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SHAPE OPTIMIZATION OF A POLYMER DISTRIBUTOR USING AN EULERIAN RESIDENCE TIME MODEL*

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Abstract. We consider the optimal shape design of polymer distributors for the industrial spinning process, where long residence times are known to have a negative impact on the quality of the fibers. To this end we introduce a cost function based on the material age and the pressure energy required for the fluid transport. We obtain the shape derivative of the cost function without using the material derivative of the state based on a recent differentiability result for the Lagrangian formulation of shape optimization problems. Numerical experiments for a three-dimensional distributor verify the feasibility of our approach.

Key words. shape optimization, polymer distributor, partial differential equations, residence time

AMS subject classifications. 49Q10, 35Q35, 76B75, 90C90

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1. Introduction.

Polymer spin packs are widely used for the production of synthetic fibers and nonwoven materials. Typically molten polymer enters the spin pack and passes a cavity where it is distributed onto several layers of filter. After passing these filters it is pressed through small capillaries where the fibers are spun. The spin pack is heated, but temperature can damage the material and lead to degradation of the sensitive polymer if residence times are too long. Typically the critical part is the cavity distributing the polymer from the small inflow tube onto the much larger filter, because a considerable amount of time is spent here.

Shape optimization has already been used for the design of spin pack cavities [18, 19, 20, 21], where the authors used an indirect objective based on the wall shear stress, since increasing the wall shear stress reduces stagnation and thus improves the residence time. However, up to now an indirect objective based on the wall shear stress was used, since increasing the wall shear stress reduces stagnation and thus improves the residence time. For the first time, this work now uses residence time directly to optimize the shape of a spin pack cavity, which is done by adding an advection-diffusion-reaction equation to the state system. State constraints on the residence time are imposed with a Moreau regularization term in the cost function. Using this approach it becomes possible to directly control the material age at the outflow of the distributor cavity.

The main theoretical result is Theorem 4.2, which gives the shape differentiability of the cost function and the corresponding distributed shape derivative using the material derivative free Lagrange approach proposed in [33]. This shape derivative gives rise to Algorithm 5.1, which is used to optimize the residence time of the fluid within a three-dimensional distributor cavity.

The paper is structured in the following way: Section 2 introduces the mathematical model and the optimization problem. Section 3 provides important results on

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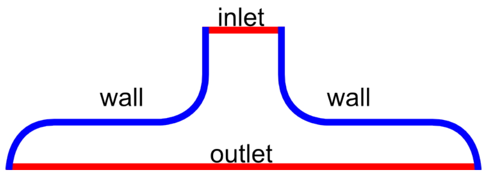


FIG. 1. *Schematic two-dimensional boundary description.*

shape calculus, which are then used in section 4 to derive the main theoretical result. Finally, a gradient descent algorithm is derived and tested in section 5.

2. Problem formulation. This section is devoted to the definition of the distributor cavity optimization problem. In subsection 2.1 we state the equations of fluid transport within the distributor. The introduction of a transport equation for the residence time of the fluid is preferable to a Lagrangian particle tracking approach, since it allows us to use ideas from PDE-constrained optimization and avoids the problem of choosing a representative sample size. Subsection 2.2 is devoted to the corresponding weak formulation and the optimal shape design problem is introduced in subsection 2.3.

2.1. Mathematical model. Let $\mathcal{P}(\mathbb{R}^3)$ be the power set of $\mathbb{R}^3$, $\mathcal{A} \subset \mathcal{P}(\mathbb{R}^3)$ the set of admissible geometries as defined in subsection 2.3, and $\Omega \in \mathcal{A}$. The flow under consideration is modeled with the stationary Stokes equations due to its high viscosity, whose nondimensionalized form reads

$$\begin{aligned} -Re^{-1}\Delta \boldsymbol{u} + \nabla p &= 0 \text{ in } \Omega, \\ \nabla \cdot \boldsymbol{u} &= 0 \text{ in } \Omega, \end{aligned} \tag{2.1}$$

where $\boldsymbol{u} \in \mathbb{R}^3$ denotes the fluid velocity, $p \in \mathbb{R}$ the pressure and $Re \ll 1$ the Reynolds number. Subdividing the boundary $\partial\Omega := \Gamma = \Gamma^{in} \cup \Gamma^{w} \cup \Gamma^{out}$ as in Figure 1, we prescribe the boundary conditions

$$\begin{aligned} \boldsymbol{u} \cdot \boldsymbol{n} &= u_{in} \text{ on } \Gamma^{in}, \\ \boldsymbol{u} &= 0 \text{ on } \Gamma^{w}, \\ \eta_{out}(\boldsymbol{u} \cdot \boldsymbol{n}) - p &= 0 \text{ on } \Gamma^{out}, \\ \boldsymbol{u} \times \boldsymbol{n} &= 0 \text{ on } \Gamma^{in} \cup \Gamma^{out}, \end{aligned} \tag{2.2}$$

with the outer unit normal vector $\boldsymbol{n}$, the parabolic inflow profile u_{in} on the inlet Γ^{in}, no-slip boundary conditions on the wall Γ^{w}, and the porosity constant $\eta_{out} > 0$ on the outflow Γ^{out}. We assume $u_{in} < 0$ almost everywhere on Γ^{in}, such that no backward flow occurs at the inflow boundary, and that both Γ^{in} and Γ^{out} are simply connected. Further, $\boldsymbol{a} \times \boldsymbol{b}$ denotes the cross-product of $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3$ and the last condition in (2.2) therefore demands an inflow velocity profile without tangential components. The condition on Γ^{out} linking the normal component of the velocity and the pressure is inspired by Darcy's law of a porous medium [24] and we refer the reader to [20] for a more in-depth explanation in the context of polymer spin packs.

Given a numerical solution of (2.1) and (2.2), the *residence time* or *material age* of the fluid could be easily obtained by a Lagrangian tracking approach. Since a nondiscrete approach, however, enables the use of methods from PDE-constrained shape optimization, we model the continuous residence time τ with the additional advection-diffusion-reaction equation and boundary conditions

$$
\begin{aligned}
\boldsymbol{u} \cdot \nabla \tau - Pe^{-1} \Delta \tau &= f(\boldsymbol{u}) \text{ in } \Omega, \\
\tau &= 0 \text{ on } \Gamma^{in}, \\
\partial_n \tau &= 0 \text{ on } \Gamma^{w} \cup \Gamma^{out},
\end{aligned} \tag{2.3}
$$

following [12], where the isotropic diffusion term with Péclet number $Pe \gg 1$ is added for regularity reasons only.

In the following we will motivate our choice for the reaction term f, which is often chosen to be the indicator function χ_M of a predefined region of interest $M \subsetneq \Omega$ excluding near-wall regions; see, e.g., [9]. For the application under consideration, where we want to approximate and compare the residence time patterns on different domains with the same topology, this approach is not feasible.

Since we are interested in the fluid residence time everywhere within the distributor, it is tempting to choose $M = \Omega$ and therefore $f(\boldsymbol{u}) = 1$ in (2.3). This choice, however, would cause the solution of (2.3) to grow boundlessly in the vicinity of Γ^w for $Pe \to \infty$, which is a reformulation of the fact that the no-slip condition causes the fluid at the wall to be trapped in the distributor indefinitely and (2.3) with $f(\boldsymbol{u}) = 1$ does not admit a stationary solution in this limit.

It is therefore not practicable to include the near-wall region or any other stagnation zone in (2.3), which inspires the definition of the preliminary reaction term

$$
\tilde{f}(\boldsymbol{u}) := \begin{cases} 1, & ||\boldsymbol{u}||_2 > u_{stag}, \\ 0 & \text{otherwise}, \end{cases}
$$

where the stagnation threshold $u_{stag} > 0$ is chosen to be at least three orders of magnitude smaller than the maximal velocity at the inflow. The introduction of u_{stag} on the one hand prevents the aforementioned singular behavior close to Γ^w and on the other hand allows us to numerically identify near-stagnation through relatively high local variations of τ, which will be demonstrated in subsection 5.3. Anticipating the need to differentiate (2.1)–(2.3) with respect to the state in section 4, we finally choose f to be a smooth approximation of $\tilde{f}$ using a bump function [17].

2.2. Well-posedness of the weak formulation. In this section we consider the well-posedness of the weak form of (2.1)–(2.3), for which we define the function spaces

$$
\begin{aligned}
&X(\Omega) := \{\boldsymbol{v} \in H^1(\Omega)^3 \mid \boldsymbol{v}|_{\Gamma^w} = 0, \boldsymbol{v} \times \boldsymbol{n}|_{\Gamma^{in} \cup \Gamma^{out}} = 0\}, \quad M(\Omega) := L^2(\Omega), \\
&X_0(\Omega) := \{\boldsymbol{v} \in X(\Omega) \mid (\boldsymbol{v} \cdot \boldsymbol{n})|_{\Gamma^{in}} = 0\}, \quad B(\Omega) := H^{1/2}(\Gamma^{in}), \\
&R(\Omega) := H^1(\Omega), \quad R_0(\Omega) := \{\sigma \in R(\Omega) \mid \sigma|_{\Gamma^{in}} = 0\},
\end{aligned}
$$

equipped with the standard L^2-norms. Note that the restriction of $\boldsymbol{v} \in H^1(\Omega)^3$ on Γ^{in} can be identified with an element in $B(\Omega)$ due to the trace theorem [35].

Given $\boldsymbol{u} \in X(\Omega)$, $\boldsymbol{v} \in X_0(\Omega)$, $q \in M(\Omega)$, $\tau \in R_0(\Omega)$, $\sigma \in R_0(\Omega)$, and $\Psi_{in} \in B(\Omega)$ we further define the mappings

$$
\begin{aligned}
\mathrm{a}(\Omega, \boldsymbol{u}, \boldsymbol{v}) &= \int_\Omega Re^{-1}(\nabla \times \boldsymbol{u}) \cdot (\nabla \times \boldsymbol{v}) \mathrm{d}\boldsymbol{x} + \int_{\Gamma^{out}} \eta_{out}(\boldsymbol{u} \cdot \boldsymbol{n})(\boldsymbol{v} \cdot \boldsymbol{n}) \mathrm{d}s, \\
\mathrm{b}(\Omega, \boldsymbol{u}, q) &= \int_\Omega q \nabla \cdot \boldsymbol{u} \mathrm{d}\boldsymbol{x}, \\
\mathrm{c}(\Omega, \boldsymbol{u}, \tau, \sigma) &= \int_\Omega \boldsymbol{u} \cdot \nabla \tau \, \sigma + Pe^{-1} \nabla \tau \cdot \nabla \sigma \mathrm{d}\boldsymbol{x}, \\
k_1(\Omega, \boldsymbol{u}, \sigma) &= \int_\Omega f(\boldsymbol{u}) \sigma \mathrm{d}\boldsymbol{x}, \\
l_1(\Omega, \boldsymbol{u}, \Psi_{in}) &= \int_{\Gamma^{in}} (\boldsymbol{u} \cdot \boldsymbol{n} - u_{in}) \Psi_{in} \mathrm{d}s
\end{aligned}
\tag{2.4}
$$

and derive the weak form (2.5) of (2.1)–(2.3) based on the decomposition

$$\Delta \boldsymbol{u} = \nabla(\nabla \cdot \boldsymbol{u}) - \nabla \times (\nabla \times \boldsymbol{u})$$

of the Laplacian [8]. Here the bilinear forms a and b correspond to the left-hand side of the weak incompressible Stokes equation and c to the left-hand side of the weak residence time equation. Furthermore the functional l_1 accounts for the inflow condition and the right-hand side k_1 for the increment of the material age along the streamlines. With these definitions the well-posedness of the forward problem is addressed in the following theorem.

THEOREM 2.1. *The problem*

$$
\begin{aligned}
&\text{Given } \Omega \in \mathcal{A} \text{ seek } q = (\boldsymbol{q}_u, q_p, q_\tau) \in X(\Omega) \times M(\Omega) \times R_0(\Omega) \text{ such that} \\
&\mathrm{a}(\Omega, \boldsymbol{q}_u, \Psi_u) - \mathrm{b}(\Omega, \Psi_u, q_p) = 0 \qquad \forall\, \Psi_u \in X_0(\Omega), \\
&\mathrm{b}(\Omega, \boldsymbol{q}_u, \Psi_p) = 0 \qquad \forall\, \Psi_p \in M(\Omega), \\
&\boldsymbol{q}_u \cdot \boldsymbol{n} = u_{in} \qquad \text{on } \Gamma^{in}, \\
&\mathrm{c}(\Omega, \boldsymbol{q}_u, q_\tau, \Psi_\tau) = k_1(\Omega, \boldsymbol{q}_u, \Psi_\tau) \quad \forall\, \Psi_\tau \in R(\Omega)
\end{aligned}
\tag{2.5}
$$

possesses a unique solution and the estimates

$$||\boldsymbol{q}_u||_{H^1(\Omega)^3} + ||q_p||_{L^2(\Omega)} \leq c\, ||u_{in}||_{L^2(\Gamma^{in})}, \tag{2.6a}$$

$$||q_\tau||_{H^1(\Omega)} \leq c\, ||k_1(\Omega, \boldsymbol{q}_u, \cdot)||_{H^{-1}(\Omega)} \tag{2.6b}$$

hold.

Proof. The continuity of the operators a, b, and c and the boundedness of k_1 and $||u_{in}||_{L^2(\Gamma^{in})}$ are readily seen.

Since τ is decoupled from $\boldsymbol{u}$ and p in (2.5), we prove the well-posedness of the Stokes equations first. This problem with homogeneous Dirichlet boundary conditions at the inflow is considered in [13] and its well-posedness for meas$(\Gamma^{out}) \neq 0$ is shown. The nonhomogeneous case is handled via the lifting of the boundary conditions (see, e.g., [8]) since $X_0(\Omega) \times M(\Omega)$ is reflexive and the trace operator from $X(\Omega)$ to $B(\Omega)$ exists due to [35]. Equation (2.6a) is then obtained in a straightforward manner.

We proceed with the convection-diffusion equation. The operator $\mathrm{c}(\Omega, \boldsymbol{q}_u, \cdot, \cdot)$ is continuous on $R_0(\Omega) \times R(\Omega)$. For $\tau \in R_0(\Omega)$ we obtain the estimate

$$\begin{aligned} \mathrm{c}(\Omega, \boldsymbol{q}_u, \tau, \tau) &= \int_\Omega (\boldsymbol{q}_u \cdot \nabla\tau)\tau \mathrm{d}\boldsymbol{x} + Pe^{-1}||\nabla\tau||^2_{L^2(\Omega)} \\ &= \int_\Omega -\frac{1}{2}(\nabla \cdot \boldsymbol{q}_u)\tau^2 \mathrm{d}\boldsymbol{x} + Pe^{-1}||\nabla\tau||^2_{L^2(\Omega)} + \frac{1}{2}\int_{\Gamma^{out}} (\boldsymbol{q}_u \cdot \boldsymbol{n})\tau^2 \mathrm{d}s \\ &\geq c||\nabla\tau||^2_{L^2(\Omega)} \\ &\geq c||\tau||^2_{H^1(\Omega)}, \end{aligned}$$

with a constant $c > 0$, where the first equality holds due to

$$\begin{aligned} \int_\Omega (\Phi_u \cdot \nabla\Phi_\tau)\Psi_\tau \mathrm{d}\boldsymbol{x} = &- \int_\Omega (\Phi_u \cdot \nabla\Psi_\tau)\Phi_\tau \mathrm{d}\boldsymbol{x} - \int_\Omega (\nabla \cdot \Phi_u)\Phi_\tau\Psi_\tau \mathrm{d}\boldsymbol{x} \\ &+ \int_{\Gamma^{out}} (\Phi_u \cdot \boldsymbol{n})\Phi_\tau\Psi_\tau \mathrm{d}s \end{aligned} \tag{2.7}$$

for all $(\Phi_u, \Phi_\tau, \Psi_\tau) \in X(\Omega) \times R_0(\Omega) \times R(\Omega)$.

In the second to last inequality the pointwise negativity of $\boldsymbol{q}_u \cdot \boldsymbol{n}$ on Γ^{in} from (2.2), the incompressibility condition, and the simple connectivity of Γ^{in} and Γ^{out} yield $\boldsymbol{q}_u \cdot \boldsymbol{n} > 0$ on Γ^{out}. The last inequality is due to an application of the Poincaré–Friedrichs inequality [8, p. 490]. Since the operator $\mathrm{c}(\boldsymbol{q}_u, \cdot, \cdot)$ is elliptic, the convection-diffusion-reaction equation has a unique solution due to the Lax–Milgram theorem [3], which also yields (2.6b). ◻

2.3. Optimization problem. Throughout this paper we are interested in finding a distributor cavity by deforming $\Gamma^d \subset \Gamma^w$ ensuring that the material age at Γ^{out} is below a given maximally acceptable value $\overline{\tau}$. Additionally we want to avoid a huge decrease in the pressure energy from the inlet to the outlet due to excessive fluid acceleration. For this purpose we define the cost function

$$J(\Omega, \sigma, v) := \int_{\Gamma^{out}} g(\sigma)\mathrm{d}s + \alpha_1 \int_\Omega \nabla v : \nabla v \,\mathrm{d}\boldsymbol{x} + \alpha_2 \int_{\Gamma^d} 1 \,\mathrm{d}s \tag{2.8}$$

with $\alpha_1, \alpha_2 > 0$. Here $g(\sigma) := {}^\gamma(\max\{0, \sigma - \overline{\tau}\})$ is the Moreau regularization with parameter γ (see, e.g., [2]) of the state constraint

$$\sigma \leq \overline{\tau} \text{ on } \Gamma^{out}. \tag{2.9}$$

The volume integral in (2.8) can be understood as the weak form of the pressure power loss from inflow to outflow due to Lemma 2.2, which has been used, e.g., for the shape optimization of ducts [14, 25]. The surface area penalization term is added to guarantee the existence of a local minimizer [1].

LEMMA 2.2. *Let* $(\boldsymbol{u}, p) \in C^2(\Omega)^3 \times C^1(\Omega)$ *be a solution of* (2.1)–(2.2). *Then it holds that*

$$\int_{\Gamma^{in} \cup \Gamma^{out}} -p(\boldsymbol{u} \cdot \boldsymbol{n})\mathrm{d}s = Re^{-1}||\nabla \boldsymbol{u}||^2_{L^2(\Omega)^{3\times 3}}. \tag{2.10}$$

Proof. As shown in [27], the incompressibility of the fluid together with the vanishing of $\boldsymbol{u} \times \boldsymbol{n}$ on Γ yields

$$\int_\Gamma \partial_n \boldsymbol{u} \cdot \boldsymbol{u} \mathrm{d}s = \int_\Gamma (\partial_n \boldsymbol{u} \cdot \boldsymbol{n})(\boldsymbol{u} \cdot \boldsymbol{n}) + (\partial_n \boldsymbol{u} \times \boldsymbol{n}) \cdot (\boldsymbol{u} \times \boldsymbol{n})\mathrm{d}s = 0.$$

Using integration by parts and (2.1) we deduce

$$Re^{-1}||\nabla \boldsymbol{u}||^2_{L^2(\Omega)^{3\times 3}} = -Re^{-1}\int_\Omega \Delta \boldsymbol{u}\cdot \boldsymbol{u}\mathrm{d}\boldsymbol{x} = -\int_\Omega \nabla p\cdot \boldsymbol{u}\mathrm{d}\boldsymbol{x},$$

and by using the incompressibility and boundary conditions we obtain

$$\int_\Omega \nabla p\cdot \boldsymbol{u}\mathrm{d}\boldsymbol{x} = \int_\Omega \nabla\cdot(p\,\boldsymbol{u})\mathrm{d}\boldsymbol{x} = \int_\Gamma p(\boldsymbol{u}\cdot\boldsymbol{n})\mathrm{d}s = \int_{\Gamma^{in}\cup\Gamma^{out}} p(\boldsymbol{u}\cdot\boldsymbol{n})\mathrm{d}s,$$

which completes the proof. ∎

Due to Theorem 2.1 we can define the reduced cost function

$$\tilde{J}(\Omega) := J(\Omega, q_\tau(\Omega), \boldsymbol{q}_u(\Omega)) = \int_{\Gamma^{out}} g(q_\tau)\mathrm{d}s + \alpha_1\int_\Omega \nabla\boldsymbol{q}_u : \nabla\boldsymbol{q}_u\,\mathrm{d}\boldsymbol{x} + \alpha_2\int_{\Gamma^d} 1\,\mathrm{d}s,$$

with the solution $q = (\boldsymbol{q}_u, q_p, q_\tau) \in X(\Omega)\times M(\Omega)\times R_0(\Omega)$ of the weak state equations and consider the PDE-constrained optimization problem

$$\begin{aligned} &\text{Seek } \hat{\Omega}\in\mathcal{A} \text{ such that}\\ &\tilde{J}(\hat{\Omega}) = \min_\Omega \tilde{J}(\Omega)\\ &\text{subject to (2.5)}\end{aligned} \tag{2.11}$$

in order to improve the initial distributor design. Here $\mathcal{A}\subset\mathcal{P}(\mathbb{R}^3)$ denotes the set of sufficiently smooth domains where the nondeformable boundary part $\Gamma\setminus\Gamma^d$ is the same as for the initial domain. In particular, we want to keep the inlet and outlet as well as the inflow pipe unchanged to fit the optimized cavity into the existing configuration of the spin pack.

3. Results from shape calculus. This section is devoted to the main ingredients from shape calculus used throughout this paper. After introducing the notation and recalling important definitions in subsection 3.1, we quote a differentiability result from [33] in subsection 3.2, which we use for the computation of the adjoint equations and the shape derivative of the cost function in section 4.

3.1. Preliminaries. We define by

$$\boldsymbol{\Theta}^1(\mathbb{R}^3) := \{\boldsymbol{\theta}\in C^{1,1}(\mathbb{R}^3)^3 : ||\boldsymbol{\theta}||_{C^{1,1}(\mathbb{R}^3)^3} < 0.5$$

the space of admissible deformations. The norm on $C^{1,1}(\mathbb{R}^3)^3$ is defined through

$$||g||_{C^{1,1}(\mathbb{R}^3)^3} := \sup_{|\mu|\le 1}||D^\mu g||_\infty + \sup_{\substack{|\mu|=1\\ \boldsymbol{x},\boldsymbol{y}\in\Omega\\ \boldsymbol{x}\neq\boldsymbol{y}}} \frac{|D^\mu g(\boldsymbol{x}) - D^\mu g(\boldsymbol{y})|}{|\boldsymbol{x}-\boldsymbol{y}|}, \tag{3.1}$$

where $\mu\in\mathbb{N}^3$ is a multi-index. For $\Omega\subset\mathbb{R}^3$, and $t\mathcal{V}\in\boldsymbol{\Theta}^1(\mathbb{R}^3)$ for all $t\in[0,1]$ the transformations

$$\begin{aligned} T_{t\mathcal{V}}&\colon \Omega\to\mathbb{R}^3,\\ &\boldsymbol{x}\mapsto T_{t\mathcal{V}}(\boldsymbol{x}) := (I+t\mathcal{V})(\boldsymbol{x})\end{aligned} \tag{3.2}$$

are diffeomorphisms due to the Neumann series and we set $\Omega_{t\mathcal{V}} := T_{t\mathcal{V}}(\Omega)$. We further denote by $\mathbf{D}T_{t\mathcal{V}} = \mathbb{I} + t\mathbf{D}\mathcal{V}$ the Jacobian of the transformation $T_{t\mathcal{V}}$ and by

$$M(t) := \mathbf{D}T_{t\mathcal{V}}^{-T}, \tag{3.3a}$$

$$\xi(t) := \det \mathbf{D}T_{t\mathcal{V}}, \tag{3.3b}$$

$$\xi_\Gamma(t) := \xi(t)|\mathbf{D}T_{t\mathcal{V}}^{-T}\boldsymbol{n}| \tag{3.3c}$$

the transposed inverse of the Jacobian of the transformation as well as the volume and surface elements of the transformation, which satisfy $M(0) = \mathbb{I}$ and $\xi(0) = \xi_\Gamma(0) = 1$. The following lemma, which will be useful in section 4, addresses the derivatives of (3.3a)–(3.3c), and a chain rule for the differential operators gradient, divergence, and curl composed with a smooth transformation of the domain.

Lemma 3.1. *For $g \in W^{1,1}_{loc}(\mathbb{R}^3)$, $G \in W^{1,1}_{loc}(\mathbb{R}^3)^3$, and $\mathcal{V} \in \mathbf{\Theta}^1(\mathbb{R}^3)$ it holds that*

$$\xi'(0) = \nabla \cdot \mathcal{V}, \quad {\xi_\Gamma}'(0) = \nabla_\Gamma \cdot \mathcal{V}, \quad M'(0) = -\boldsymbol{D}\mathcal{V}^T, \tag{3.4}$$

with the tangential divergence $\nabla_\Gamma \cdot \mathcal{V}$. Further,

$$\begin{aligned} \nabla(g \circ T_{t\mathcal{V}}^{-1}) &= (M(t)\,\nabla g) \circ T_{t\mathcal{V}}^{-1}, \\ \nabla \cdot (G \circ T_{t\mathcal{V}}^{-1}) &= \operatorname{tr}(\boldsymbol{D}G\, M^T(t)) \circ T_{t\mathcal{V}}^{-1}, \\ (\nabla \times (G \circ T_{t\mathcal{V}}^{-1}))_i &= -\epsilon_{ijk}(\boldsymbol{D}G\, M^T(t))_{jk} \circ T_{t\mathcal{V}}^{-1}. \end{aligned} \tag{3.5}$$

Proof. The proofs of (3.4) and the first equality in (3.5) can be found in [5]. An application of the chain rule together with (3.3a) yields

$$\mathbf{D}(G \circ T_{t\mathcal{V}}^{-1}) = (\mathbf{D}G \circ T_{t\mathcal{V}}^{-1})\,\mathbf{D}T_{t\mathcal{V}}^{-1} = (\mathbf{D}G\, M^T(t)) \circ T_{t\mathcal{V}}^{-1}.$$

The statement concerning the divergence is then derived from

$$\nabla \cdot (G \circ T_{t\mathcal{V}}^{-1}) = \operatorname{tr}(\mathbf{D}(G \circ T_{t\mathcal{V}}^{-1}))$$

and the one concerning the curl from

$$(\nabla \times (G \circ T_{t\mathcal{V}}^{-1}))_i = -\epsilon_{ijk}\big(\mathbf{D}(G \circ T_{t\mathcal{V}}^{-1})\big)_{jk}$$

using the summation convention and the Levi–Civita symbol ϵ_{ijk}. ◻

We now define derivatives of the cost function with respect to changes of the domain.

Definition 3.2 (see [32]). *$J\colon \mathcal{A} \to \mathbb{R}$ is said to have the Eulerian semiderivative in direction $\mathcal{V} \in C^{1,1}(\mathbb{R}^3)^3$ if the limit*

$$dJ(\Omega)[\mathcal{V}] := \lim_{t \searrow 0} \frac{J(T_{t\mathcal{V}}(\Omega)) - J(\Omega)}{t}$$

exists. It is called shape differentiable if the Eulerian semiderivative exists for all $\mathcal{V} \in C^{1,1}(\mathbb{R}^3)^3$ and the mapping $\mathcal{V} \mapsto dJ(\Omega)[\mathcal{V}]$ is linear and continuous. $dJ(\Omega)[\mathcal{V}]$ is then called the shape derivative of J.

3.2. A differentiability result. We now cite a recent differentiability result from [33], which generalizes the well-known Correa–Seeger theorem [5] and which can be used to compute the Eulerian semiderivative of PDE-constrained cost functions without material derivatives of the state.

Let E and F be Banach spaces, $T > 0$, and let

$$\begin{aligned} \mathscr{G}\colon [0,T] \times E \times F &\to \mathbb{R},\\ (t,\Phi,\Psi) &\mapsto \mathscr{G}(t,\Phi,\Psi) \end{aligned}$$

be affine with respect to Ψ. Furthermore define

$$E(t) := \{q \in E \,|\, D_\Psi \mathscr{G}(t,q,0)[\hat{\Psi}] = 0 \quad \forall\, \hat{\Psi} \in F\}$$

and let the following hypothesis be satisfied.

Assumption 3.3 (H0). For every $(t,\Psi) \in [0,T] \times F$ the set $E(t)$ is single-valued and we write $E(t) = \{q^t\}$. Further assume that

(i) the function $[0,1] \ni r \mapsto \mathscr{G}(t, q^0 + r(q^t - q^0), \Psi)$ is absolutely continuous, and

(ii) for all $\hat{\Phi} \in E$, the function $r \mapsto D_\Phi \mathscr{G}(t, q^0 + r(q^t - q^0), \Psi)[\hat{\Phi}]$ belongs to $L^1[0,1]$.

For $t \in [0,T]$ and $q^t \in E(t)$ we set

$$Y(t,q^t,q^0) := \left\{ \lambda \in F \,\middle|\, \forall\, \hat{\Phi} \in E : \int_0^1 D_{\hat{\Phi}} \mathscr{G}(t, q^0 + r(q^t - q^0), \lambda)[\hat{\Phi}] \mathrm{d}r = 0 \right\},$$

which is called the solution set of the *averaged adjoint equation* with respect to t, q^t, and q^0. Then the following holds.

Theorem 3.4 (see [33]). *Let assumption* (H0) *and the following conditions be satisfied:*

(H1) *For all $t \in [0,T]$ and all $\Psi \in F$ the derivative $\partial_t \mathscr{G}(t,q^0,\Psi)$ exists.*

(H2) *For all $t \in [0,T]$ the set $Y(t,q^t,q^0)$ is single-valued and we write*

$$Y(t,q^t,q^0) = \{\lambda^t\}.$$

(H3) *For every sequence of nonnegative numbers $(t_n)_{n\in\mathbb{N}}$ converging to zero, there exists a subsequence $(t_{n_k})_{k\in\mathbb{N}}$ such that*

$$\lim_{\substack{k\to\infty\\ r\searrow 0}} \partial_t \mathscr{G}(r, q^0, \lambda^{t_{n_k}}) = \partial_t \mathscr{G}(0, q^0, \lambda^0).$$

Then for $\Psi \in F$ we obtain

$$\frac{d}{dt}(\mathscr{G}(t,q^t,\Psi))\bigg|_{t=0} = \partial_t \mathscr{G}(0,q^0,\lambda^0).$$

4. Shape gradient of the cost function. In this section we derive the Eulerian semiderivative of the cost function by an application of the material derivative free Lagrange approach [33]. After introducing the associated Lagrangian and an investigation of the adjoint equations in subsection 4.1, the subsequent subsection 4.2 is devoted to the validation of the prerequisites for the application of Theorem 3.4. To the best of our knowledge the continuous model (2.3) for the fluid residence time has not been considered as a PDE constraint in gradient-based optimal shape design so far and a result similar to Theorem 4.2 has not yet been derived in the literature.

4.1. Lagrangian and adjoint equations. Set $E(\Omega) := X(\Omega) \times M(\Omega) \times R_0(\Omega)$ and $F(\Omega) := X_0(\Omega) \times M(\Omega) \times R(\Omega) \times B(\Omega)$. For $\Phi := (\Phi_u^T, \Phi_p, \Phi_\tau) \in E(\Omega)$ and $\Psi := (\Psi_u^T, \Psi_p, \Psi_\tau, \Psi_{in}) \in F(\Omega)$ we define

$$\begin{aligned}\mathrm{Q}(\Omega, \Phi, \Psi) := {} & \mathrm{a}(\Omega, \Phi_u, \Psi_u) - \mathrm{b}(\Omega, \Psi_u, \Phi_p) + \mathrm{b}(\Omega, \Phi_u, \Psi_p) \\ & + l_1(\Omega, \Phi_u, \Psi_{in}) + \mathrm{c}(\Omega, \Phi_u, \Phi_\tau, \Psi_\tau) - k_1(\Omega, \Phi_u, \Psi_\tau)\end{aligned} \tag{4.1}$$

for the PDE constraint using the definitions from subsection 2.2 and introduce the Lagrangian

$$G(\Omega, \Phi, \Psi) := J(\Omega, \Phi_\tau, \Phi_u) + \mathrm{Q}(\Omega, \Phi, \Psi) \tag{4.2}$$

associated with the optimization problem (2.11).

The adjoint state equations are obtained by differentiating (4.2) with respect to Φ at $\Phi = q := (\boldsymbol{q}_u^T, q_p, q_\tau)^T$ and $\Psi = \lambda := (\lambda_u^T, \lambda_p, \lambda_\tau, \lambda_{in})^T$ and solving

$$D_\Phi G(\Omega, q, \lambda)[\Phi] = 0 \quad \forall\, \Phi \in E(\Omega). \tag{4.3}$$

We sort for the different components of Φ in (4.3) and obtain the adjoint transport equation

$$\begin{aligned}&\int_\Omega -(\boldsymbol{q}_u \cdot \nabla\lambda_\tau)\Phi_\tau + Pe^{-1}\nabla\lambda_\tau \cdot \nabla\Phi_\tau \mathrm{d}\boldsymbol{x} + \int_{\Gamma^{out}} (\boldsymbol{q}_u \cdot \boldsymbol{n})\lambda_\tau\Phi_\tau \mathrm{d}s \\ &= -\int_{\Gamma^{out}} \partial_{\Phi_\tau} g(q_\tau)\Phi_\tau \mathrm{d}s \quad \forall\, \Phi_\tau \in R_0(\Omega)\end{aligned}$$

as well as the adjoint Stokes equation

$$\begin{aligned}&\int_\Omega Re^{-1}(\nabla \times \Phi_u) \cdot (\nabla \times \lambda_u)\mathrm{d}\boldsymbol{x} + \int_\Omega \lambda_p \nabla \cdot \Phi_u \mathrm{d}\boldsymbol{x} \\ &+ \int_{\Gamma^{out}} \eta_{out}(\Phi_u \cdot \boldsymbol{n})(\lambda_u \cdot \boldsymbol{n})\mathrm{d}s + \int_{\Gamma^{in}} (\Phi_u \cdot \boldsymbol{n})\,\lambda_{in}\mathrm{d}s \\ &= \int_\Omega \Phi_u \cdot (\nabla q_\tau \lambda_\tau + \partial_{\Phi_u} f(\boldsymbol{q}_u)\lambda_\tau)\mathrm{d}\boldsymbol{x} - 2\,\alpha_1 \int_\Omega \nabla \boldsymbol{q}_u : \nabla\Phi_u \mathrm{d}\boldsymbol{x} \quad \forall\, \Phi_u \in X(\Omega),\end{aligned}$$

with incompressibility condition

$$\int_\Omega \Phi_p \nabla \cdot \lambda_u \mathrm{d}\boldsymbol{x} = 0 \quad \forall\, \Phi_p \in M(\Omega).$$

For the sake of brevity we introduce

$$\begin{aligned}\mathrm{d}(\Omega, \boldsymbol{q}_u, \lambda_\tau, \Phi_\tau) :=& \mathrm{c}(\Omega, -\boldsymbol{q}_u, \lambda_\tau, \Phi_\tau) + \int_{\Gamma^{out}} (\boldsymbol{q}_u \cdot \boldsymbol{n})\lambda_\tau\Phi_\tau \mathrm{d}s, \\ k_2(\Omega, q_\tau, \Phi_\tau) :=& \int_{\Gamma^{out}} -\partial_{\Phi_\tau} g(q_\tau)\Phi_\tau \mathrm{d}s, \\ m(\Omega, \boldsymbol{q}_u, q_\tau, \lambda_\tau, \Phi_u) :=& \int_\Omega \Phi_u \cdot (\nabla q_\tau \lambda_\tau + \partial_{\Phi_u} f(\boldsymbol{q}_u)\lambda_\tau)\mathrm{d}\boldsymbol{x} - 2\,\alpha_1 \int_\Omega \nabla\boldsymbol{q}_u : \nabla\Phi_u \mathrm{d}\boldsymbol{x}, \\ l_2(\Omega, \Phi_u, \lambda_{in}) :=& \int_{\Gamma^{in}} (\Phi_u \cdot \boldsymbol{n})\,\lambda_{in}\mathrm{d}s.\end{aligned}$$

Here the operator d describes the transport of the adjoint material age λ_τ along the negative fluid streamlines and the right-hand-side k_2 accounts for the adjoint inflow conditions depending on the integrand g of the cost function. The right-hand-side m sums up all terms that can be evaluated once the solution of (2.5) as well as λ_τ are given, and l_2 stems from the differentiation of the weak form of the inflow condition. Given these abbreviations the well-posedness of the adjoint equations (4.3) is addressed in the following theorem.

THEOREM 4.1. *The problem*

$$\begin{aligned} &\text{Given } \Omega \in \mathcal{A} \text{ and } (\boldsymbol{q}_u, q_p, q_\tau) \in E(\Omega) \text{ solving (2.5) seek} \\ &\qquad (\lambda_u, \lambda_p, \lambda_\tau, \lambda_{in}) \in F(\Omega) \text{ s.t.} \\ &\mathrm{d}(\Omega, \boldsymbol{q}_u, \lambda_\tau, \Phi_\tau) = k_2(\Omega, q_\tau, \Phi_\tau) \qquad \forall\, \Phi_\tau \in R_0(\Omega) \\ &\mathrm{a}(\Omega, \lambda_u, \Phi_u) + \mathrm{b}(\Omega, \Phi_u, \lambda_p) = m(\Omega, \boldsymbol{q}_u, q_\tau, \lambda_\tau, \Phi_u) \qquad \forall\, \Phi_u \in X(\Omega) \\ &\mathrm{b}(\Omega, \lambda_u, \Phi_p) = 0 \qquad \forall\, \Phi_p \in M(\Omega) \\ &l_2(\Omega, \Phi_u, \lambda_{in}) = 0 \qquad \forall\, \Phi_u \in X(\Omega) \end{aligned} \tag{4.4}$$

possesses a unique solution and the estimates

$$||\lambda_\tau||_{H^1(\Omega)} \le c||k_2(\Omega, q_\tau, \cdot)||_{H^{-1}(\Omega)} \tag{4.5a}$$

$$||\lambda_u||_{H^1(\Omega)^3} + ||\lambda_p||_{L^2(\Omega)} \le c||m(\Omega, \boldsymbol{q}_u, q_\tau, \lambda_\tau, \cdot)||_{H^{-1}(\Omega)^3} \tag{4.5b}$$

hold.

Proof. The ellipticity of d follows from Theorem 2.1 and therefore the standard estimates (4.5a) and (4.5b) hold.

4.2. Computation of the shape gradient. After introducing the adjoint equations in the previous section, we now address the shape differentiability of the cost function following ideas from [11, 33].

THEOREM 4.2. *The function J is shape differentiable and its shape derivative in direction $\mathcal{V}$ is given by*

$$\begin{aligned} dJ(\Omega)[\mathcal{V}] = &- \int_\Omega Re^{-1}((\epsilon_{ijk}(\boldsymbol{D}\boldsymbol{q}_u\, \boldsymbol{D}\mathcal{V}))_{jk}\, \boldsymbol{e_i}) \cdot (\nabla \times \lambda_u)\mathrm{d}\boldsymbol{x} \\ &- \int_\Omega Re^{-1}(\nabla \times \boldsymbol{q}_u) \cdot (\epsilon_{ijk}(\boldsymbol{D}\lambda_u\, \boldsymbol{D}\mathcal{V})_{jk}\, \boldsymbol{e_i})\mathrm{d}\boldsymbol{x} \\ &- \int_\Omega \big(\lambda_p \operatorname{tr}(\boldsymbol{D}\boldsymbol{q}_u\, \boldsymbol{D}\mathcal{V}) - q_p \operatorname{tr}(\boldsymbol{D}\lambda_u\, \boldsymbol{D}\mathcal{V})\big)\mathrm{d}\boldsymbol{x} \\ &- \int_\Omega \big(\boldsymbol{q}_u \cdot (\boldsymbol{D}\mathcal{V}^T\, \nabla q_\tau)\big)\lambda_\tau \mathrm{d}\boldsymbol{x} \\ &- \int_\Omega Pe^{-1}\big((\boldsymbol{D}\mathcal{V}^T\, \nabla q_\tau) \cdot \nabla\lambda_\tau + (\boldsymbol{D}\mathcal{V}^T\, \nabla\lambda_\tau) \cdot \nabla q_\tau\big)\mathrm{d}\boldsymbol{x} \\ &+ \int_\Omega \big(Re^{-1}(\nabla \times \boldsymbol{q}_u) \cdot (\nabla \times \lambda_u) - q_p(\nabla \cdot \lambda_u)\big)(\nabla \cdot \mathcal{V})\mathrm{d}\boldsymbol{x} \\ &+ \int_\Omega \lambda_p(\nabla \cdot \boldsymbol{q}_u)(\nabla \cdot \mathcal{V})\mathrm{d}\boldsymbol{x} \\ &+ \int_\Omega \big(\boldsymbol{q}_u \cdot \nabla q_\tau\, \lambda_\tau + Pe^{-1}\nabla q_\tau \cdot \nabla\lambda_\tau - f(\boldsymbol{q}_u)\lambda_\tau\big)(\nabla \cdot \mathcal{V})\mathrm{d}\boldsymbol{x} \\ &+ \alpha_1 \int_\Omega \big(\boldsymbol{Q}(\mathcal{V})\, \nabla\boldsymbol{q}_u\big) : \nabla\boldsymbol{q}_u \mathrm{d}\boldsymbol{x} + \alpha_2 \int_{\Gamma^d} \nabla_\Gamma \cdot \mathcal{V}\mathrm{d}s, \end{aligned} \tag{4.6}$$

where $\boldsymbol{Q}(\mathcal{V}) := (\nabla \cdot \mathcal{V})\mathbb{I} - \boldsymbol{D}\mathcal{V}^T - \boldsymbol{D}\mathcal{V}$, $\boldsymbol{e_i} \in \mathbb{R}^3$ *denotes the ith standard basis vector, and* $q \in X(\Omega)$ *and* $\lambda \in F(\Omega)$ *are the unique solutions of* (2.5) *and* (4.4), *respectively.*

Proof. For the differentiation of $G(\Omega_{t\mathcal{V}}, \hat{\Phi}, \hat{\Psi})$ with $\hat{\Phi} \in E(\Omega_{t\mathcal{V}})$ and $\hat{\Psi} \in F(\Omega_{t\mathcal{V}})$ we parametrize $E(\Omega_{t\mathcal{V}})$ and $F(\Omega_{t\mathcal{V}})$ by elements of $E(\Omega)$ and $F(\Omega)$ composed with $T_{t\mathcal{V}}^{-1}$ and introduce

$$
\begin{aligned}
\mathscr{G}(t, \Phi, \Psi) :=& \; G(\Omega_{t\mathcal{V}}, \Phi \circ T_{t\mathcal{V}}^{-1}, \Psi \circ T_{t\mathcal{V}}^{-1}) \\
=& \int_{T_{t\mathcal{V}}(\Gamma^{in})} g(\Phi_\tau \circ T_{t\mathcal{V}}^{-1})\mathrm{d}s + \alpha_2 \int_{T_{t\mathcal{V}}(\Gamma^d)} 1\mathrm{d}s \\
&+ \alpha_1 \int_{\Omega_{t\mathcal{V}}} \nabla(\Phi_u \circ T_{t\mathcal{V}}^{-1}) : \nabla(\Phi_u \circ T_{t\mathcal{V}}^{-1})\mathrm{d}\boldsymbol{x} \\
&+ Re^{-1} \int_{\Omega_{t\mathcal{V}}} \nabla \times (\Phi_u \circ T_{t\mathcal{V}}^{-1}) \cdot \nabla \times (\Psi_u \circ T_{t\mathcal{V}}^{-1})\mathrm{d}\boldsymbol{x} \\
&+ \int_{T_{t\mathcal{V}}(\Gamma^{out})} \eta_{out}\big((\Phi_u \circ T_{t\mathcal{V}}^{-1}) \cdot \boldsymbol{n}\big) \big((\Psi_u \circ T_{t\mathcal{V}}^{-1}) \cdot \boldsymbol{n}\big)\mathrm{d}s \\
&+ \int_{T_{t\mathcal{V}}(\Gamma^{in})} ((\Phi_u \circ T_{t\mathcal{V}}^{-1}) \cdot \boldsymbol{n} - u_{in})\mathrm{d}s \\
&- \int_{\Omega_{t\mathcal{V}}} (\Phi_p \circ T_{t\mathcal{V}}^{-1})\nabla \cdot (\Psi_u \circ T_{t\mathcal{V}}^{-1})\mathrm{d}\boldsymbol{x} + \int_{\Omega_{t\mathcal{V}}} (\Psi_p \circ T_{t\mathcal{V}}^{-1})\nabla \cdot (\Phi_u \circ T_{t\mathcal{V}}^{-1})\mathrm{d}\boldsymbol{x} \\
&+ \int_{\Omega_{t\mathcal{V}}} (\Phi_u \circ T_{t\mathcal{V}}^{-1}) \cdot \nabla(\Phi_\tau \circ T_{t\mathcal{V}}^{-1}) \, (\Psi_\tau \circ T_{t\mathcal{V}}^{-1})\mathrm{d}\boldsymbol{x} \\
&+ Pe^{-1} \int_{\Omega_{t\mathcal{V}}} \nabla(\Phi_\tau \circ T_{t\mathcal{V}}^{-1}) \cdot \nabla(\Psi_\tau \circ T_{t\mathcal{V}}^{-1})\mathrm{d}\boldsymbol{x} \\
&- \int_{\Omega_{t\mathcal{V}}} f(\Phi_u \circ T_{t\mathcal{V}}^{-1})(\Psi_\tau \circ T_{t\mathcal{V}}^{-1})\mathrm{d}\boldsymbol{x}.
\end{aligned}
$$

An application of the transformation rule mapping the integrals defined on $\Omega_{t\mathcal{V}}$ to Ω in conjunction with Lemma 3.1 yields

(4.7)

$$
\begin{aligned}
\mathscr{G}(t, \Phi, \Psi) =& \int_{\Gamma^{out}} g(\Phi_\tau)\xi_\Gamma(t)\mathrm{d}s + \alpha_2 \int_{\Gamma^d} \xi_\Gamma(t)\mathrm{d}s \\
&+ \alpha_1 \int_\Omega (M(t)\, \nabla\Phi_u) : (M(t)\, \nabla\Phi_u)\xi(t)\mathrm{d}\boldsymbol{x} \\
&+ \int_\Omega Re^{-1}(\epsilon_{ijk}(\mathbf{D}\Phi_u\, M(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\, M(t))_{jk})\xi(t)\mathrm{d}\boldsymbol{x} \\
&+ \int_{\Gamma^{out}} \eta_{out}(\Phi_u \cdot \boldsymbol{n})(\Psi_u \cdot \boldsymbol{n})\xi_\Gamma(t)\mathrm{d}s + \int_{\Gamma^{in}} (\Phi_u \cdot \boldsymbol{n} - u_{in})\Psi_{in}\xi_\Gamma(t)\mathrm{d}s \\
&- \int_\Omega \Phi_p \mathrm{tr}(\mathbf{D}\Psi_u\, M^T(t))\xi(t)\mathrm{d}\boldsymbol{x} + \int_\Omega \Psi_p \mathrm{tr}(\mathbf{D}\Phi_u\, M^T(t))\xi(t)\mathrm{d}\boldsymbol{x} \\
&+ \int_\Omega \Big(\Phi_u \cdot (M(t)\, \nabla\Phi_\tau)\Psi_\tau + Pe^{-1}(M(t)\, \nabla\Phi_\tau) \cdot (M(t)\, \nabla\Psi_\tau)\Big)\xi(t)\mathrm{d}\boldsymbol{x} \\
&- \int_\Omega f(\Phi_u)\Psi_\tau\xi(t)\mathrm{d}\boldsymbol{x}.
\end{aligned}
$$

Note that by definition $\mathscr{G}$ is affine with respect to Ψ and that

$$J(\Omega_{t\mathcal{V}}) = \mathscr{G}(t, q^t, \Psi) \quad \forall\, \Psi \in F(\Omega), \tag{4.8}$$

where $q^t := ((\boldsymbol{q}_u^t)^T, q_p^t, q_\tau^t)^T \in E(\Omega)$ with $\boldsymbol{q}_u^t \cdot \boldsymbol{n} = u_{in}$ on Γ^{in} solves the forward equations on the transformed domain after pull-back to the reference domain

$$\mathrm{Q}_t(\Omega, q^t, \Psi) = 0 \quad \forall\, \Psi \in F(\Omega) \tag{4.9}$$

with

(4.10)

$$\begin{aligned}
\mathrm{Q}_t(\Omega, q^t, \Psi) := &\int_\Omega Re^{-1}(\epsilon_{ijk}(\mathbf{D}\boldsymbol{q}_u^t\, M(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\, M(t))_{jk})\xi(t)\mathrm{d}\boldsymbol{x} \\
&+ \int_{\Gamma^{out}} \eta_{out}(\boldsymbol{q}_u^t \cdot \boldsymbol{n})(\Psi_u \cdot \boldsymbol{n})\xi_\Gamma(t)\mathrm{d}s + \int_{\Gamma^{in}} (\Phi_u \cdot \boldsymbol{n} - u_{in})\Psi_{in}\xi_\Gamma(t)\mathrm{d}s \\
&- \int_\Omega q_p^t \mathrm{tr}(\mathbf{D}\Psi_u\, M^T(t))\xi(t)\mathrm{d}\boldsymbol{x} + \int_\Omega \Psi_p \mathrm{tr}(\mathbf{D}\boldsymbol{q}_u^t\, M^T(t))\xi(t)\mathrm{d}\boldsymbol{x} \\
&+ \int_\Omega \Big(\boldsymbol{q}_u^t \cdot (M(t)\,\nabla q_\tau^t)\Psi_\tau + Pe^{-1}(M(t)\,\nabla q_\tau^t)\cdot(M(t)\,\nabla\Psi_\tau)\Big)\xi(t)\mathrm{d}\boldsymbol{x} \\
&- \int_\Omega f(\boldsymbol{q}_u^t)\Psi_\tau \xi(t)\mathrm{d}\boldsymbol{x}.
\end{aligned}$$

In order to apply Theorem 3.4 for the computation of the shape derivative, we verify that $\mathscr{G}$ with $E = E(\Omega)$ and $F = F(\Omega)$ satisfies assumptions (H0)–(H3) and start by showing that (4.9) is indeed well-posed.

Verification of (H0). We assume that $\mathcal{V} \in \boldsymbol{\Theta}^1(\mathbb{R}^3)$ is chosen such that for $t > 0$ small enough, the perturbed domain possesses the same smoothness properties as Ω and $\Gamma \setminus \Gamma^d$ is unchanged, i.e., $\Omega_{t\mathcal{V}} \in \mathcal{A}$. Due to Theorem 2.1 there exists a solution $q_t \in E(\Omega_{t\mathcal{V}})$ of

$$\mathrm{Q}(\Omega_{t\mathcal{V}}, q_t, \hat{\Psi}) = 0 \quad \forall\, \hat{\Psi} \in F(\Omega_{t\mathcal{V}}),$$

which is bounded by (2.6a) and (2.6b). The definitions of Q and Q_t from (4.1) and (4.10) together with the reparametrization of the function spaces yield

$$\mathrm{Q}_t(\Omega, \Phi, \Psi) = \mathrm{Q}(\Omega_{t\mathcal{V}}, \Phi \circ T_{t\mathcal{V}}^{-1}, \Psi \circ T_{t\mathcal{V}}^{-1}) = \mathrm{Q}(\Omega_{t\mathcal{V}}, \hat{\Phi}, \hat{\Psi}),$$

which implies that $q^t := q_t \circ T_{t\mathcal{V}} \in E(\Omega)$ solves (4.9). The boundedness of q^t can then be inferred from the boundedness of q_t and $T_{t\mathcal{V}}$.

Conditions (H0)(i) and (H0)(ii) are satisfied due to the continuity of the functions $[0, 1] \ni r \mapsto \mathscr{G}(t, q^0 + r(q^t - q^0), \Psi)$ and $[0, 1] \ni r \mapsto D_\Phi\mathscr{G}(t, q^0 + r(q^t - q^0), \Psi)[\Phi]$.

Verification of (H1). Condition (H1) is satisfied since $M(t)$, $\xi(t)$ and $\xi_\Gamma(t)$ are continuously differentiable.

Verification of (H2). Defining the averaged solution $q^{t,r} := q + r(q^t - q)$, we consider the solution set $\{\lambda^t\} \subset E(\Omega)$ with $\lambda^t := ((\lambda_u^t)^T, \lambda_p^t, \lambda_\tau^t, \lambda_{in}^t)^T$ of the averaged adjoint equation

$$\int_0^1 D_\Phi\mathscr{G}(t, q^{t,r}, \lambda^t)[\Phi]\,\mathrm{d}r = 0 \quad \forall \Phi \in E(\Omega). \tag{4.11}$$

Proceeding similarly to subsection 4.1, we derive the averaged adjoint transport equation

$$
\begin{aligned}
&\int_0^1 \int_\Omega -(\boldsymbol{q}_u^{t,r} \cdot (M(t)\nabla \lambda_\tau^t))\Phi_\tau \xi(t) \mathrm{d}\boldsymbol{x}\, \mathrm{d}r \\
&+ \int_0^1 \int_\Omega Pe^{-1} (M(t)\,\nabla \lambda_\tau^t) \cdot (M(t)\,\nabla \Phi_\tau)\xi(t)\mathrm{d}\boldsymbol{x}\, \mathrm{d}r \\
&+ \int_0^1 \int_{\Gamma^{out}} (\boldsymbol{q}_u^{t,r} \cdot \boldsymbol{n})\Phi_\tau \lambda_\tau^t \xi_\Gamma(t)\mathrm{d}s\, \mathrm{d}r \\
&= -\int_0^1 \int_{\Gamma^{out}} \partial_{\Phi_\tau} g(q_\tau^{t,r})\Phi_\tau \xi_\Gamma(t)\mathrm{d}s\, \mathrm{d}r \quad \forall\, \Phi_\tau \in R(\Omega),
\end{aligned} \tag{4.12}
$$

as well as the averaged adjoint Stokes equation

$$
\begin{aligned}
&\int_0^1 \int_\Omega Re^{-1} (\epsilon_{ijk}(\mathbf{D}\Phi_u\, M(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\lambda_u^t\, M(t))_{jk})\xi(t)\mathrm{d}\boldsymbol{x}\, \mathrm{d}r \\
&+ \int_0^1 \int_\Omega \lambda_p^t \mathrm{tr}(\mathbf{D}\Phi_u\, M^T(t))\xi(t)\mathrm{d}\boldsymbol{x}\, \mathrm{d}r \\
&+ \int_0^1 \int_{\Gamma^{out}} \eta_{out}(\Phi_u \cdot \boldsymbol{n})(\lambda_u^t \cdot \boldsymbol{n})\xi_\Gamma(t)\mathrm{d}s\, \mathrm{d}r + \int_0^1 \int_{\Gamma^{in}} (\Phi_u \cdot \boldsymbol{n})\lambda_{in}\xi_\Gamma(t)\mathrm{d}s\, \mathrm{d}r \\
&= \int_0^1 \int_\Omega \Phi_u \cdot \Big((\lambda_\tau^t\, M(t)\, \nabla q_\tau^{t,r}) + \partial_{\Phi_u} f(\boldsymbol{q}_u^{t,r})\lambda_\tau^t \Big)\xi(t)\mathrm{d}\boldsymbol{x}\, \mathrm{d}r \\
&- \int_0^1 \int_\Omega 2\,\alpha_1 (M(t)\,\nabla \boldsymbol{q}_u^{t,r}) : (M(t)\,\nabla \Phi_u)\xi(t)\mathrm{d}\boldsymbol{x}\, \mathrm{d}r \quad \forall\, \Phi_u \in X(\Omega),
\end{aligned} \tag{4.13}
$$

with incompressibility condition

$$
\int_0^1 \int_\Omega -\Phi_p \mathrm{tr}(\mathbf{D}\lambda_u^t\, M^T(t))\xi(t)\mathrm{d}\boldsymbol{x}\, \mathrm{d}r = 0 \quad \forall\, \Phi_p \in M(\Omega). \tag{4.14}
$$

Analogous to the well-posedness of (4.9), the existence of a unique solution of (4.11) for $t > 0$ sufficiently small can be inferred from the well-posedness of the adjoint equations on $\Omega_{t\mathcal{V}}$ given by Theorem 4.1.

Verification of (H3). We make sure this assumption holds by showing that there is a sequence $(\lambda^{t_k})_{k\in\mathbb{N}}$ with $t_k \searrow 0$ as $k \to \infty$, where $\{\lambda^{t_{n_k}}\} = Y(t_k, q^{t_k}, q)$ converges weakly in $F(\Omega)$ to λ, and that $(t, \Psi) \mapsto \partial_t \mathscr{G}(t, q, \Psi)$ is weakly sequentially continuous.

The boundedness of the sequence $(||q^t||_{E(\Omega)})_{t\geq 0}$ guarantees the boundedness of the sequence $(||\lambda^t||_{F(\Omega)})_{t\geq 0}$ for t sufficiently small. This can be seen by taking $\Phi_\tau = \lambda_\tau^t$, $\Phi_u = \lambda_u^t$, and $\Phi_p = \lambda_p^t$ in (4.12)–(4.14), respectively, and using the continuity of the integrals at $t = 0$. Due to the boundedness of the sequence of averaged adjoint solutions there exists a weakly converging subsequence $\lambda^{t_{n_k}}$ with limit $w \in F(\Omega)$. The strong convergence $q^t \to q$ in $E(\Omega)$, which is proved in Lemma 4.3, can be used to pass to the limit $t \searrow 0$ in (4.12)–(4.14) and we obtain

$$
\lambda^{t_{n_k}} \rightharpoonup \lambda \text{ for } k \to \infty,
$$

where $\lambda \in F(\Omega)$ solves the adjoint problem (4.4). The uniqueness of the limit yields $w = \lambda$.

Since condition (H1) is satisfied, we can compute the partial derivative

$$
\begin{aligned}
&\partial_t \mathscr{G}(t,\Phi,\Psi)\\
&= \int_{\Gamma^{out}} g(\Psi_\tau){\xi_\Gamma}'(t)\mathrm{d}s + \int_{\Gamma^d} \alpha_2 {\xi_\Gamma}'(t)\mathrm{d}s\\
&+ \int_\Omega \alpha_1 (M'(t)\,\nabla\Phi_u) : (M(t)\,\nabla\Phi_u)\xi(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega \alpha_1 (M(t)\,\nabla\Phi_u) : (M'(t)\,\nabla\Phi_u)\xi(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega \alpha_1 (M(t)\,\nabla\Phi_u) : (M(t)\,\nabla\Phi_u)\xi'(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega Re^{-1}(\epsilon_{ijk}(\mathbf{D}\Phi_u\, M'^T(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\, M^T(t))_{jk})\xi(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega Re^{-1}(\epsilon_{ijk}(\mathbf{D}\Phi_u\, M^T(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\, M'^T(t))_{jk})\xi(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega Re^{-1}(\epsilon_{ijk}(\mathbf{D}\Phi_u\, M^T(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\, M^T(t))_{jk})\xi'(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_{\Gamma^{out}} \eta_{out}(\Phi_u\cdot\boldsymbol{n})(\Psi_u\cdot\boldsymbol{n}){\xi_\Gamma}'(t)\mathrm{d}s + \int_{\Gamma^{in}} (\Phi_u\cdot\boldsymbol{n} - u_{in})\Psi_{in}{\xi_\Gamma}'(t)\mathrm{d}s\\
&+ \int_\Omega -\Phi_p \mathrm{tr}(\mathbf{D}\Psi_u\, M'^T(t))\xi(t)\mathrm{d}\boldsymbol{x} + \int_\Omega -\Phi_p \mathrm{tr}(\mathbf{D}\Psi_u\, M^T(t))\xi'(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega \Psi_p \mathrm{tr}(\mathbf{D}\Phi_u\, M'^T(t))\xi(t)\mathrm{d}\boldsymbol{x} + \int_\Omega \Psi_p \mathrm{tr}(\mathbf{D}\Phi_u\, M^T(t))\xi'(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega \Phi_u\cdot(M'(t)\,\nabla\Phi_\tau)\Psi_\tau\xi(t)\mathrm{d}\boldsymbol{x} + \int_\Omega \Phi_u\cdot(M(t)\,\nabla\Phi_\tau)\Psi_\tau\xi'(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega Pe^{-1}(M'(t)\,\nabla\Phi_\tau)\cdot(M(t)\,\nabla\Psi_\tau)\xi(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega Pe^{-1}(M(t)\,\nabla\Phi_\tau)\cdot(M'(t)\,\nabla\Psi_\tau)\xi(t)\mathrm{d}\boldsymbol{x}\\
&+ \int_\Omega Pe^{-1}(M(t)\,\nabla\Phi_\tau)\cdot(M(t)\,\nabla\Psi_\tau)\xi'(t)\mathrm{d}\boldsymbol{x} - \int_\Omega f(\Phi_u)\Psi_\tau\xi'(t)\mathrm{d}\boldsymbol{x},
\end{aligned}
$$

from which we see that for fixed $\Phi \in E(\Omega)$ the mapping $(t,\Psi) \mapsto \partial_t\mathscr{G}(t,\Phi,\Psi)$ is weakly sequentially continuous. Therefore (H3) is satisfied. Due to (4.8) we obtain

$$
dJ(\Omega)[\mathcal{V}] = \partial_t\mathscr{G}(0,q,\lambda) \tag{4.15}
$$

with the solutions $q \in E(\Omega)$ of the forward problem (2.5) and $\lambda \in F(\Omega)$ of the adjoint problem (4.4). Since Γ^{in} and Γ^{out} are kept fixed, the boundary integrals in (4.15) vanish. For the evaluation of the remaining volume integrals we take (3.4) from Lemma 3.1 into account. ∎

Next, Lemma 4.3 addresses the convergence in norms of the solutions of (4.9), which was used to verify assumption (H3) in Theorem 4.2. A continuity result for the instationary incompressible Navier–Stokes equations with different boundary conditions has been derived in [22]. Since we consider a nonstandard formulation of the stationary incompressible Stokes equations with an additional advection-diffusion-reaction equation (2.5) in this paper, Lemma 4.3 represents a new result.

Lemma 4.3. *The sequence of solutions $\{q^t\}_t \in E(\Omega)$ of (4.9) converges to the solution $q \in E(\Omega)$ of problem (2.5) in the sense of norms, i.e., it holds that*

$$\lim_{t \searrow 0} ||q^t - q||_{E(\Omega)} = 0.$$

Proof. The proof is split into three parts. In the first part we prove the continuity result for the fluid velocity, which is then used for the continuity of pressure and residence time in the second and third parts, respectively. Throughout the proof we denote by $c > 0$ a generic constant.

Continuity of the velocity. In order to prove $\lim_{t\searrow 0} ||\boldsymbol{q}_u^t - \boldsymbol{q}_u||_{H^1(\Omega)^3} = 0$ we subtract the fluid velocity equation on the unperturbed domain

$$\begin{aligned} 0 &= \int_\Omega Re^{-1}(\nabla \times \boldsymbol{q}_u) \cdot (\nabla \times \Psi_u)\mathrm{d}\boldsymbol{x} \\ &\quad + \int_{\Gamma^{out}} \eta_{out}(\boldsymbol{q}_u \cdot \boldsymbol{n})(\Psi_u \cdot \boldsymbol{n})\mathrm{d}s - \int_\Omega q_p \nabla \cdot \Psi_u \mathrm{d}\boldsymbol{x} \quad \forall\, \Psi_u \in X_0(\Omega) \end{aligned}$$

from the corresponding equation on the perturbed domain

$$\begin{aligned} 0 &= \int_\Omega Re^{-1}(\epsilon_{ijk}(\mathbf{D}\boldsymbol{q}_u^t\, M(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\, M(t))_{jk})\xi(t)\mathrm{d}\boldsymbol{x} \\ &+ \int_{\Gamma^{out}} \eta_{out}(\boldsymbol{q}_u^t \cdot \boldsymbol{n})(\Psi_u \cdot \boldsymbol{n})\xi_\Gamma(t)\mathrm{d}s - \int_\Omega q_p^t \mathrm{tr}(\mathbf{D}\Psi_u\, M^T(t))\xi(t)\mathrm{d}\boldsymbol{x} \quad \forall\, \Psi_u \in X_0(\Omega) \end{aligned}$$

for $t > 0$. Carefully adding zeros, this amounts to

$$\begin{aligned} & Re^{-1}\int_\Omega (\nabla \times (\boldsymbol{q}_u^t - \boldsymbol{q}_u)) \cdot (\nabla \times \Psi_u)\mathrm{d}\boldsymbol{x} + \eta_{out}\int_{\Gamma^{out}} ((\boldsymbol{q}_u^t - \boldsymbol{q}_u)\cdot \boldsymbol{n})(\Psi_u \cdot \boldsymbol{n})\mathrm{d}s \\ &= -Re^{-1}\int_\Omega (\epsilon_{ijk}(\mathbf{D}\boldsymbol{q}_u^t\, M(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\,(\xi(t)M(t) - \mathbb{I}))_{jk}))\mathrm{d}\boldsymbol{x} \\ &- Re^{-1}\int_\Omega (\epsilon_{ijk}(\mathbf{D}\boldsymbol{q}_u^t\,(M(t) - \mathbb{I}))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u)_{jk}))\mathrm{d}\boldsymbol{x} \\ &- \eta_{out}\int_{\Gamma^{out}} (\boldsymbol{q}_u^t \cdot \boldsymbol{n})(\Psi_u \cdot \boldsymbol{n})(\xi_\Gamma(t) - 1)\mathrm{d}s \\ &+ \int_\Omega (q_p^t - q_p)\mathrm{tr}(\mathbf{D}\Psi_u)\mathrm{d}\boldsymbol{x} + \int_\Omega q_p^t \mathrm{tr}(\mathbf{D}\Psi_u(M(t) - \mathbb{I}))\xi(t)\mathrm{d}\boldsymbol{x} \\ &+ \int_\Omega q_p^t \mathrm{tr}(\mathbf{D}\Psi_u)(\xi(t) - 1)\mathrm{d}\boldsymbol{x} \quad \forall\, \Psi_u \in X_0(\Omega). \end{aligned} \tag{4.16}$$

The first term on the right-hand side of (4.16) can be estimated by

$$\begin{aligned} &\int_\Omega |(\epsilon_{ijk}(\mathbf{D}\boldsymbol{q}_u^t\, M(t))_{jk})(\epsilon_{ijk}(\mathbf{D}\Psi_u\,(\xi(t)M(t) - \mathbb{I}))_{jk}))|\mathrm{d}\boldsymbol{x} \\ &\le c||\mathbf{D}\boldsymbol{q}_u^t\, M(t)||_{L^2(\Omega)^{3\times 3}}\, ||\mathbf{D}\Psi_u\,(\xi(t)M(t) - \mathbb{I})||_{L^2(\Omega)^{3\times 3}} \\ &\le c||M(t)||_{L^\infty(\Omega)^{3\times 3}}\, ||\mathbf{D}\boldsymbol{q}_u^t||_{L^2(\Omega)^{3\times 3}}\, ||\mathbf{D}\Psi_u||_{L^2(\Omega)^{3\times 3}}\, ||\xi(t)M(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}} \\ &\le c||\xi(t)M(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}} \end{aligned}$$

using Hölder's inequality, the boundedness of the state variables, and the boundedness of the Jacobian of the transformation for $t \in [0, T]$.

The second and fifth terms can be estimated similarly using

$$||\mathrm{tr}(\mathbf{D}\Psi_u(M(t)-\mathbb{I}))||_{L^2(\Omega)} \leq c||M(t)-\mathbb{I}||_{L^\infty(\Omega)^{3\times 3}}\,||\mathbf{D}\Psi_u||_{L^2(\Omega)^{3\times 3}}. \tag{4.17}$$

For the third term we get

$$\begin{aligned}\int_{\Gamma^{out}} |(\boldsymbol{q}_u^t\cdot\boldsymbol{n})(\Psi_u\cdot\boldsymbol{n})(\xi_\Gamma(t)-1)|\mathrm{d}s &\leq c||\boldsymbol{q}_u^t||_{H^1(\Omega)^3}\,||\Psi_u||_{H^1(\Omega)^3}\,||\xi_\Gamma(t)-1||_{L^\infty(\Gamma^{out})}\\ &\leq c||\xi_\Gamma(t)-1||_{L^\infty(\Gamma^{out})}\end{aligned}$$

using Hölder's inequality, the trace theorem [35], and the boundedness of the state.

With the same techniques as before, the sixth term is bounded by

$$\int_\Omega |q_p^t\mathrm{tr}(\mathbf{D}\Psi_u)(\xi(t)-1)|\mathrm{d}\boldsymbol{x} \leq c||\xi(t)-1||_{L^\infty(\Omega)}.$$

The fourth term requires a little more care. Subtracting the incompressibility equation for $t=0$ from the corresponding equation for $t>0$ gives

$$\begin{aligned}\int_\Omega \Psi_p\mathrm{tr}(\mathbf{D}(\boldsymbol{q}_u-\boldsymbol{q}_u^t))\mathrm{d}\boldsymbol{x} &= \int_\Omega \Psi_p\mathrm{tr}(\mathbf{D}\boldsymbol{q}_u^t(M^T(t)-\mathbb{I}))\xi(t)\mathrm{d}\boldsymbol{x}\\ &\quad+\int_\Omega \Psi_p\mathrm{tr}(\mathbf{D}\boldsymbol{q}_u^t)(\xi(t)-1)\mathrm{d}\boldsymbol{x}\quad\forall\Psi_p\in M(\Omega).\end{aligned}$$

If we now set $\Psi_p=\mathrm{tr}(\mathbf{D}(\boldsymbol{q}_u-\boldsymbol{q}_u^t))$ in this equation and use (4.17), we obtain

$$||\mathrm{tr}(\mathbf{D}(\boldsymbol{q}_u-\boldsymbol{q}_u^t))||_{L^2(\Omega)} \leq c(||M(t)-\mathbb{I}||_{L^\infty(\Omega)^{3\times3}}+||\xi(t)-1||_{L^\infty(\Omega)}),$$

which can then be used to bound the fourth term of (4.16) by

$$\begin{aligned}\int_\Omega |(q_p^t-q_p)\mathrm{tr}(\mathbf{D}\Psi_u)|\mathrm{d}\boldsymbol{x} &\leq (||q_p||_{L^2(\Omega)}+||q_p^t||_{L^2(\Omega)})||\mathrm{tr}(\mathbf{D}\Psi_u)||_{L^2(\Omega)}\\ &\leq c(||M(t)-\mathbb{I}||_{L^\infty(\Omega)^{3\times3}}+||\xi(t)-1||_{L^\infty(\Omega)}).\end{aligned}$$

We now consider the left-hand side of (4.16). Setting $\Psi_u=\boldsymbol{q}_u^t-\boldsymbol{q}_u$ we obtain

$$\begin{aligned}c||\boldsymbol{q}_u^t-\boldsymbol{q}_u||^2_{H^1(\Omega)^3} &\leq Re^{-1}||\nabla\times(\boldsymbol{q}_u^t-\boldsymbol{q}_u)||^2_{L^2(\Omega)^3}\\ &\leq Re^{-1}||\nabla\times(\boldsymbol{q}_u^t-\boldsymbol{q}_u)||^2_{L^2(\Omega)^3}+\eta_{out}\int_{\Gamma^{out}}((\boldsymbol{q}_u^t-\boldsymbol{q}_u)\cdot\boldsymbol{n})^2\mathrm{d}s.\end{aligned}$$

Here we have used the ellipticity result from [13] as well as the Poincaré–Friedrichs inequality, which can be applied due to $(\boldsymbol{q}_u^t-\boldsymbol{q}_u)\cdot\boldsymbol{n}=0$ a.e. on Γ^{in}.

Summing up we derived

$$\begin{aligned}||\boldsymbol{q}_u^t-\boldsymbol{q}_u||^2_{H^1(\Omega)^3} &\leq c\big(||\xi(t)M(t)-\mathbb{I}||_{L^\infty(\Omega)^{3\times3}}+||M(t)-\mathbb{I}||_{L^\infty(\Omega)^{3\times3}}\\ &\quad+||\xi(t)-1||_{L^\infty(\Omega)}+||\xi_\Gamma(t)-1||_{L^\infty(\Gamma^{out})}\big).\end{aligned}$$

Since the right-hand side of the above inequality continuously depends on t and $M(0)=\mathbb{I}$ as well as $\xi(0)=\xi_\Gamma(0)=1$ hold, we obtain $\lim_{t\searrow0}||\boldsymbol{q}_u^t-\boldsymbol{q}_u||_{H^1(\Omega)^3}=0$.

Continuity of the pressure. Given the continuity result for the velocity, the statement $\lim_{t\searrow0}||q_p^t-q_p||_{L^2(\Omega)}=0$ holds due to Lemma 4.17 of [22].

Continuity of the residence time. We subtract the equation on the unperturbed domain

$$0 = \int_\Omega \boldsymbol{q}_u \cdot \nabla q_\tau \Psi_\tau \mathrm{d}\boldsymbol{x} + \int_\Omega Pe^{-1} \nabla q_\tau \cdot \nabla \Psi_\tau \mathrm{d}\boldsymbol{x} - \int_\Omega f(\boldsymbol{q}_u)\Psi_\tau \mathrm{d}\boldsymbol{x} \quad \forall \Psi_\tau \in R(\Omega)$$

from the equation on the perturbed domain

$$\begin{aligned} 0 = &\int_\Omega \boldsymbol{q}_u^t \cdot M(t)\, \nabla q_\tau^t \Psi_\tau \xi(t) \mathrm{d}\boldsymbol{x} + \int_\Omega Pe^{-1} (M(t)\, \nabla q_\tau^t) \cdot (M(t)\, \nabla \Psi_\tau)\xi(t) \mathrm{d}\boldsymbol{x} \\ &- \int_\Omega f(\boldsymbol{q}_u^t)\Psi_\tau \xi(t) \mathrm{d}\boldsymbol{x} \quad \forall \Psi_\tau \in R(\Omega) \end{aligned}$$

for $t > 0$. After adding zeros and inserting $\Psi_\tau = q_\tau^t - q_\tau$, this is equal to

$$\begin{aligned} &\int_\Omega Pe^{-1} \nabla (q_\tau^t - q_\tau) \cdot \nabla (q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} + \int_\Omega \boldsymbol{q}_u \cdot \nabla (q_\tau^t - q_\tau)(q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} \\ &= - \int_\Omega \boldsymbol{q}_u^t \cdot (\xi(t) M(t) - \mathbb{I})\, \nabla q_\tau^t (q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} - \int_\Omega (\boldsymbol{q}_u^t - \boldsymbol{q}_u) \cdot \nabla q_\tau^t (q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} \\ &\quad - \int_\Omega Pe^{-1} ((\xi(t) M(t) M^T(t) - \mathbb{I})\, \nabla q_\tau^t) \nabla (q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} \\ &\quad + \int_\Omega (f(\boldsymbol{q}_u^t) - f(\boldsymbol{q}_u))(q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} + \int_\Omega f(\boldsymbol{q}_u^t)(\xi(t) - 1)(q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x}. \end{aligned} \tag{4.18}$$

The first integral on the left-hand side of (4.18) is equal to $Pe^{-1} ||\nabla (q_\tau^t - q_\tau)||^2_{L^2(\Omega)}$. For the second one, we have

$$2 \int_\Omega \boldsymbol{q}_u \cdot \nabla (q_\tau^t - q_\tau)(q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} = \int_{\Gamma^{out}} (\boldsymbol{q}_u \cdot \boldsymbol{n})(q_\tau^t - q_\tau)^2 \mathrm{d}s \geq 0$$

due to (2.7), the weak incompressibility condition, and the simple connectivity of Γ^{in} and Γ^{out}. An application of the Poincaré–Friedrichs inequality then yields

$$\begin{aligned} c^{-1} ||q_\tau^t - q_\tau||^2_{H^1(\Omega)} \leq &\int_\Omega Pe^{-1} \nabla (q_\tau^t - q_\tau) \cdot \nabla (q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x} \\ &+ \int_\Omega \boldsymbol{q}_u \cdot \nabla (q_\tau^t - q_\tau)(q_\tau^t - q_\tau) \mathrm{d}\boldsymbol{x}. \end{aligned} \tag{4.19}$$

In order to estimate the terms on the right-hand side of (4.18) we note that for $\Omega \subset \mathbb{R}^3$ bounded the inclusion

$$H^1(\Omega) \hookrightarrow L^6(\Omega) \tag{4.20}$$

holds due to the Sobolev embedding theorem. An application of Hölder's inequality together with (4.20) and the boundedness of the state variables then yields

$$\begin{aligned} &\int_\Omega |\boldsymbol{q}_u^t \cdot (\xi(t) M(t) - \mathbb{I})\, \nabla q_\tau^t (q_\tau^t - q_\tau)| \mathrm{d}\boldsymbol{x} \\ &\leq ||\xi(t) M(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}}\, ||\boldsymbol{q}_u^t||_{L^6(\Omega)^3}\, ||\nabla q_\tau^t||_{L^{3/2}(\Omega)^3}\, ||q_\tau^t - q_\tau||_{L^6(\Omega)} \\ &\leq c||\xi(t) M(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}}\, ||\boldsymbol{q}_u^t||_{H^1(\Omega)^3}\, ||\nabla q_\tau^t||_{L^2(\Omega)^3}\, ||q_\tau^t - q_\tau||_{H^1(\Omega)} \\ &\leq c||\xi(t) M(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}}\, ||q_\tau^t - q_\tau||_{H^1(\Omega)}. \end{aligned}$$

The second integral can be bounded in the same manner by

$$\begin{aligned}\int_\Omega |(\boldsymbol{q}_u^t - \boldsymbol{q}_u)\cdot \nabla q_\tau^t (q_\tau^t - q_\tau)|\mathrm{d}\boldsymbol{x} &\le ||\boldsymbol{q}_u^t - \boldsymbol{q}_u||_{L^6(\Omega)^3}\, ||\nabla q_\tau^t||_{L^{3/2}(\Omega)^3}\, ||q_\tau^t - q_\tau||_{L^6(\Omega)} \\ &\le c||\boldsymbol{q}_u^t - \boldsymbol{q}_u||_{H^1(\Omega)^3}\, ||\nabla q_\tau^t||_{L^2(\Omega)}\, ||q_\tau^t - q_\tau||_{H^1(\Omega)} \\ &\le c||\boldsymbol{q}_u^t - \boldsymbol{q}_u||_{H^1(\Omega)^3}\, ||q_\tau^t - q_\tau||_{H^1(\Omega)}.\end{aligned}$$

For the third integral we obtain

$$\begin{aligned}&\int_\Omega |Pe^{-1}((\xi(t)M(t)M^T(t) - \mathbb{I})\,\nabla q_\tau^t)\nabla(q_\tau^t - q_\tau)|\mathrm{d}\boldsymbol{x} \\ &\le Pe^{-1}||\xi(t)M(t)M^T(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}}\, ||\nabla q_\tau^t||_{L^2(\Omega)^3}\, ||\nabla(q_\tau^t - q_\tau)||_{L^2(\Omega)^3} \\ &\le c||\xi(t)M(t)M^T(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}}\, ||q_\tau^t - q_\tau||_{H^1(\Omega)}.\end{aligned}$$

The fourth integral can be estimated through

$$\begin{aligned}\int_\Omega (f(\boldsymbol{q}_u^t) - f(\boldsymbol{q}_u))(q_\tau^t - q_\tau)\mathrm{d}\boldsymbol{x} &\le ||f(\boldsymbol{q}_u^t) - f(\boldsymbol{q}_u)||_{L^2(\Omega)}\, ||q_\tau^t - q_\tau||_{L^2(\Omega)} \\ &\le c||\boldsymbol{q}_u^t - \boldsymbol{q}_u||_{H^1(\Omega)^3}\, ||q_\tau^t - q_\tau||_{H^1(\Omega)}\end{aligned}$$

by the Lipschitz continuity of f. The fifth integral is bounded by

$$\begin{aligned}\int_\Omega |f(\boldsymbol{q}_u^t)(\xi(t) - 1)(q_\tau^t - q_\tau)|\mathrm{d}\boldsymbol{x} &\le ||f(\boldsymbol{q}_u^t)||_{L^2(\Omega)}\, ||\xi(t) - 1||_{L^\infty(\Omega)}\, ||q_\tau^t - q_\tau||_{L^2(\Omega)} \\ &\le c||\xi(t) - 1||_{L^\infty(\Omega)}\, ||q_\tau^t - q_\tau||_{H^1(\Omega)}.\end{aligned}$$

Combining (4.19) with these estimates and dividing by $||q_\tau^t - q_\tau||_{H^1(\Omega)}$ yields

$$\begin{aligned}||q_\tau^t - q_\tau||_{H^1(\Omega)} \le c\,Pe\,\big(&||\xi(t)M(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}} + ||\boldsymbol{q}_u^t - \boldsymbol{q}_u||_{H^1(\Omega)^3} \\ &+ ||\xi(t)M(t)M^T(t) - \mathbb{I}||_{L^\infty(\Omega)^{3\times 3}} + ||\xi(t) - 1||_{L^\infty(\Omega)}\big).\end{aligned}$$

Passing to the limit, the right-hand side of the above equation vanishes due to the first part of the proof and the regularity of the transformation and we therefore obtain $\lim_{t\searrow 0} ||q_\tau^t - q_\tau||_{H^1(\Omega)} = 0$. ∎

5. Melt distributor optimization. After the derivation of the shape gradient in section 4 we now turn our attention toward the numerical implementation. Subsection 5.1 is devoted to the mesh deformation procedure based on the main theorem, Theorem 4.2. After addressing details of the discretization in subsection 5.2, we validate our approach in subsection 5.3 by applying a gradient descent method on the distributor shown in Figure 2.

5.1. Gradient descent method. For the computation of a geometry that yields a decrease in the cost function, we define the space of deformations

$$D := \left\{ W \in H^1(\Omega)^3 \,\middle|\, W|_{\Gamma\setminus\Gamma^d} = 0 \right\}$$

and identify the shape derivative (4.6) with an element $\mathcal{G} \in D$ by solving

$$\mathcal{A}(\mathcal{G}, \mathcal{V}) = dJ(\Omega)[\mathcal{V}] \quad \forall\, \mathcal{V} \in D$$

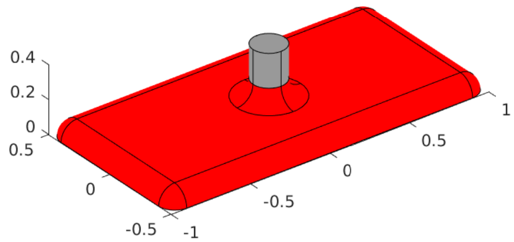


FIG. 2. *Initial distributor geometry and deformable boundary* Γ^d.

with an elliptic bilinear form $\mathcal{A}$. We employ the approach of solving the linear elasticity equations with the volume and surface parts of the shape gradient acting as body forces and surface tractions; see, e.g., [7, 28]. For this purpose we introduce the strain and stress tensors

$$\sigma(\mathcal{G}) := \lambda \operatorname{tr}(\epsilon(\mathcal{G}))\mathbb{I} + 2\mu\epsilon(\mathcal{G}), \quad \epsilon(\mathcal{G}) := \frac{1}{2}(\nabla\mathcal{G} + \nabla\mathcal{G}^T)$$

with the first and second Lamé parameters λ and μ. Proceeding in a similar manner as [28] we set $\nu = \lambda = 0$ and choose $\mu := \sqrt{\mu^*}$ with the solution μ^* of

$$\begin{aligned} \Delta\mu^* &= 0 \text{ in } \Omega, \\ \mu^* &= \mu^*_{max} \text{ on } \Gamma^d, \\ \mu^* &= \mu^*_{min} \text{ on } \Gamma \setminus \Gamma^d \end{aligned} \tag{5.1}$$

for $\mu^*_{min} = 1$ and $\mu^*_{max} = 100$ and determine the shape gradient $\mathcal{G} \in H$ by numerically solving

$$\mathcal{A}(\mathcal{G}, \mathcal{V}) := \int_\Omega \sigma(\mathcal{G}) : \epsilon(\mathcal{V}) \mathrm{d}\boldsymbol{x} = dJ(\Omega)[\mathcal{V}] \quad \forall\, \mathcal{V} \in D. \tag{5.2}$$

We note that the negative gradient $-\mathcal{G} \in D \setminus \{0\}$ satisfies

$$dJ(\Omega)[-\mathcal{G}] = -\mathcal{A}(\mathcal{G}, \mathcal{G}) < 0$$

due to the ellipticity of $\mathcal{A}$ and therefore yields a direction of descent. Given the step size $t > 0$ and the solution $\mathcal{G} \in D$ of (5.2) we deform the mesh used for the discretization of (2.5), (4.4), (5.1), and (5.2) by applying the transformation

$$T_{t\mathcal{V}} := \mathbb{I} + t(-\mathcal{G})$$

to each vertex without changing their connectivity. For $t > 0$ small enough this defines a diffeomorphism [31] keeping $\Gamma \setminus \Gamma^d$ fixed and therefore yields a valid geometry $T_{t\mathcal{V}}(\Omega) \in \mathcal{A}$ satisfying $J(T_{t\mathcal{V}}(\Omega)) < J(\Omega)$.

From the Hadamard theorem [32] we know that changes in the cost function are solely due to normal deformations of the boundary, which introduce changes in the domain. We therefore use the norm

$$||\mathcal{G}||_{\Gamma^d} := \sqrt{\int_{\Gamma^d} (\mathcal{G} \cdot \boldsymbol{n})^2 \mathrm{d}s} \tag{5.3}$$

instead of (3.1) or any other norm defined on Ω and perform the gradient descent method outlined in Algorithm 5.1. In order to find a step size that yields a decrease in the cost function, we perform a backtracking approach via the Armijo rule, where the initial step size t_k of iteration k is computed based on the first-order change of J at each iteration [36]. Explicitly, we set

$$t_k := \max\left\{ \min\left\{ t_{k-1}\left(\frac{||\mathcal{G}_{k-1}||_{\Gamma^d}}{||\mathcal{G}_k||_{\Gamma^d}}\right)^2, 10\, t_1\right\}, 0.1\, t_1\right\} \quad \text{for } k = 2, 3, \dots, \tag{5.4}$$

which also prevents too large deviations from the initial step size of the first iteration.

Remeshing is generally believed to be unavoidable in the context of shape optimization [23]. If mesh elements would overlap during the deformation process in Algorithm 5.1, we create a new mesh on the last valid geometry with comparable overall element size and halve the initial step size. The approach of *restricted mesh deformations* described in the recent paper [10] might yield more robust mesh deformations and thereby eliminate the necessity to remesh during the shape deformation process. Another approach to obtain mesh deformations preserving the mesh quality is based on conformal mappings [15]. The author's approach up to now has been limited to the two-dimensional setting, but it might be transferable to the three-dimensional case.

Algorithm 5.1 terminates if the computed descent direction does not yield a decrease in the cost function. In order to ensure that this only happens close to a stationary point, we track the gradient norms during the iterations given by (5.3) together with the decrease in the cost function. However, we do not use the norms for a termination criterion, since we have no a priori knowledge on their rate of convergence.

Remark 5.1. We note that there exist more sophisticated second-order methods for shape optimization [29, 30], which require the approximation of the shape Hessian of J. This is a nontrivial analytical and numerical task in its own right and since the gradient descent method in conjunction with the step size rule (5.4) yielded satisfactory results for our application, we did not further pursue it.

Algorithm 5.1 Gradient descent method.

```
Set Ω ← Ω_0
Set converged ← false
repeat
    Compute state and adjoint variables from (2.5) and (4.4).
    Compute shape gradient from (5.1) and (5.2).
    if Step size t yields decrease in the cost function then
        Ω ← T_{tV}(Ω)
    else
        converged ← true
    end if
until converged
```

5.2. Discretization. We implemented Algorithm 5.1 in MATLAB, which is linked with COMSOL Multiphysics used for mesh creation as well as the assembly and solving of the discretized state equations via the API LiveLink.

The weak forward and adjoint Stokes equation are discretized with the well-known Taylor–Hood element and for the forward and adjoint transport equations we use linear Lagrange elements applying both streamline- and crosswind-stabilization; see

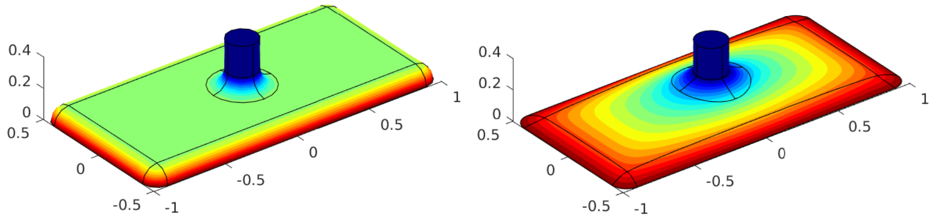


FIG. 3. *Height profiles of the initial and optimized geometry for $\overline{\tau} = 15$.*

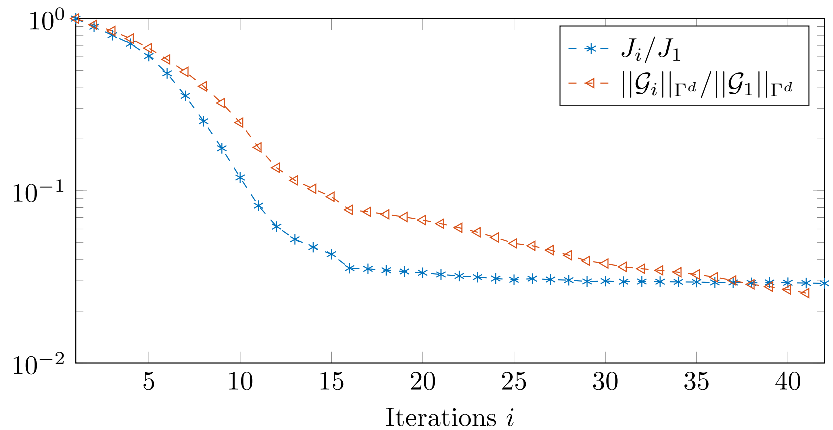


FIG. 4. *Relative objective function values and gradient norms.*

[4, 6]. The resulting linear systems are solved with preconditioned GMRES methods, where in the case of the forward and adjoint Stokes system we use a Vanka-type preconditioner, which can be considered as a block Gauss–Seidel method [16, 34], and for the forward and adjoint transport equation we apply an ILU method [26]. The linear systems arising from the discretization of (5.1) and (5.2) with quadratic Lagrange elements are positive-definite; thus we apply the CG method here.

5.3. Numerical experiments. In this section we apply Algorithm 5.1 to the initial design from Figure 2 using the parameters $Re = 7.1 \cdot 10^{-2}$ and $\eta_{out} = 3.5 \cdot 10^7$, which are given from the industrial context, as well as $Pe = 10^{-5}$, $\gamma = 2$, $\alpha_1 = 2 \cdot 10^{-2}$, and $\alpha_2 = 2$. The initial and optimized cavities for $\overline{\tau} = 15$ are shown in Figure 3, where an initial mesh consisting of 79265 tetrahedrons is used. During the iterations the deformable boundary Γ^d is smoothly flattened in the vicinity of the corners of the cavity and lifted close to the inflow tube.

Figure 4 shows the decrease in the cost function and the relative gradient norms given by (5.3) during the iterations. The cost function drops monotonously except for slight increases as in the 26th iteration due to the remeshing procedure described in subsection 5.1. After 25 iterations almost no more decrease in the objective is obtained and the algorithm terminates after 42 iterations with a relative gradient norm below 3% of the norm on Ω_0. This, in conjunction with the cost function barely changing after iteration 25, indicates that a stationary point has been attained.

We now investigate the influence of the acceptable material age $\overline{\tau}$ on the optimized shapes and the pressure energy drop (2.10) by varying the maximally acceptable

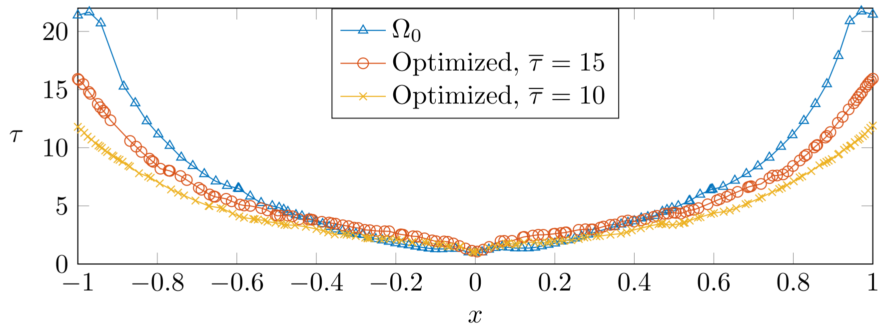
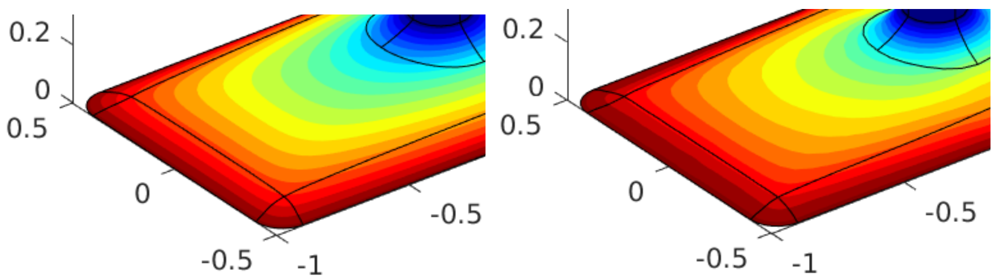


FIG. 5. *Residence times along the longitudinal symmetry axis of* Γ^{out}.



(a)

(b)

FIG. 6. *Height profiles of the optimized geometries.* (a) $\overline{\tau} = 15$ *(volume of* Ω_0 *reduced by* 26.0%*).* (b) $\overline{\tau} = 10$ *(volume of* Ω_0 *reduced by* 40.2%*).*

residence time $\overline{\tau}$ while keeping all other constants unchanged. The material ages τ along the longitudinal axis of Γ^{out} for the initial and the two optimized geometries are depicted in Figure 5, where the relatively large values of τ at the outermost parts result from relatively small flow velocities in the vicinity of Γ^w. Since the cost function incorporates the Moreau regularization of the state constraint (2.9), the residence time in this region does not exactly fall below $\overline{\tau}$ for both cases.

As expected, a lower acceptable residence time leads to a flatter optimal design with a smaller volume, which can be seen from Figure 6 comparing the height profiles of the optimized geometries for $\overline{\tau} = 15$ and $\overline{\tau} = 10$. While for $\overline{\tau} = 15$ the pressure energy drop from (2.10) is only 1.03% higher than for the initial design, it is increased by 38.51% for the optimized geometry using $\overline{\tau} = 10$. This may seem like a large increase in the energy required to transport the fluid through the cavity; however, in an industrial spin pack typically 70% to 90% of the total pressure drop occurs in the fine capillaries where the fibers are spun and most of the remaining pressure drop occurs in filter screens [21]. The distributor considered here is responsible for most of the residence time but only for a very small fraction of the overall pressure drop. Therefore, even an increase in pressure by about 40% within the cavity has only a minor effect on the pressure of the whole system.

6. Conclusion. In this work we considered the optimal shape design of a polymer distributor for the industrial fiber spinning process, where we are interested in avoiding material degradation due to long residence times within the geometry. In contrast to previous work in this area optimizing the wall shear stress of the fluid and thereby indirectly controlling the residence time, we chose to model the residence time with an advection-diffusion-reaction equation. In addition to a regularized state constraint for the material age at the outflow we incorporated the weak form of the pressure energy drop into the objective, such that unreasonably narrow geometries, which reduce the time required for the transport process by excessively accelerating the fluid, are penalized.

We derived the volume formulation of the shape derivative of the cost function using a shape-Lagrangian approach and thereby avoid the material derivatives of the state variables. The resulting expression is generally applicable for gradient-based optimal shape design of pipes transporting viscous Newtonian fluids that can be described with the incompressible Stokes equations together with the Darcy boundary condition of a porous medium at the outlet. In order to compute a smooth deformation of the volume mesh that satisfies the geometric constraint of keeping the inlet and outlet as well as the inflow pipe of the distributor fixed, the shape derivative is projected based on the equations of linear elasticity.

Our numerical experiments show that the maximal material age of the fluid at the outflow boundary can be controlled by changing the shape of the distributor. The more stringent the maximally acceptable residence time at the outflow is chosen, the flatter the optimized geometry becomes, leading to a relatively high increase of pressure drop within the distributor cavity. However, since the distributor only accounts for a small percentage of the total pressure drop within the system, this is acceptable for the industrial application.

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