipated energy (2.4) using Proposition 3.1 and the chain rule (see also [6, 22, 12] for details). In the following, to simplify the writing, we define the region sign s_i as

$$s_i = \begin{cases} 1 & \text{if} \quad i = 1, \\ -1 & \text{if} \quad i = 2. \end{cases}$$

Proposition 3.5 (Shape derivative of the dissipation energy)**.** *Let $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}}$ and, for $i = 1, 2$, let $(\boldsymbol{v}_i, q_i) \in \mathcal{V}_0(\Omega_i) \times \mathrm{L}^2(\Omega_i)$ be the solution of the following adjoint equation of the Navier-Stokes equations associated to the dissipation energy:*

$$\left\{ \begin{array}{rll} -\nu_i \Delta \boldsymbol{v}_i + (\nabla \boldsymbol{u}_i)^t \boldsymbol{v}_i - (\nabla \boldsymbol{v}_i) \boldsymbol{u}_i + \dfrac{1}{\rho_i} \nabla q_i & = -2\nu_i \Delta \boldsymbol{u}_i & \text{in } \Omega_i, \\ \mathrm{div}(\boldsymbol{v}_i) & = 0 & \text{in } \Omega_i, \\ \boldsymbol{v}_i & = 0 & \text{on } \Gamma_{\mathrm{D},i} \cup \Gamma_{\mathrm{e},i} \cup \Gamma, \\ \sigma(\boldsymbol{v}_i, q_i)\boldsymbol{n} + (\boldsymbol{u}_i \cdot \boldsymbol{n})\boldsymbol{v}_i & = 4\nu \varepsilon(\boldsymbol{u}_i)\boldsymbol{n} & \text{on } \Gamma_{\mathrm{N},i}. \end{array} \right. , \tag{3.10}$$

If $(\boldsymbol{u}_i, p_i), (\boldsymbol{v}_i, q_i) \in \mathrm{H}^2(\Omega_i)^d \times \mathrm{H}^1(\Omega_i)$, then the shape derivative of the dissipation energy is given by

$$D_i'(\Gamma)(\boldsymbol{\theta}) = 2\nu_i \int_{\Gamma} s_i (\varepsilon(\boldsymbol{u}_i) : \varepsilon(\boldsymbol{v}_i) - |\varepsilon(\boldsymbol{u}_i)|^2)(\boldsymbol{\theta} \cdot \boldsymbol{n}) \, \mathrm{d}s. \tag{3.11}$$

Heat exchanged. We define the two following mappings $f_i \in (\mathrm{H}^1(\Omega_i))'$ and $\boldsymbol{g}_i \in (\mathrm{H}^1(\Omega_i)^d)'$, given by:

$$\begin{array}{rcl} \langle f_i, \mathsf{S} \rangle_{(\mathrm{H}^1(\Omega_i))', \mathrm{H}^1(\Omega_i)} & = & \displaystyle\int_{\Omega_i} s_i \boldsymbol{u}_i \cdot \nabla \mathsf{S}_i \, \mathrm{d}x, \quad \forall \mathsf{S} \in \mathrm{H}^1(\Omega_i), \\ \langle \boldsymbol{g}_i, \boldsymbol{w} \rangle_{(\mathrm{H}^1(\Omega_i)^d)', \mathrm{H}^1(\Omega_i)^d} & = & \displaystyle\int_{\Omega_i} s_i \boldsymbol{w} \cdot \nabla \mathsf{T}_i \, \mathrm{d}x, \quad \forall \boldsymbol{w} \in \mathrm{H}^1(\Omega_i)^d, \end{array}$$

where $\boldsymbol{u}_i$ and T_i are the respective solutions of (2.1) and (2.2).

Proposition 3.6 (Shape derivative of the exchanged heat)**.** *Let $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}}$ and let introduce $\mathsf{R} = (\mathsf{R}_1, \mathsf{R}_2) \in \mathcal{H}_0(\Omega_1, \Omega_2)$ the adjoint of the approximated-convection diffusion equation* (2.1) *associated to the heat exchanged:*

$$\left\{ \begin{array}{rcl} -\,\mathrm{div}(\kappa_i \nabla \mathsf{R}_i + \mathsf{R}_i \boldsymbol{u}_i) & = & f_i \ \text{in } \Omega_i, i = 1, 2, \\ \mathsf{R}_i & = & 0 \ \text{on } \Gamma_{\mathrm{D},i}, i = 1, 2, \\ \kappa_i \dfrac{\partial \mathsf{R}_i}{\partial \boldsymbol{n}} & = & 0 \ \text{on } \Gamma_{\mathrm{N,i}} \cup \Gamma_{\mathrm{e,i}}, i = 1, 2, \\ \left\langle \kappa \dfrac{\partial \mathsf{R}}{\partial \boldsymbol{n}} \right\rangle & = & -\dfrac{\kappa_s}{\eta} [\mathsf{R}] - \kappa_s H \langle \mathsf{R} \rangle \ \text{on } \Gamma, \\ \left[\kappa \dfrac{\partial \mathsf{R}}{\partial \boldsymbol{n}} \right] & = & \eta \, \mathrm{div}_\tau (\kappa_s \nabla_\tau \langle \mathsf{R} \rangle) \ \text{on } \Gamma, \\ \kappa_i \dfrac{\partial \mathsf{R}_i}{\partial \boldsymbol{n}} & = & 0 \ \text{on } \partial\Gamma, i = 1, 2, \end{array} \right. \tag{3.12}$$

and $(\boldsymbol{v}_i, q_i) \in \mathcal{V}_0(\Omega_i) \times \mathrm{L}^2(\Omega_i)$ *the adjoint of the Navier-Stokes equations* (2.1) *associated to the heat exchanged:*

$$\left\{ \begin{array}{rcl} -\nu_i \Delta \boldsymbol{v}_i + (\nabla \boldsymbol{u}_i)^t \boldsymbol{v}_i - (\nabla \boldsymbol{v}_i)\boldsymbol{u}_i + \dfrac{1}{\rho_i}\nabla q_i & = & -\mathsf{R}_i \nabla \mathsf{T}_i + \boldsymbol{g}_i \text{ in } \Omega_i, \\ \mathrm{div}(\boldsymbol{v}_i) & = & 0 \text{ in } \Omega_i, \\ \boldsymbol{v}_i & = & 0 \text{ on } \Gamma_{\mathrm{D},i} \cup \Gamma \cup \Gamma_{\mathrm{e,i}}, \\ \sigma(\boldsymbol{v}_i, q_i)\boldsymbol{n} & = & 0 \text{ on } \Gamma_{\mathrm{N,i}}, \end{array} \right. \tag{3.13}$$

for each $i = 1, 2$.

The heat exchanged W *defined in* (2.3) *is shape differentiable and if* $\mathsf{T} = (\mathsf{T}_1, \mathsf{T}_2) \in \mathrm{H}^2(\Omega_1, \Gamma) \times \mathrm{H}^2(\Omega_2, \Gamma)$*,* $\mathsf{R} = (\mathsf{R}_1, \mathsf{R}_2) \in \mathrm{H}^2(\Omega_1, \Gamma) \times \mathrm{H}^2(\Omega_2, \Gamma)$ *and* $(\boldsymbol{u}_i, p_i), (\boldsymbol{v}_i, q_i) \in \mathrm{H}^2(\Omega_i)^d \times \mathrm{H}^1(\Omega_i)$*, then the shape derivative* $W'(\Gamma)(\boldsymbol{\theta})$ *can be expressed in the following surface shape derivative form:*

$$\begin{aligned} W'(\Gamma)(\boldsymbol{\theta}) = & \int_\Gamma \left(2[\nu \varepsilon(\boldsymbol{u}) : \varepsilon(\boldsymbol{v})] - [\kappa \nabla \mathsf{T} \cdot \nabla \mathsf{R}] + 2\left[\kappa \frac{\partial \mathsf{T}}{\partial \boldsymbol{n}} \frac{\partial \mathsf{R}}{\partial \boldsymbol{n}}\right] \right) (\boldsymbol{\theta} \cdot \boldsymbol{n}) \, \mathrm{d}s \\ & - \int_\Gamma \left(\eta \kappa_s (H\mathrm{I} - 2\nabla_\tau \boldsymbol{n}) \nabla_\tau \langle \mathsf{T} \rangle \cdot \nabla_\tau \langle \mathsf{R} \rangle + \frac{\kappa_s}{\eta} H [\mathsf{T}][\mathsf{R}] \right) (\boldsymbol{\theta} \cdot \boldsymbol{n}) \, \mathrm{d}s \\ & - \kappa_s \int_\Gamma \left(H^2 [\mathsf{T}] \langle \mathsf{R} \rangle - \Delta_\tau([\mathsf{T}]\langle \mathsf{R} \rangle) + \frac{\partial H}{\partial \boldsymbol{n}} [\mathsf{T}] \langle \mathsf{R} \rangle \right) (\boldsymbol{\theta} \cdot \boldsymbol{n}) \, \mathrm{d}s. \end{aligned} \tag{3.14}$$

Remark 3.7. *Both adjoint equations* (3.12) *and* (3.13) *are well-posed. The adjoint of the approximated convection-diffusion equation is well-posed by Lax-Milgram, analogously to* (2.2) *(see [10]). The equation* (3.10) *is a linearization of the Navier-Stokes (transposed) and the proof is an adaptation of the Navier-Stokes case (see [19, Chapter IV] or [9] for details).*

Proof. Step 1: differentiability. The crucial point is the differentiability in a neighborhood of 0, of $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}} \mapsto \overline{\mathsf{T}}_{\boldsymbol{\theta}} \in \mathcal{H}^1(\Omega_1, \Omega_2)$ and $\boldsymbol{\theta} \in \Theta_{\mathrm{ad}} \mapsto \overline{u}_{\boldsymbol{\theta},i} \in \mathrm{H}^1(\Omega_i)^d, i = 1, 2$. The first one was proved in Proposition 3.2 and the second one in [9]. Then, recalling that

$$W(\Gamma^{\boldsymbol{\theta}}) = \sum_{i=1}^{2} \int_{\Omega_i^{\boldsymbol{\theta}}} s_i \boldsymbol{u}_{\boldsymbol{\theta},i} \cdot \nabla \mathsf{T}_{\boldsymbol{\theta},i} \, \mathrm{d}x,$$

and doing a change of variables (similarly to the proof of Proposition 3.2), we obtain

$$W(\Gamma^{\boldsymbol{\theta}}) = \sum_{i=1}^{2} \int_{\Omega_i} s_i (\mathrm{I} + \nabla \boldsymbol{\theta})^{-1} \overline{\boldsymbol{u}}_{\boldsymbol{\theta},i} \cdot \nabla \overline{\mathsf{T}}_{\boldsymbol{\theta},i} |\det(\mathrm{I} + \nabla \boldsymbol{\theta})| \, \mathrm{d}x. \tag{3.15}$$

Using the chain rule (the differentiability of the other terms is classical, though it was discussed in the proof of Proposition 3.2), we conclude that W is shape differentiable.

Step 2: shape derivative computation. Since $\boldsymbol{u}_i \in \mathrm{H}^2(\Omega_i)^d$ and $\mathsf{T}_i \in \mathrm{H}^2(\Omega_i, \Gamma)$, $i = 1, 2$, then thanks to Proposition 3.4, $\boldsymbol{u}_i' \in \mathrm{H}^1(\Omega_i)^d$ and $\mathsf{T}_i' \in \mathrm{H}^1(\Omega_i, \Gamma)$. Differentiating (2.3), using the classical formulas of shape derivatives of integral functionals and by chain rule,

$$W'(\Gamma)(\boldsymbol{\theta}) = \sum_{i=1}^{2} \int_{\Omega_i} s_i \left(\boldsymbol{u}_i \cdot \nabla \mathsf{T}_i' + \boldsymbol{u}_i' \cdot \nabla \mathsf{T}_i \right) \, \mathrm{d}x + \sum_{i=1}^{2} \int_\Gamma s_i (\boldsymbol{u}_i \cdot \nabla \mathsf{T}_i)(\boldsymbol{\theta} \cdot \boldsymbol{n}_i) \, \mathrm{d}s,$$

where $\boldsymbol{n}_i$ is the unitary normal at Γ, exterior to Ω_i. Using that $\boldsymbol{u}_i = 0$ on Γ, we obtain:

$$W'(\Gamma)(\boldsymbol{\theta}) = \sum_{i=1}^{2} \int_{\Omega_i} s_i \left(\boldsymbol{u}_i \cdot \nabla \mathsf{T}_i' + \boldsymbol{u}_i' \cdot \nabla \mathsf{T}_i \right) \, \mathrm{d}x. \tag{3.16}$$

Then, we proceed as it is standard, this is, we multiply each equation of the shape derivative of the states by its respective adjoint, and then we integrate by parts using the boundary conditions that satisfy each solution. Conversely, we multiply the adjoint equation by the corresponding shape derivative and then we integrate. Hence, multiplying (3.8) by R, (3.3) by $\boldsymbol{v}_i$, (3.12) by T', (3.13) by $\boldsymbol{u}_i'$ and integrating in Ω (or Ω_i in the Navier-Stokes case), we get

$$\sum_{i=1}^{2}\int_{\Omega_i}(\kappa_i\nabla\mathsf{T}_i'\cdot\nabla\mathsf{R}_i+\mathsf{R}_i\boldsymbol{u}_i\cdot\nabla\mathsf{T}_i'+\mathsf{R}_i\boldsymbol{u}_i'\cdot\nabla\mathsf{T}_i)\,\mathrm{d}x$$
$$+\int_\Gamma\left(\eta\kappa_s\nabla_\tau\langle\mathsf{T}'\rangle\cdot\nabla_\tau\langle\mathsf{R}\rangle+\kappa_s H[\mathsf{T}']\langle\mathsf{R}\rangle+\frac{\kappa_s}{\eta}[\mathsf{T}'][\mathsf{R}]\right)\mathrm{d}s$$
$$=\int_\Gamma(\xi_1(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n})[\mathsf{R}]+\xi_2(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n})\langle\mathsf{R}\rangle)\,\mathrm{d}s,\quad(3.17)$$

$$\int_{\Omega_i}\left(2\nu_i\varepsilon(\boldsymbol{u}_i'):\varepsilon(\boldsymbol{v}_i)+(\nabla\boldsymbol{u}_i')\boldsymbol{u}_i\cdot\boldsymbol{v}_i+(\nabla\boldsymbol{u}_i)\boldsymbol{u}_i'\cdot\boldsymbol{v}_i-\frac{q_i}{\rho_i}\operatorname{div}(\boldsymbol{u}_i')-\frac{p_i'}{\rho_i}\operatorname{div}(\boldsymbol{v}_i)\right)\mathrm{d}x=0,\quad(3.18)$$

$$\sum_{i=1}^{2}\int_{\Omega_i}(\kappa_i\nabla\mathsf{R}_i\cdot\nabla\mathsf{T}_i'+\mathsf{R}_i\boldsymbol{u}_i\cdot\nabla\mathsf{T}_i')\,\mathrm{d}x$$
$$+\int_\Gamma\left(\eta\kappa_s\nabla_\tau\langle\mathsf{R}\rangle\cdot\nabla_\tau\langle\mathsf{T}'\rangle+\kappa_s H[\mathsf{R}]\langle\mathsf{T}'\rangle+\frac{\kappa_s}{\eta}[\mathsf{R}][\mathsf{T}']\right)\mathrm{d}s=\sum_{i=}^{2}\int_{\Omega_i}s_i\nabla\mathsf{T}_i'\cdot\boldsymbol{u}_i\,\mathrm{d}x,\quad(3.19)$$

and

$$\int_{\Omega_i}\left(2\nu_i\varepsilon(\boldsymbol{v}_i):\varepsilon(\boldsymbol{u}_i')+(\nabla\boldsymbol{u}_i')\boldsymbol{u}_i\cdot\boldsymbol{v}_i+(\nabla\boldsymbol{u}_i)\boldsymbol{u}_i'-\frac{q_i}{\rho_i}\operatorname{div}(\boldsymbol{u}_i')-\frac{p_i'}{\rho_i}\operatorname{div}(\boldsymbol{v}_i)\right)\mathrm{d}x$$
$$+\int_{\Omega_i}\mathsf{R}_i\nabla\mathsf{T}_i\cdot\boldsymbol{u}_i'\,\mathrm{d}x+\int_\Gamma s_i\sigma(\boldsymbol{v}_i,q_i)\boldsymbol{n}\cdot\frac{\partial\boldsymbol{u}_i}{\partial\boldsymbol{n}}(\boldsymbol{\theta}\cdot\boldsymbol{n})\,\mathrm{d}s=\sum_{i=1}^{2}\int_{\Omega_i}s_i\nabla\mathsf{T}_i\cdot\boldsymbol{u}_i'\,\mathrm{d}x.\quad(3.20)$$

Using the above identities in (3.16), we obtain

$$W'(\Gamma)(\boldsymbol{\theta})=\int_\Gamma\left([\sigma(\boldsymbol{v},q)\boldsymbol{n}\cdot\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{n}}(\boldsymbol{\theta}\cdot\boldsymbol{n})]+\xi_1(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n})[\mathsf{R}]+\xi_2(\mathsf{T},\boldsymbol{\theta}\cdot\boldsymbol{n})\langle\mathsf{R}\rangle\right)\mathrm{d}s.$$

Integrating by parts and using that $\left[\sigma(\boldsymbol{v},q)\boldsymbol{n}\cdot\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{n}}(\boldsymbol{\theta}\cdot\boldsymbol{n})\right]=2[\varepsilon(\boldsymbol{u}):\varepsilon(\boldsymbol{v})]$, we get

$$W'(\Gamma)(\boldsymbol{\theta})\quad=\quad\int_\Gamma f\,(\boldsymbol{\theta}\cdot\boldsymbol{n})\,\mathrm{d}s,$$

where

$$f=2[\nu\varepsilon(\boldsymbol{u}):\varepsilon(\boldsymbol{v})]-[\kappa\nabla_\tau\mathsf{T}\cdot\nabla_\tau\mathsf{R}]-\eta\kappa_s(H\mathrm{I}-2\nabla_\tau\boldsymbol{n})\nabla_\tau\langle\mathsf{T}\rangle\cdot\nabla_\tau\langle\mathsf{R}\rangle+\frac{\kappa_s}{\eta}H[\mathsf{T}][\mathsf{R}]$$
$$-\kappa_s\left(H^2[\mathsf{T}]\langle\mathsf{R}\rangle-\Delta_\tau([\mathsf{T}]\langle\mathsf{R}\rangle)+\frac{\partial H}{\partial\boldsymbol{n}}[\mathsf{T}]\langle\mathsf{R}\rangle\right)+\eta\kappa_s\Delta_\tau(\langle\mathsf{R}\rangle)\left\langle\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right\rangle$$
$$-\frac{\kappa_s}{\eta}[\mathsf{R}]\left[\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right]-\kappa_s H\langle\mathsf{R}\rangle\left[\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right].$$

Since R is the solution of the adjoint of the convection-diffusion equation (3.13),

$$\eta\kappa_s\Delta_\tau(\langle\mathsf{R}\rangle)\left\langle\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right\rangle-\frac{\kappa_s}{\eta}[\mathsf{R}]\left[\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right]-\kappa_s H\langle\mathsf{R}\rangle\left[\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right]=\left[\kappa\frac{\partial\mathsf{R}}{\partial\boldsymbol{n}}\frac{\partial\mathsf{T}}{\partial\boldsymbol{n}}\right],$$

leading to the same expression as in (3.14). □

4 Numerical methods used to solve the involved problems

4.1 Shape optimization framework

The level-set method. In the context of shape optimization, the level set evolution method was introduced by Allaire *et al.* in [4]. The domain Ω is fixed, we describe each subdomain Ω_i by means of a level set function $\phi:\Omega\to\mathbb{R}$ to track the interface Γ that we aim to optimize. Then, the mesh on Ω is done based on the level-set ϕ, identifying Γ to the zero level set of ϕ:

$$\begin{cases} x\in\Omega_1 & \Longleftrightarrow & \phi(x)<0,\\ x\in\Gamma & \Longleftrightarrow & \phi(x)=0,\\ x\in\Omega_2 & \Longleftrightarrow & \phi(x)>0.\end{cases}$$

After initialization, at the step n of the shape optimization process, we compute the level set ϕ^n by solving the following equation,

$$\begin{cases}\dfrac{\partial\phi^n}{\partial t}+\boldsymbol{\theta}\cdot\nabla\phi^n=0, & 0<t<\tau,\ x\in\Omega,\\ \phi^n(0,x)=\phi^{n-1}(x), & x\in\Omega,\end{cases}\tag{4.1}$$

where $\tau>0$ is the descent step in the shape optimization algorithm and $\boldsymbol{\theta}$ is an appropriate velocity field, such that $\tau\|\boldsymbol{\theta}\|_{\mathrm{L}^\infty(\Omega)^d}$ is of the order of mesh size h. Numerically speaking, Equation (4.1) can be computed by ADVECT (see [7]) and the remeshing step by MMG (see [13]).

Null space optimization method. As constrained optimization algorithm, we rely on the *null space algorithm* introduced in [17] under the implementation of Feppon [15]. This method first decreases the violation of the constraint in order to be feasible, then minimizes the objective function. The used descent direction $\boldsymbol{\theta}$ is obtained by an extension-regularization procedure: *find* $\boldsymbol{\theta}\in\Theta_{\mathrm{er}}=\{\boldsymbol{\psi}\in\mathrm{H}^1(\Omega)^d;\ \boldsymbol{\psi}=0 \text{ on } \partial\Omega;\ \boldsymbol{\psi}=0 \text{ in } \Omega^\delta_{\mathrm{D},1}\cup\Omega^\delta_{\mathrm{D},2}\}$, *such that* for all $\boldsymbol{\psi}\in\Theta_{\mathrm{er}}$,

$$\int_\Omega 100h^2\nabla\boldsymbol{\theta}:\nabla\boldsymbol{\psi}+\boldsymbol{\theta}\cdot\boldsymbol{\psi}\,\mathrm{d}x=J'(\Gamma)(\boldsymbol{\psi}),\tag{4.2}$$

where h is the mesh size and $J(\Gamma)$ is a linear combination between the functionals involved in the problem: $W(\Gamma),D_1(\Gamma),D_2(\Gamma)$ and $V(\Gamma)$, which weights are given by the optimization algorithm. The output deformation field is such that $\|\boldsymbol{\theta}\|_{\mathrm{L}^\infty(\Omega)^d}$ is of the order of the mesh size scale h and the the optimization step τ can be chosen as 1.

4.2 Numerical resolution with FEM

Navier-Stokes equations. We use the augmented Lagrangian preconditionner proposed by [24] to solve the Navier-Stokes equations (2.1). In this method, one penalizes the divergence and uses a Newton iteration method with a field split structure. We also penalize the divergence for the adjoint equation (3.13). We use the softwares FreeFem++ (see [20]) and PETSc (see [5]).

Nitsche extended finite element method for a Ventcel transmission problem with discontinuities at the interface The approximate convection-diffusion (2.2) and its adjoint equations can not be implemented directly due to the use of the broken Sobolev spaces such as $\mathcal{H}_0(\Omega_1, \Omega_2)$. Allaire *et al* proposed a method in [3] to approximate this kind of equations in order to use any finite element software with spaces of continuous functions. However this method involves to duplicate the degrees of freedom, which we do not want for our 3D simulations. Indeed, it becomes very expensive in our context. In the case of the variational formulation (2.8) of the convection-diffusion problem (2.2), the associated bilinear form, denoted by $a(\cdot,\cdot)$, can be split as $a(\cdot,\cdot) = b(\cdot,\cdot) + c(\cdot,\cdot)$, where

$$\begin{aligned} b(\phi, \mathsf{S}) &= \sum_{i=1}^{2} \int_{\Omega_i} (\kappa_i \nabla\phi_i \cdot \nabla \mathsf{S}_i + \mathsf{S}_i \boldsymbol{u}_i \cdot \nabla\phi_i)\, \mathrm{d}x + \int_\Gamma (\eta\kappa_{\mathrm{s}} \nabla_\tau \langle\phi\rangle \cdot \nabla_\tau \langle \mathsf{S}\rangle + \kappa_{\mathrm{s}} H[\phi]\langle \mathsf{S}\rangle)\, \mathrm{d}s, \\ c(\phi, \mathsf{S}) &= \frac{\kappa_{\mathrm{s}}}{\eta} \int_\Gamma [\phi][\mathsf{S}]\, \mathrm{d}s, \end{aligned}$$

defined for any $\phi, \mathsf{S} \in \mathcal{H}^1(\Omega_1, \Omega_2)$. In our the case, the model comes from an asymptotic development and the parameter η is takes small values. The term $c(\mathsf{T}, \mathsf{S})$ then produces poor conditioning and the resolution based on this formulation is then slow and unprecise.

We hence use instead the Nitsche approach [25] introduced in [8] to stabilize our formulation with respect to η by improving the conditioning of the matrix. Since this is a dedicated method, we briefly present it. For the sake of simplicity, in this part, we suppose T_{D} to be a $\mathbb{P}^1$ function (defined in all Ω).

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

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

Then, we define the following mesh-depending bilinear form, for any $\mathsf{T}_h, \mathsf{S}_h \in \mathrm{P}^1_h$,

$$a_h(\mathsf{T}_h, \mathsf{S}_h) = a(\mathsf{T}_h, \mathsf{S}_h) - \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{\gamma\eta h_F}{\eta + \gamma\kappa_{\mathrm{s}} h_F} \left(\left\langle \kappa \frac{\partial \mathsf{T}_h}{\partial \boldsymbol{n}} \right\rangle + \frac{\kappa_{\mathrm{s}}}{\eta}[\mathsf{T}_h], \left\langle \kappa \frac{\partial \mathsf{S}_h}{\partial \boldsymbol{n}} \right\rangle + \frac{\kappa_{\mathrm{s}}}{\eta}[\mathsf{S}_h] \right)_{\mathrm{L}^2(F)}.$$

where $\gamma > 0$ is a stabilization parameter, that it chosen small enough in order to guarantee the coercivity of a_h. To approximate the solution of (2.2), we consider the Nitsche type formulation:

$$\begin{aligned} &\textit{Find } \mathsf{T}_h \in \mathrm{P}^1_h \textit{ with } \mathsf{T}_h = \mathsf{T}_{\mathrm{D}} \textit{ on } \Gamma_{\mathrm{D}}, \textit{ such that} \\ &a_h(\mathsf{T}_h, \mathsf{S}_h) = 0, \quad \forall \mathsf{S}_h \in \mathrm{P}^1_{h,0}. \end{aligned} \tag{4.3}$$

By adapting the arguments of [8, Theorem 4.6]), we can easily provide error estimates stated as usually in Nitsche method in the mesh-dependent norm on P^1_h defined by:

$$|||\cdot|||_h^2 = \sum_{i=1}^{2} \|\kappa_i^{1/2} \nabla \cdot\|^2_{\mathrm{L}^2(\Omega_i)^d} + \|(\kappa_s\eta)^{1/2} \nabla_\tau \langle\cdot\rangle\|^2_{\mathrm{L}^2(\Gamma)^d} + \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{\kappa_s}{\eta + \gamma\kappa_s h_F} \|[\cdot]\|^2_{\mathrm{L}^2(F)}.$$

Theorem 4.1 (Error estimate in energy norm)**.** *Let $\mathsf{T} \in \mathcal{H}_{\mathsf{T}_{\mathrm{D}}}(\Omega_1, \Omega_2)$ the solution of the continuous convection-diffusion equation* (2.2) *and T_h the solution of the (discrete) Nitsche problem* (4.3)*. If in addition $\mathsf{T} \in \mathcal{H}^2(\Omega_1, \Omega_2)$, for γ sufficiently small, there exists a constant $C > 0$ independent of h and η such that:*

$$|||\mathsf{T} - \mathsf{T}_h|||_h \le Ch \left(\sum_{i=1}^{2} \|\kappa_i^{1/2} (\mathsf{T}_i - \mathsf{T}_{\mathrm{D,i}})\|^2_{\mathrm{H}^2(\Omega_i)} + \|(\kappa_s\eta)^{1/2} \langle \mathsf{T}\rangle\|^2_{\mathrm{H}^2(\Gamma)} + \sum_{F \in \mathcal{F}_{h,\Gamma}} \frac{\kappa_s}{\gamma h_F} \|[\mathsf{T}]\|^2_{\mathrm{H}^1(F)} \right)^{1/2}.$$

We proceed in a similar way concerning the adjoint equation (3.12).

Numerical computation of the curvature terms. We conclude this part by highlighting some original features and difficulties in computing the shape derivatives involved in the problem under consideration. In particular, we recall how to compute numerically a regularized version of the discretized unit normal and a discretized version of the mean curvature. Finally, the term $\partial_{\boldsymbol{n}} H$ in the shape derivative expressions (3.14) is delicate to treat: consequently, we now explain how we deal with it. The issue comes when we use the level formalism and in particular $\mathbb{P}^1$ finite elements as discretization of the signed distance function d_{Ω_1}.

Let us first explain how to compute the extensions of the unit normal and the mean curvature. As we said earlier in (3.1), we have that

$$\boldsymbol{n} = \nabla d_{\Omega_1} \quad \text{and} \quad H = \Delta d_{\Omega_1} \quad \text{on } \Gamma.$$

Numerically, we compute d_{Ω_1} by using MSHDIST [14], discretized as a $\mathbb{P}^1$ function denoted d_h in the following. Then, we follow the work [18] that proposes a variational method to regularize and approximate the mean curvature in the following two steps. Firstly, we solve the following problem:

$$\begin{gathered} \textit{Find } \boldsymbol{g}_h \in (\mathrm{H}^1(\Omega) \cap \mathbb{P}^1)^d \textit{ such that,} \\ \forall \boldsymbol{\varphi}_h \in (\mathrm{H}^1(\Omega) \cap \mathbb{P}^1)^d, \qquad \int_\Omega \boldsymbol{g}_h \cdot \boldsymbol{\varphi}_h \,\mathrm{d}x = \int_\Omega \nabla d_h \cdot \boldsymbol{\varphi}_h \,\mathrm{d}x. \end{gathered}$$

The output $\boldsymbol{g}_h$ is a regularized version of $\boldsymbol{n}_h = \nabla d_h$, since it is $\mathbb{P}^1$ instead of $\mathbb{P}^0$. Similarly, we compute a discretized version of the mean curvature H to be $\mathbb{P}^1$, denoted by H_h by solving the problem:

$$\begin{gathered} \textit{Find } H_h \in \mathrm{H}^1(\Omega) \cap \mathbb{P}^1 \textit{ such that,} \\ \forall \phi_h \in \mathrm{H}^1(\Omega) \cap \mathbb{P}^1, \qquad \int_\Omega \left(10h^2 \nabla H_h \cdot \nabla \phi_h + H_h \phi_h\right) \,\mathrm{d}x = \int_\Omega \mathrm{div}(g_h)\phi_h \,\mathrm{d}x. \end{gathered}$$

To compute $\partial_{\boldsymbol{n}} H$, we use the identity $\partial_{\boldsymbol{n}} H = -\|\nabla \boldsymbol{n}\|_F^2$, where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix. Hence we use the previous formula, also used in [23], with $\boldsymbol{g}_h$ as discretization of $\boldsymbol{n}$. For the sake of completeness, we detail the proof this relation: $\boldsymbol{n} = \nabla d_{\Omega_1}$ is an extension of the unit normal to $\partial\Omega_1$, unitary in a neighborhood of $\partial\Omega_1$ $\|\boldsymbol{n}\|^2 = \|\nabla d_{\Omega_1}\|^2 = 1$ in a neighborhood of $\partial\Omega_1$. Differentiating this identity, in particular we get $\Delta(\|\boldsymbol{n}\|^2) = 0$ on $\partial\Omega_1$, and using the identity $\Delta(\boldsymbol{u} \cdot \boldsymbol{v}) = \mathrm{I}\Delta \boldsymbol{u} \cdot \boldsymbol{v} + \mathrm{I}\Delta \boldsymbol{v} \cdot \boldsymbol{u} + 2\nabla \boldsymbol{u} : \nabla \boldsymbol{v}$ with $\boldsymbol{u} = \boldsymbol{v} = \boldsymbol{n}$, we obtain:

$$2\mathrm{I}\Delta \boldsymbol{n} \cdot \boldsymbol{n} + 2\|\nabla \boldsymbol{n}\|_F^2 = 0.$$

4.3 Summary: brief description of the algorithm used

To summarize the complete shape optimization procedure, we present below each step with the associated computational code or library we use in Algorithm 1.

5 Numerical results

In this final section, we present the numerical simulations that we have performed in the three-dimensional case. We will focus on two typical situations in heat exchangers: crossflow and co-current flow. The purpose of these simulations is to illustrate our results and prove the feasibility and effectiveness of the proposed method. We performed medium/large scale numerical simulations, ranging from 100 to 500 thousand vertices and 1 to 2.5 million tetrahedra. In this way, we illustrate the ability of the method studied to provide new designs that increase the performance of the initial design of the heat exchanger while verifying the constraints.

Algorithm 1 Level-set mesh evolution method

Require an initial split domain $\Omega_1^0, \Omega_2^0 \subset \Omega$.
for $n = 0, \ldots, n_{\text{maxiter}}$ **do**
  Current subdomains Ω_1^n, Ω_2^n represented by the mesh $\mathcal{T}_{\Omega_i^n} \subset \mathcal{T}_\Omega$, $i = 1, 2$.
  Solve (2.1): the Navier-Stokes equations. ▷ FreeFem++
  Solve (3.10): the adjoint equation of the Navier-Stokes equations associated to the dissipation energy. ▷ FreeFem++
  Solve (2.2): the convection-diffusion equation, using Nitsche method. ▷ C++ in-house code
  Solve (3.12): the adjoint equation of the convection-diffusion equation associated to the heat exchanged, using Nitsche method. ▷ C++ in-house code
  Solve (3.13): the adjoint equation of the Navier-Stokes equations associated to the heat exchanged. ▷ FreeFem++
  Compute the gradients by extension-regularization. ▷ FreeFem++
  Compute the deformation field $\boldsymbol{\theta}$. ▷ Null-space algorithm
  Update the level-set function ϕ^{n+1} by advection. ▷ mshdist and advect
  Remesh thanks to ϕ^{n+1}. ▷ mmg
end for

We will solve the problem (2.6) for two different test cases where we choose $D_{0,i}$, $i = 1, 2$ as k times ($k \in \mathbb{N}^*$) the initial dissipation of the fluid i and V_0 as the initial volume of the hot fluid. In the following, we consider the box $\Omega = [0,1] \times [0,1] \times [0,1]$. Moreover, we fix some constants $r_1, r_2, y_c, Y_c > 0$ (described below for each case) and we then define

$$\begin{aligned}
\Gamma_{\mathrm{D},1} &= \{(x,y,0) \in \Omega; (x-0.5)^2 + (y-y_c)^2 = r_1^2\}, \\
\Gamma_{\mathrm{N},1} &= \{(x,y,1) \in \Omega; (x-0.5)^2 + (y-Y_c)^2 = r_1^2\}, \\
\Gamma_{\mathrm{D},2} &= \{(x,0,z) \in \Omega; (x-0.5)^2 + (z-0.5)^2 = r_2^2\}, \\
\Gamma_{\mathrm{N},2} &= \{(x,1,z) \in \Omega; (x-0.5)^2 + (z-0.5)^2 = r_2^2\}.
\end{aligned}$$

Additionally, we consider the following inlet velocity

$$\begin{aligned}
\boldsymbol{u}_{\mathrm{D},1} &= (0, 0, (r_1^2 - (x-0.5)^2 - (y-y_c)^2)/r_1^2), \\
\boldsymbol{u}_{\mathrm{D},2} &= (0, (r_2^2 - (x-0.5)^2 - (z-0.5)^2)/r_2^2, 0),
\end{aligned}$$

that follows a parabolic profile, and the inlet temperature $\mathsf{T}_{\mathrm{D},1} = 10$, $\mathsf{T}_{\mathrm{D},2} = 0$. Finally, we use the parameters given in Table 1.

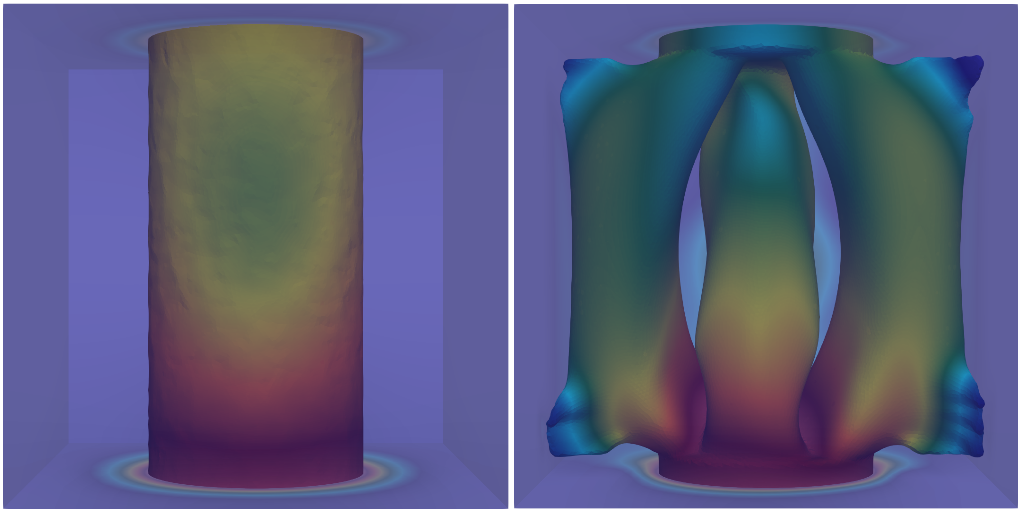
κ_1	4×10^{-3}	$m^2 s^{-1}$	κ_2	10^{-3}	$m^2 s^{-1}$	κ_s	10^{-2}	$m^2 s^{-1}$
ν_1	2	$m^2 s^{-1}$	ν_2	1	$m^2 s^{-1}$	η	10^{-2}	

Table 1: Values of the physical parameters

5.1 First example: Crossflow cylinder case

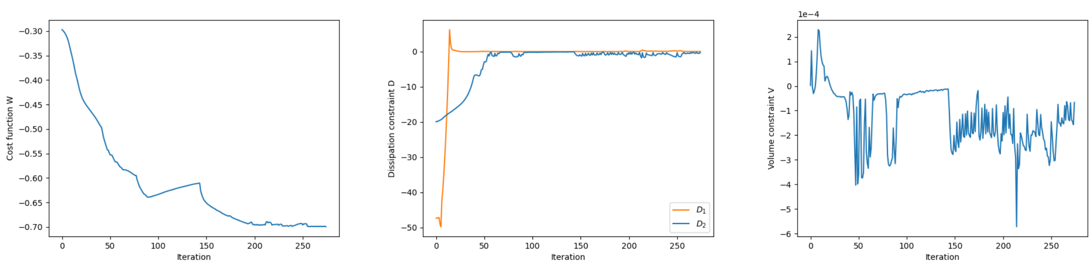
In this case, we choose $y_c = Y_c = 0.5$, $r_1 = r_2 = 0.25$ and $D_{0,i}$, $i = 1, 2$ to be $k = 5$ times the initial dissipation value of the respective fluid, which gives in the presented simulation $D_{0,1} = 60$, $D_{0,2} = 25$ and $V_0 = \pi r_1^2 \approx 0.194$. It should be noted that the most time-consuming part is the resolution of the Navier-Stokes equations, since the degrees of freedom are about 2 and 4 millions for the cold and hot Navier-Stokes equations, respectively.

The obtained results are shown in Figures 2. The convergence history for the functionals is



(a) Initial domain Ω.　　(b) Final domain Ω.

Figure 2: Initial and final domain Ω for the first example.



(a) Objective function W.　　(b) Dissipation constraints D_i.　　(c) Volume constraint V.

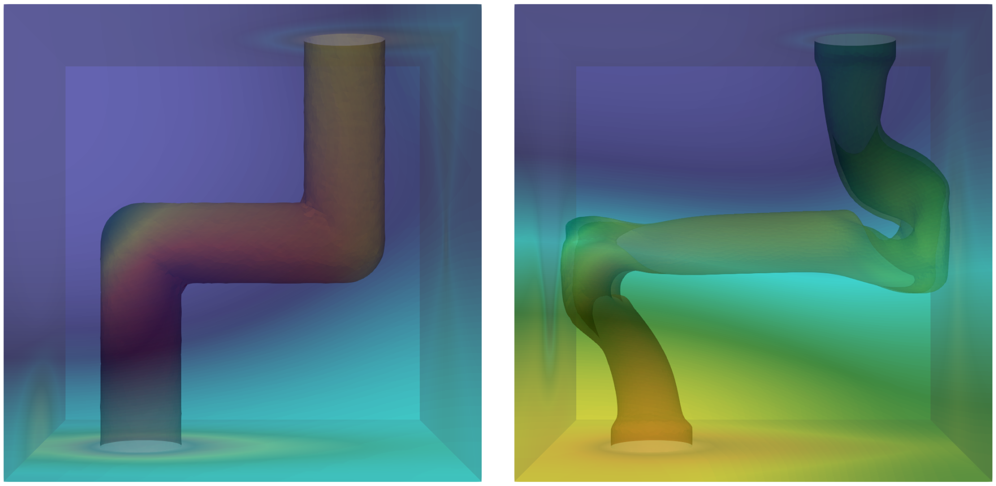
Figure 3: Convergence history for the first example.

depicted on Figure 3, where the exchanged heat improved is about 135%.

We observe that there is a change in the topology. This can be explained by the fact that, since we are considering a co-current flow, the cold fluid has to 'pass through' the thermal fluid instead of 'avoiding' it to increase the heat exchanged. In addition, the contact surface has increased, which makes sense because it allows more exchange zones.

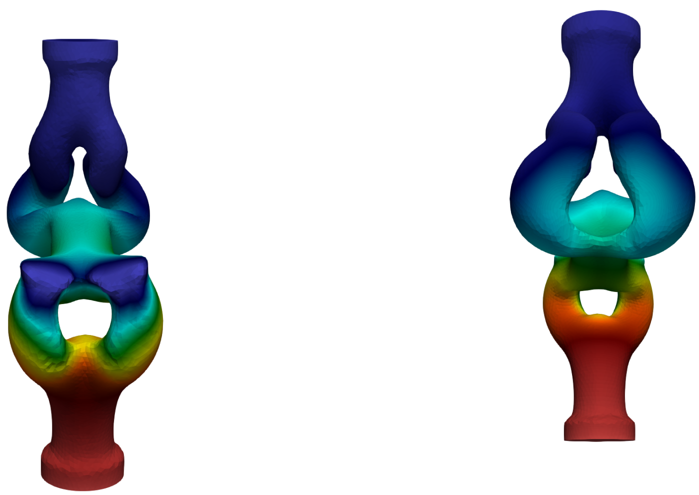
5.2 Second example: Co-current flow tube case

In this case, we consider $y_c = 0.25$, $Y_c = 0.75$, $r_1 = 0.1, r_2 = 0.1$ and $D_{0,i}$, $i = 1, 2$ to be 5 times the initial dissipation value of the respective value, which gives in the presented simulations $D_{0,1} = 85$, $D_{0,2} = 5$, and $V_0 \approx 0.0456$. We consider here a more complicated initial configuration and thinner hot domain. Here, the hot and cold Navier-Stokes equations have about 0.5 and 1.5 millions degrees of freedom, respectively. The obtained results are shown in Figures 4 and 5. The convergence history is depicted on Figure 6, where the exchanged heat improved in about 50%.



(a) Initial domain Ω. (b) Final domain Ω.

Figure 4: Initial and final domain Ω for the second example.

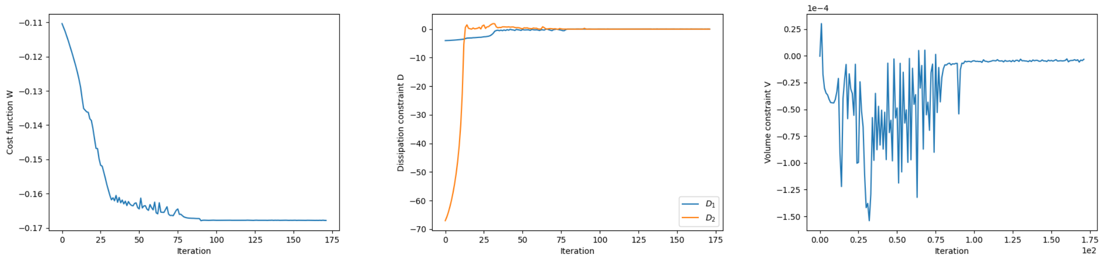


(a) Left view. (b) Right view.

Figure 5: Lateral views of the tube at the last performed iteration.

Acknowledgement

R. Zelada was partially funded by the National Agency for Research and Development (ANID) Scholarship Program BECA DOCTORADO NACIONAL 2021-21211704. F. Caubet and M. Dambrine were funded by the ANR projects SHAPO (ANR-18-CE40-0013) and STOIQUES (ANR-24-CE40-2216).



(a) Objective function W.

(b) Dissipation constraints D_i.

(c) Volume constraint V.

Figure 6: Convergence history for the second example.

References

[1] L. Afraites, M. Dambrine, and D. Kateb. On second order shape optimization methods for electrical impedance tomography. *SIAM Journal on Control and Optimization*, 47(3):1556–1590, 2008.

[2] G. Allaire. *Conception optimale de structures*, volume 58 of *Mathématiques & Applications (Berlin) [Mathematics & Applications]*. Springer-Verlag, Berlin, 2007. With the collaboration of Marc Schoenauer (INRIA) in the writing of Chapter 8.

[3] G. Allaire, B. Bogosel, and M. Godoy. Shape optimization of an imperfect interface: steady-state heat diffusion. *J. Optim. Theory Appl.*, 191(1):169–201, 2021.

[4] G. Allaire, C. Dapogny, and P. Frey. A mesh evolution algorithm based on the level set method for geometry and topology optimization. *Struct. Multidiscip. Optim.*, 48(4):711–715, 2013.

[5] S. Balay, S. Abhyankar, M. F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, A. Dener, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, D. A. May, L. C. McInnes, R. T. Mills, T. Munson, K. Rupp, P. Sanan, B. F. Smith, S. Zampini, H. Zhang, and H. Zhang. PETSc users manual. Technical Report ANL-95/11 - Revision 3.11, Argonne National Laboratory, 2019.

[6] J. A. Bello, E. Fernández-Cara, J. Lemoine, and J. Simon. The differentiability of the drag with respect to the variations of a Lipschitz domain in a Navier-Stokes flow. *SIAM Journal on Control and Optimization*, 35(2):626–640, 1997.

[7] C. Bui, C. Dapogny, and P. Frey. An accurate anisotropic adaptation method for solving the level set advection equation. *Internat. J. Numer. Methods Fluids*, 70(7):899–922, 2012.

[8] D. Capatina, F. Caubet, M. Dambrine, and R. Zelada. Nitsche extended finite element method of a Ventcel transmission problem with discontinuities at the interface. *ESAIM: Mathematical Modelling and Numerical Analysis*, 2025. DOI: https://doi.org/10.1051/m2an/2025014.

[9] F. Caubet. Instability of an inverse problem for the stationary Navier-Stokes equations. *SIAM J. Control Optim.*, 51(4):2949–2975, 2013.

[10] F. Caubet, C. Conca, M. Dambrine, and R. Zelada. How to insulate a pipe? working paper or preprint, Nov. 2024.

[11] F. Caubet, C. Conca, M. Dambrine, and R. Zelada. Shape optimization for heat exchangers with a thin layer. In *Sixteenth International Conference Zaragoza-Pau on Mathematics and its Applications*, volume 43, pages 51–61. Prensas de la Universidad de Zaragoza, 2024.

[12] F. Caubet and M. Dambrine. Stability of critical shapes for the drag minimization problem in stokes flow. *Journal de Mathématiques Pures et Appliquées*, 100(3):327–346, 2013.

[13] C. Dapogny, C. Dobrzynski, and P. Frey. Three-dimensional adaptive domain remeshing, implicit domain meshing, and applications to free and moving boundary problems. *J. Comput. Phys.*, 262:358–378, 2014.

[14] C. Dapogny and P. Frey. Computation of the signed distance function to a discrete contour on adapted triangulation. *Calcolo*, 49(3):193–219, 2012.

[15] F. Feppon. Null space optimizer, 2019. `https://gitlab.com/florian.feppon/null-space-optimizer` [Accessed: 21/10/2024].

[16] F. Feppon, G. Allaire, F. Bordeu, J. Cortial, and C. Dapogny. Shape optimization of a coupled thermal fluid-structure problem in a level set mesh evolution framework. *SeMA J.*, 76(3):413–458, 2019.

[17] F. Feppon, G. Allaire, and C. Dapogny. Null space gradient flows for constrained optimization with applications to shape optimization. *ESAIM Control Optim. Calc. Var.*, 26:Paper No. 90, 45, 2020.

[18] F. Feppon, G. Allaire, and C. Dapogny. A variational formulation for computing shape derivatives of geometric constraints along rays. *ESAIM Math. Model. Numer. Anal.*, 54(1):181–228, 2020.

[19] V. Girault and P.-A. Raviart. *Finite element methods for Navier-Stokes equations*, volume 5 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 1986. Theory and algorithms.

[20] F. Hecht. New development in freefem++. *J. Numer. Math.*, 20(3-4):251–265, 2012.

[21] A. Henrot and M. Pierre. *Variation et optimisation de formes*, volume 48 of *Mathématiques & Applications (Berlin) [Mathematics & Applications]*. Springer, Berlin, 2005. Une analyse géométrique. [A geometric analysis].

[22] A. Henrot and Y. Privat. What is the optimal shape of a pipe? *Arch. Ration. Mech. Anal.*, 196(1):281–302, 2010.

[23] M. Hintermüller and W. Ring. A second order shape optimization approach for image segmentation. *SIAM J. Appl. Math.*, 64(2):442–467, 2003/04.

[24] J. Moulin, P. Jolivet, and O. Marquet. Augmented Lagrangian preconditioner for large-scale hydrodynamic stability analysis. *Comput. Methods Appl. Mech. Engrg.*, 351:718–743, 2019.

[25] J. Nitsche. über ein Variationsprinzip zur Lösung von Dirichlet-Problemen bei Verwendung von Teilräumen, die keinen Randbedingungen unterworfen sind. *Abh. Math. Sem. Univ. Hamburg*, 36:9–15, 1971.

[26] R. Temam. *Navier-Stokes equations.* AMS Chelsea Publishing, Providence, RI, 2001. Theory and numerical analysis, Reprint of the 1984 edition.