Topology optimization of turbulent rotating flows using Spalart–Allmaras model

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Abstract

The design of rotating fluid devices, such as flow machines, mixers, and separators, with a focus on performance improvement is of high interest. They usually operate under high Reynolds numbers featuring turbulent flows. In this research, the topology optimization model of turbulent flows is expanded by adapting the Spalart–Allmaras (SA) model with the Rotation/Curvature Correction to consider a density-based material model. This correction improves the turbulence evaluation when rotating frames are considered. The SA model considers the distance to the nearest wall to calculate the turbulent viscosity. However, in the TO, it uses the distance to the nearest solid element, which is calculated by using a novel Eikonal equation with a penalization model. The algorithm is implemented by using a finite element model to solve the state equations. The pyadjoint libraries are used to perform the automatic sensitivity derivation. The objective function considered minimizes energy dissipation. The algorithm is evaluated by performing the optimization of rotating flows with high Reynolds numbers. Several optimized topologies for different domains and angular velocities are shown.

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1. Introduction

A large number of fluid flow problems encountered in daily life are turbulent. Typical examples are flows around cars, airplanes, and buildings, where wakes formed by the flow around those bodies are turbulent. Thus, understanding and choosing the suitable turbulence model are essential matters for the CFD code to represent the real problem. Different turbulence models were developed to address the solution of these flows and the choice of the turbulence model can have a significant influence on the simulation accuracy [1]. This choice becomes especially important when an optimization problem is considered, given that the algorithms are guided by the problem modeling.

In the topology optimization method, the material is distributed (fluid or solid) over a domain, aiming to maximize (or minimize) an objective function under defined constraints. This method was first introduced to fluid domains

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by Borrvall and Petersson [2], in which they apply the technique to 2D flow channel problems, in order to minimize the energy dissipation over the domain. Gersborg-Hansen [3], Gersborg-Hansen et al. [4] and Olesen et al. [5] extended this approach by using Navier–Stokes equations for an extended Reynolds number range and considering additional effects, such as body force and non-linearities. Evgrafov [6] reassesses the work of Borrvall and Petersson [2] and compares the Brinkman model used with a different approach by considering the fluid viscosity as a problem variable. Evgrafov also studied the application of topology optimization to slightly compressible fluid [7].

In the work of Deng et al. [8], the topology optimization method is applied to the flow channel problem, aiming to minimize the pressure loss, considering Navier–Stokes formulation and the presence of body forces. The system problem is solved with the adjoint method, and the solver is implemented by using the commercial software COMSOL Multiphysics. Another work aiming at the optimization of flow channels is Sá et al. [9], in which they use a topological derivative method to obtain the topology of fluid flow channels.

The topology optimization method applied to flow machines has been studied in the work Romero and Silva [10], in which the fluid flow in the device is modeled as Navier–Stokes flow with the addition of a rotating reference system, giving rise to the effects of Centrifugal force and Coriolis force. In a similar work, Sá et al. [11] performed the rotor optimization of Newtonian pumps by using an optimization based on the topological derivative concept. In these works, various configurations are proposed for the machine rotor, exploring the influence of the initial domain and the effects of changes in the boundary conditions. As a result, non-intuitive geometries found in the literature are obtained. The design of flow machine impellers is also studied for flow with axial symmetry by considering 2D-swirl flows [12], such as in the design of Tesla pumps [13].

The more recent topics on topology optimization for fluid flows involve expanding the formulation to consider turbulence models. The work of Papoutsis-Kiachagias and Giannakoglou [14] is one of the first works to consider turbulence in topology optimization, they performed both the shape and topology optimization of gliders and other industrial applications by using the continuous adjoint approach. The work of Yoon [15] presents the optimization of flows inside channels for different Reynolds numbers by using the Spalart–Allmaras model. Other recent works also show the inclusion of the $k − \omega$ model in topology optimization [16,17]. The work [18] introduces the topology optimization considering the $k − \epsilon$ model, however, it still presents limitations when implementing the law of the wall.

In this work, a topology optimization model of the Spalart–Allmaras turbulence model is used [19], coupled with strategies to increase its accuracy [20] and to adjust the rotational frame [21]. The topology optimization model of turbulence flows is expanded by adapting the Spalart–Allmaras model with the Rotation/Curvature Correction to consider a material model. Also, a novel Eikonal equation with a penalization model is used. The optimization problem considers a rotating domain and the energy dissipation functional as objective function. The algorithm is implemented by using the FEniCS software to solve the state equations via the finite element method. The automatic sensitivity derivation is performed by using the pyadjoint libraries and the Interior Point Optimizer (IPOpt) is used to update the design variable. The algorithm is evaluated with respect to the optimization constants, and several examples are analyzed by changing the boundary conditions and domain size.

This paper is organized as follows: In Section 2, the state equations are presented, which involves the Reynolds Averaged Navier–Stokes model in a rotational frame, the modified Spalart–Allmaras model, and the Eikonal equation, which is the equation used to calculate the distance to the walls. Section 3 reveals the material model used and the changes in each state equation to accommodate it. In Section 4, the numerical implementation is presented. In Section 5, the numerical results are shown in three parts. First, the optimization of high Reynolds flows is analyzed with the coupled RANS–SA model for different optimization constants. Then, the algorithm is analyzed for different domain geometries and rotational velocities. Finally, in Section 6, conclusions are derived.

## 2. State equations

In this work, the topology optimization is performed by considering the RANS equations are used coupled with the Spalart–Allmaras turbulence model. Thus, these equations are modified to consider the material model as follows.
2.1. Reynolds averaged Navier–Stokes equations (RANS)

The model used considers the variable fields in a rotational reference frame. Therefore, the velocity is decomposed in two parts:

$$\bar{u}_{abs} = \bar{u} + \omega \times r$$

where \( \bar{u}_{abs} \) is the time-averaged velocity in the stationary (or absolute) frame, \( \bar{u} \) is the time-averaged velocity in the relative frame, \( \omega \) is the relative frame rotation speed, and \( r \) is the distance to the rotation axis.

Following the same approach presented by [15], the time-averaged version of the Navier–Stokes equations in a rotational frame becomes:

$$\rho(\bar{u} \cdot \nabla)\bar{u} = \nabla \cdot T + \rho f - 2\rho \omega \times \bar{u} - \rho \omega \times \omega \times r - \kappa(\omega)\bar{u}$$

where \( \bar{p} \) is the time-averaged pressure, \( T = -\bar{p}I + (\mu + \mu_T)(\nabla \bar{u} + \nabla \bar{u}^T) \). The notation used considers \((\nabla \bar{u})_{ij} = \partial u_j / \partial x_i \). Hence, the FEniCS implementation uses the "nabla_grad" operator and the first term becomes \( \text{dot}(\bar{u}, \text{nabla_grad}(\bar{u})) \) [22].

The continuity equation for the RANS model is given by:

$$\nabla \cdot \bar{u} = 0$$

For simplicity, \( \bar{u} \) and \( \bar{p} \) are substituted by \( u \) and \( p \) from now on.

The RANS equations are solved by using the finite element model with the Galerkin method. The Taylor–Hood elements used, in which the velocity field has a quadratic interpolation and the pressure field has a linear interpolation, as shown in Fig. 1.

2.2. Spalart–Allmaras turbulence model

The Spalart–Allmaras (SA) turbulence model, introduced in [19]. The SA equation does not solve directly for the turbulent viscosity \( \mu_T \), but rather for the modified turbulent viscosity \( \nu_t \) which is used to compute the eddy viscosity. When the relative frame velocity is considered, some modifications to the traditional model become necessary. The terms related to eddy production and destruction are proportional to the absolute velocity. Meanwhile, the convective term, which is responsible for the convection of the turbulence inside the domain, is proportional to the relative velocity frame. Thus, the equation used is:

$$\left( u_{abs} \cdot \nabla \right) \nu_t = P(u) - D(u) + \frac{1}{\sigma_v} \left[ \nabla \cdot ((\nu + \nu_t)\nabla \nu_t) + c_{b2} (\nabla \nu_t)^2 \right],$$

where \( u_{abs} \) is the velocity in the absolute frame (\( u_{abs} = u + \omega \times r \)), and \( u \) is the velocity in the relative frame.

The eddy viscosity \( \nu_t \) is given by [19]:

$$\nu_T = \nu_t f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}}, \quad \chi = \frac{\nu_t}{\nu}$$

where \( \nu \) is the fluid kinematic viscosity.
The production and wall destruction terms are

\[
P = f_{r1} c_{b1} (1 - f_{i2}) \tilde{S} v_l, \quad D = \left( c_{w1} f_w - \frac{c_{b1}}{k^2} f_{i2} \right) \left[ \frac{v_l}{d} \right]^2
\]  

(6)

The function \( f_w \) is given by

\[
f_w = g \left[ 1 + \frac{c_{w3}}{g^6 + c_{w3}} \right]^{\frac{1}{6}},
\]

\[
g = r + c_{w2}(r^6 - r),
\]

\[
r = \min \left( \frac{v_l}{S \kappa d^2}, r_{lim} \right).
\]

Laminar suppression term is given by

\[
 f_{i2} = c_{i3} \exp(-c_{i4} \chi^2)
\]

(8)

Here \( \tilde{S} \) is the modified vorticity, with the modifications to prevent negative values \([23]\):

\[
\tilde{S} = \begin{cases} 
S \tilde{S} & : \tilde{S} \geq -c_{i2} S \\
S + \frac{S(c_{i2}^2 \tilde{S} + c_{i3} \bar{S})}{(c_{i3}^2 - 2c_{i2}^2) - 3} & : \tilde{S} < -c_{i2} S 
\end{cases}
\]

(10)

where \( c_{i2} = 0.7, c_{i3} = 0.9, \) \( d \) is the distance to the closest wall calculated by using the Eikonal equation, and \( S \) is the magnitude of vorticity given by:

\[
S = \sqrt{2} \Omega_u : \Omega_u, \quad \Omega_u = \frac{1}{2} (\nabla u - \nabla u^T)
\]

(11)

The remaining constants are given by

\[
c_{b1} = 0.1355, \quad \sigma_v = 2/3, \quad c_{b2} = 0.622, \quad \kappa = 0.41,
\]

\[
c_{w1} = \frac{c_{b1}}{\kappa^2 + (1 + c_{b2})/\sigma_v}, \quad c_{w2} = 0.3, \quad c_{w3} = 2,
\]

\[
c_{i1} = 7.1, \quad c_{i3} = 1.2, \quad c_{i4} = 0.5, \quad r_{lim} = 10
\]

The last term to be defined is \( f_{r1} \), which is the rotation correction. When rotational domains are considered, it is argued by Spalart and Shur \([20]\) that a correction in the turbulence production term is needed. The work of Tao et al. \([21]\) shows that RANS simulations without corrections present an isotropic model for the turbulence, which is not enough to describe some turbulence effects, such as flow separation. The rotation correction term supplement the model with anisotropy. The \( f_{r1} \) term is an empirical rotation function given by \([20]\):

\[
f_{r1}(r^*, \tilde{\tau}) = \left( 1 + c_{r1} \frac{2r^*}{1 + r^*} (1 - c_{r3} tan^{-1}(c_{r2} \tilde{\tau})) \right) - c_{r1}
\]

(12)

where the constants are \( c_{r1} = 1, c_{r2} = 12, c_{r3} = 1. \) \( \tilde{\tau} \) and \( r^* \) are functions of the strain rate (\( S_{sr} \)) and the vorticity corrected by rotation (\( W_{sr} \)):

\[
S_{RC} = \sqrt{2} S_{sr} : S_{sr}, \quad S_{sr} = \frac{1}{2} (\nabla u + \nabla u^T)
\]

\[
W_{RC} = \sqrt{2} W_{sr} : W_{sr}, \quad W_{sr} = \frac{1}{2} \left[ (\nabla u - \nabla u^T) + 2\omega_{rot} \right]
\]

(14)

where \( \omega_{rot} \) is the resulting tensor, given by:

\[
\omega_{rot} = \omega_{rot}^* = \epsilon_{mji} \omega_{mj}
\]

(15)

Finally, \( \tilde{\tau} \) and \( r^* \) definitions are given by \([24]\):

\[
r^* = \frac{S_{RC}}{W_{RC}}, \quad \tilde{\tau} = \frac{W_{RC}}{S_{RC}} \left( \frac{W_{RC}}{S_{RC}} - 1 \right)
\]

(16)
The SA equation is solved by using the finite element model with the Galerkin method. The eddy viscosity \( (\nu_t) \) has a quadratic interpolation. In topology optimization another modification is necessary, which consists of introducing a penalization term similar to the Brinkman equation to remove the eddy viscosity in solid regions. This modification is presented in Section 3.2.

2.3. Eikonal equation

The Spalart–Allmaras model uses the distance to the nearest wall in the equation. The wall distance can be calculated by iterating the mesh and using search procedures. However, this procedure can become very costly for refined meshes [25]. One way to circumvent this issue uses differential equations to calculate all distances in a single solve. Different equations describe the wall distance and can be seen in Tucker et al. [25]. In this work, a hyperbolic Eikonal equation is used:

\[
|\nabla \phi| = 1 + \mu_{eik} \nabla^2 \phi
\]  

(17)

where \( \phi \) is the distance to the nearest wall and \( \mu_{eik} \) is a pseudo-viscosity to smooth the solution. For this equation to represent the wall distance, it is solved considering \( \phi = 0 \) at the boundaries.

The Eikonal equation is solved by using the finite element model with the Galerkin method. The wall distance \( (\phi) \) is calculated by using quadratic interpolation.

Eq. (17) also needs to be modified to address the material model in the topology optimization, which consists in introducing a penalization term to guide the wall distance to zero at solid regions. This modification is presented in Section 3.3.

3. Topology optimization model

3.1. Material model

The topology optimization method involves distributing material over a specified domain by following certain requisites. Therefore, in order to determine the path to be followed by the fluid and to define a design variable to perform a topology optimization, a porous domain was introduced by Borrvall and Petersson [2], partitioning domain regions between high permeability material, interpreted as pure fluid, and low permeability material, representing solid, i.e., the porosity virtually separates fluid and solid regions [3]. This is done with the introduction of the absorption term \( \kappa \) that controls the material distribution in the domain.

The absorption coefficient \( \kappa \) can be considered as an interpolation of the material flux on the domain, which represents the transition of material between high porosity (solid, \( \kappa \gg 1 \)) and low porosity (fluid, \( \kappa = 0 \)) regions. This coefficient is a function of \( \alpha \), a pseudo-density field which is the optimization problem design variable. The choice of this function \( \alpha \rightarrow \kappa(\alpha) \) allows the design variable to assume intermediate values, between 0 and 1. In order to suppress these undesired values, a convex \( q \)-parameterized interpolation function can be chosen [2]:

\[
\kappa(\alpha) = \kappa_{\text{max}} + (\kappa_{\text{min}} - \kappa_{\text{max}}) \alpha \frac{1 + q}{\alpha + q}
\]  

(18)

with \( \kappa \in [\kappa_{\text{min}}, \kappa_{\text{max}}] \), \( \alpha \) represents points inside the domain and \( q \) is a parameter that controls \( \kappa \) curvature. Thus, for \( q \to \infty, \kappa \to \kappa_{\text{max}} + (\kappa_{\text{min}} - \kappa_{\text{max}}) \alpha \) is a linear function. Fig. 2 illustrates this behavior by considering \( \kappa_{\text{max}} = 10,000 \) and \( \kappa_{\text{min}} = 0 \). The optimization process aims to obtain values of 0 or 1 to the design variable \( \alpha \) (\( \alpha \approx 0 \) or \( \alpha \approx 1 \)), since a intermediate value would not have a physical meaning. Therefore, when \( \alpha \approx 1 \Rightarrow \kappa = \kappa_{\text{min}} \), represents a flow of pure fluid, while when \( \alpha \approx 0 \Rightarrow \kappa = \kappa_{\text{max}} \), represents a restricted flow inside a porous medium.

3.2. Spalart–Allmaras equation with material model

The work of Yoon [15] uses an exponential function in order to account for the material model in the Spalart–Allmaras equations, by adding a penalty term consisting of a high valued constant and the design variable to
the power of another constant ($\alpha^n$). However, in this work, the added term is similar to the friction force on Navier–Stokes eq., i.e., the interpolation function of Eq. (18) is added to Eq. (4). The result is given by:

$$R_{SA} = \int_{\Omega} \left[ (u_{abs} \cdot \nabla)v_t \lambda_{SA} - f_{r1} P(u) + D(u) - \frac{1}{\sigma_v} e_{k2}(\nabla v_t)^2 \right] \lambda_{SA} \, d\Omega$$

$$+ \int_{\Omega} \frac{1}{\sigma_v} (v + v_t) \nabla v_t \cdot \nabla \lambda_{SA} \, d\Omega$$

$$- \int_{\Gamma} \frac{1}{\sigma_v} (v + v_t) \lambda_{SA} \nabla v_t \cdot \mathbf{n} \, d\Gamma$$

$$+ \int_{\Omega} \kappa_{SA}(\alpha) v_t \lambda_{SA} \, d\Omega$$

where $\lambda_{SA}$ is a test function and $\kappa_{SA}(\alpha)$ is a function similar to Eq. (18), however with different constant values.

3.3. Eikonal equation with material model

The Eikonal equation is used to calculate the distance of each point of the domain to the nearest wall. However, in reality, the equation calculates the distance to the nearest node with zero value, hence, defining the boundary condition as zero gives the distance to the boundary. The addition of the material model to the equation can induce new nodes to assume the value zero and, therefore, allowing the Eikonal able to calculate the distance to the nearest solid node.

Hence, the same idea of a material model that changes the calculated value at a point is used for the Eikonal equation (Eq. (17)), by adding the interpolation function multiplied by the wall distance. By multiplying Eq. (17) by a test function and integrating by parts, the resulting weak form is given by:

$$R_{eik} = \int_{\Omega} \sqrt{\nabla \phi \cdot \nabla \phi} \, y_e - f_e \, y_e + \mu_{eik} \nabla \phi \cdot \nabla y_e \, d\Omega$$

$$- \int_{\Gamma} y_e \nabla \phi \cdot \mathbf{n} \, d\Gamma + \int_{\Omega} \kappa_{eik}(\alpha) \phi \, y_e \, d\Omega$$

where $f_e = 1$, $y_e$ is a test function, and $\kappa_{eik}(\alpha)$ is a function similar to Eq. (18), however, with different constant values.

In order to exemplify the effect of the material model, a square domain is chosen with unitary sides (Fig. 3(a)) and with the boundary conditions shown in Fig. 3(b). This example considers an unstructured mesh with 40,000 elements. Two design variable distributions are tested, one entirely filled with fluid (Fig. 3(c)), and other where
Fig. 3. Eikonal behavior with material model.
there are regions with value 1.0, representing fluid (blue), i.e., regions where the distance needs to be calculated, and regions with value 0.0, representing solid (red), where the distance should be set to zero. Also, a region with an intermediary value of 0.5 is defined to highlight the damping that occurs in gray regions. This configuration is shown in Fig. 3(d).

Fig. 3(f) shows the calculated distance for this configuration. It can be noticed that at the left portion (blue) the distance is calculated without the material damp. The case with an entirely fluid domain is shown for reference in Fig. 3(e).

By taking a slice of the domain (cut A from Figs. 3(c) and 3(d)) and analyzing the distance behavior in Fig. 3(g), we can see that for \( x \) between 0.0 and 0.33 (fluid region — blue region) the width is 0.33 and the value of a node at the middle of the blue region (\( x=0.15 \)) is 0.15, as expected. In the gray region, the calculated distance is damped and an intermediary distance value is held (around 0.07). In the solid region the distance is zero. Thus, with the proposed material model, it is possible to emulate a wall and calculate the correct distance by using the design variable.

3.4. Topology optimization problem

The optimization problem in this work has the following formulation:

\[
\text{Minimize : } \Phi_T(\alpha) \\
\alpha \\
\text{subjected to : } \\
R_{RANS} = 0, \\
R_{RANS} = 0, \\
R_{SA} = 0, \\
R_{eik} = 0, \\
\int_{\Omega} \alpha \, d\Omega \leq f |\Omega|, \\
0 \leq \alpha \leq 1
\]

(21)

where \( R_{RANS} \) is the rotational RANS momentum equation weak form (Eq. (2)), \( R_{RANS} \) is the continuity equation weak form, \( R_{SA} \) is the Spalart–Allmaras equation weak form (Eq. (19)), and \( R_{eik} \) is the Eikonal equation weak form (Eq. (20)). A fraction of the domain volume (\( f |\Omega| \)) is defined as an upper bound to create regions of fluid and leaving the remainder to be occupied by solid.

The objective function is the minimization of energy dissipation. The energy dissipation represents the loss in fluid potential power [2]. Yoon [15] proposed a form for the energy dissipation that considers the effect of material model and the turbulence viscosity, given by:

\[
\Phi_T(\alpha) = \int_{\Omega} \frac{1}{2} (\mu + \mu_T)(\nabla u + \nabla u^T) : (\nabla u + \nabla u^T) + \kappa(\alpha)u \cdot u \, d\Omega,
\]

(22)

where \( \mu \) is the fluid molecular viscosity, and \( \mu_T \) is the turbulent viscosity given by Eq. (5).

The energy dissipation functional can be divided into two parts, defined here as Viscous Dissipation and Friction Dissipation. The viscous dissipation is given by:

\[
\Phi_{visc} = \int_{\Omega} \left[ \frac{1}{2} (\mu + \mu_T)(\nabla u + \nabla u^T) : (\nabla u + \nabla u^T) \right] d\Omega
\]

(23)

and the second part (Friction Dissipation) is given by:

\[
\Phi_{fric} = \int_{\Omega} \kappa(\alpha)u \cdot u \, d\Omega
\]

(24)

4. Numerical implementation

4.1. Optimization algorithm

The topology optimization procedure consists mainly of FE model solution, gradient evaluation, and optimization algorithm. The process is iterative and consists of the following steps, which are also presented in Fig. 4:

(a) Define an Initial Distribution for the design variable (\( \alpha \));
Fig. 4. Topology optimization implementation flow chart.

(b) Solve Eikonal equation with given initial value for design variables;
(c) Solve the coupled RANS–SA equations with given initial value for design variables;
(d) Solve adjoint equations based on velocity, pressure, wall distance and eddy viscosity fields of (b) and (c);
(e) Calculate the sensitivities of objective functions and constraints;
(f) Update the design variable value with an optimization algorithm under bounded constraints (0 ≤ α ≤ 1);
(g) Verify the stop criterion.

The sensitivity verification via finite differences is displayed in the Appendix. The stop criterion is defined as a norm between two consecutive iterations:

\[ \| \alpha^k - \alpha^{k-1} \|_\infty \ll 1 \times 10^{-3} \]  

where \( \alpha \) is the design variable distribution and \( k \) is the iteration number.

4.2. FEniCS environment

In this work, the FEniCS environment [26] is used to solve the equations presented in the previous sections. The resulting FEM system is solved with the Multifrontal Massively Parallel Sparse direct Solver (MUMPS) [27]. The optimization is solved by initially by calculating the sensitivities, which is obtained by using the adjoint method implemented by the software pyadjoint [28]. This software performs the automatic sensitivity derivation from the equations implemented in the FEniCS language. Then, an optimizer is employed to update the design variable. In this work, the IPOpt optimizer [29,30] is used, which is an Interior Point Optimization algorithm.

The flow chart of the optimization procedure is represented in Fig. 4. The sequence of steps to solve the optimization involves firstly defining an initial material distribution and the boundary conditions, then the FEniCS routines are called to solve the FEM system returning the solution vector \([u_1 \ u_2 \ p \ v]\). With this, the functional is evaluated and the pyadjoint is called to perform the adjoint problem derivation. Next, this information is passed to the optimizer IPOpt, which computes the following material distribution over the domain. The process is repeated until the functional value converges, in which case the optimized solution is reached. Fig. 4 shows the steps described above.
5. Results

In order to exemplify the methodology, an impeller-like case is designed. First, the effect of changing the material model constants in the final design is analyzed. Then, the algorithm is evaluated against different boundary conditions, such as different rotational velocities and domain sizes. The boundary conditions for the following examples presented are shown in Fig. 5. The geometry sizes are displayed in Table 1. The boundary conditions vary with each example and are shown in the respective sections. The mesh used in all examples is unstructured with around 140,000 triangular elements.

5.1. Material model analysis

In this section, the RANS–SA model and the high Reynolds setup are used. Three cases are studied to verify the algorithm’s behavior by changing the values of $k_{\text{max}}$ and $q$. Usually, a high value of $k_{\text{max}}$ is needed at the end of the optimization algorithm so the fluid does not enter the solid domain. However, it is presented in the literature that starting the algorithm with a lower penalization value can lead to different local minima [2]. The boundary conditions for this section are shown in Table 2, and represent a Reynolds number around 100,000.

Table 3 presents the tested setups. The algorithm starts with $q = q_{\text{init}}$ and holds this value for 100 iterations, then the value is updated to $q = q_{\text{final}}$ for another 200 iterations. The optimized topologies and the variable fields are shown in Fig. 6. In order to present a fair comparison among the cases, the fields shown in this figure are obtained by using the highest penalization values, i.e., $k_{\text{max}} = 1 \cdot 10^4$ and $q = 0.5$.

The optimized topologies are dependent on the optimization constants values. The case with the lowest $k_{\text{max}}$ (Case 1 — Fig. 6(a)) presents a curved topology with an intermediary porosity region near the inlet. This gray area reduces the diffusion of the high eddy viscosity and locally reduces the energy dissipation value. As the value of $k_{\text{max}}$ increases, the topology tends to split in smaller channels. The velocity fields (Figs. 6(d)–6(f)) show that the

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**Table 1**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
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</tr>
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<td>$r_{\text{out}}$</td>
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</tr>
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Table 2
Boundary conditions for the \( \kappa_{\text{max}} \) and \( q \) analysis.

<table>
<thead>
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<th>Condition</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
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<td>u_{\text{in}}</td>
<td>)</td>
</tr>
<tr>
<td></td>
<td>(</td>
<td>v_{\text{in}}</td>
<td>)</td>
</tr>
<tr>
<td></td>
<td>( \omega_z )</td>
<td>10,000</td>
<td>rpm</td>
</tr>
<tr>
<td><strong>Outlet</strong></td>
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<td>( \nabla v_l \cdot n )</td>
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</tr>
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<td><strong>Walls</strong></td>
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</tr>
<tr>
<td></td>
<td>( v_l )</td>
<td>0</td>
<td>Poise</td>
</tr>
</tbody>
</table>

Table 3
Test cases and material model parameters for \( \kappa_{\text{max}} \) and \( q \) analysis.

<table>
<thead>
<tr>
<th>Cases</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial guess</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>Volume fraction ( (f) )</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>( \kappa_{\text{max}} )</td>
<td>1,000</td>
<td>10,000</td>
<td>10,000</td>
</tr>
<tr>
<td>( \kappa_{\text{min}} )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( q_{\text{init}} )</td>
<td>0.1</td>
<td>0.01</td>
<td>0.1</td>
</tr>
<tr>
<td>( q_{\text{final}} )</td>
<td>0.5</td>
<td>0.1</td>
<td>0.5</td>
</tr>
<tr>
<td>( \kappa_{\text{SA max}} )</td>
<td>10,000</td>
<td>10,000</td>
<td>10,000</td>
</tr>
<tr>
<td>( \kappa_{\text{SA min}} )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( q_{\text{SA}} )</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>( \kappa_{\text{eik max}} )</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>( \kappa_{\text{eik min}} )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( q_{\text{eik}} )</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

peak velocity is higher in Case 1 (256 [cm/s]), while the peaks in cases 2 and 3 have values close to 160 [cm/s]. This indicates that the velocity gradient in the second and third cases should also be lower than in the first case.

The pressure fields (Figs. 6(g)–6(i)) are very similar among the cases. The eddy viscosity fields (Figs. 6(m)–6(o)) show that most of the turbulence is diffused in the domain by the inlet. This indicates that the imposed turbulence condition at the inlet can be overestimated. Moreover, it is expected that the topologies would not present high turbulence viscosity values due to the eddy viscosity being present in the objective function. By observing the wall distance distributions (Figs. 6(j)–6(l)), it is possible to notice that Cases 2 and 3 topologies have channel widths smaller than the inlet, which contributes to the increase of the turbulence destruction term, and consequently to the reduction of the eddy viscosity value.

The energy dissipation function (Eq. (22)), plotted point-wise with log-scale in Figs. 6(p), 6(q), and 6(r), shows that the overall distribution in Case 3 has lower values than the other cases, i.e., there are broader regions with values below 10,000. Besides, the function value is not zero near the frontier of the solid region. This occurs due to the penalization method, which imposes the zero velocity in the solid region in a weak manner, so small velocity values may appear and so velocity gradients.

The functional values, shown in Table 4, are calculated by using the highest penalization values, i.e., \( \kappa_{\text{max}} = 1 \cdot 10^4 \) and \( q = 0.5 \). The values corroborate with the lower energy dissipation presented in the plots. The energy dissipation values are split in viscous dissipation and friction dissipation, given that the real objective is to reduce the viscous dissipation and the friction portion of the functional acts as a regularization. Case 3 displays an integrated viscous dissipation around 46% lower than Case 1 and 19% lower than Case 2. This can be explained by the channels with lower velocities, which makes difficult the diffusion, and by smaller widths, which decreases the production, and increases the destruction of the eddy viscosity due to the smaller distance to walls.
Table 4
Objective function values for optimized topologies obtained with the RANS–SA model.

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area (cm²)</td>
<td>0.33</td>
<td>0.21</td>
<td>0.33</td>
</tr>
<tr>
<td>Mass flow</td>
<td>34.62</td>
<td>33.62</td>
<td>34.62</td>
</tr>
<tr>
<td>Inlet pressure (-10⁵)</td>
<td>−4.04</td>
<td>−4.22</td>
<td>−4.26</td>
</tr>
<tr>
<td>Energy dissipation (-10⁵)</td>
<td>6.48</td>
<td>6.70</td>
<td>6.34</td>
</tr>
<tr>
<td>Viscous dissipation (-10⁵)</td>
<td>1.04</td>
<td>0.69</td>
<td>0.56</td>
</tr>
<tr>
<td>Friction dissipation (-10⁵)</td>
<td>5.44</td>
<td>6.01</td>
<td>5.78</td>
</tr>
</tbody>
</table>

*The values are calculated with \(\kappa_{\text{max}} = 1 \cdot 10^4\) and \(q = 0.5\).

Table 5
Objective function values for post-processed topologies.

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area (cm²)</td>
<td>0.32</td>
<td>0.20</td>
<td>0.27</td>
</tr>
<tr>
<td>Mass flow</td>
<td>33.88</td>
<td>33.88</td>
<td>33.88</td>
</tr>
<tr>
<td>Inlet pressure (-10⁵)</td>
<td>−3.64</td>
<td>−3.88</td>
<td>−4.22</td>
</tr>
<tr>
<td>Energy dissipation (-10⁵)</td>
<td>1.98</td>
<td>1.89</td>
<td>1.04</td>
</tr>
<tr>
<td>Viscous dissipation (-10⁵)</td>
<td>1.98</td>
<td>1.89</td>
<td>1.04</td>
</tr>
<tr>
<td>Friction dissipation (-10⁵)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

Focusing on evaluating the topologies in a more realistic approach, the results need to be analyzed without the influence of the material model, given that intermediary material values cannot be easily built with the current technology. Thus, the topologies are isolated by removing the solid region and post-processed by smoothing the contour. The results are shown in Fig. 8. The velocity fields for all cases show a big change in the peak values when compared to the cases with the material model (Fig. 6). This occurs due to the absence of gray regions, which prevents the flow deceleration caused by intermediary values in the material model. The energy dissipation peak values also increase, given that the gradient at the walls is not softened by the material model. Also, the highest values occur in the same regions. For the second and third cases, the viscous dissipation peak occurs at the edge where the channel splits, which is expected, given that it acts as an obstacle that changes the flow direction abruptly.

The convergence curve for the optimization problem (objective function by iteration) is shown in Fig. 7. It can be observed that when the value of \(q\) is increased the objective function increases as well, forming a new peak (iteration 100). This is expected given that a higher \(q\) returns a higher \(\kappa(\alpha)\) for intermediary design variable values. Also, notice that the overall lower value for Case 1 in this plot is due to the lower \(\kappa_{\text{max}}\) used during the optimization.

Table 5 shows the functional values for the post-processed topologies. In this table, the friction dissipation values are zero since there is no material model. The viscous dissipation values are around 70% higher in the post-processed topologies than in the case with the material model due to the infiltration present when the material is used. However, the relation between the cases and conclusions are maintained. Case 3 still presents the best viscous dissipation value among the tested cases, and is approximately 45% lower than the others.

5.1.1. Cross check with NS model

This section shows a comparison of the previous results with topologies obtained by considering only the Navier–Stokes (NS) equations (without the turbulence model). The cross-check analysis is shown to verify if it is worth to perform the optimization considering the complete RANS–SA model. If the optimization performed by using only the NS model could achieve a topology with performance similar to the results obtained with the RANS–SA when both are analyzed with the RANS–SA equations, the extra computational cost would not be necessary during the optimization. Given that the optimization with NS requires fewer variables and so, less computation time.

The same three cases shown before are evaluated (Table 3). The optimization starts with a homogeneous field initial guess of 0.25. The optimized topologies are post-processed, evaluated with both models (RANS–SA and NS), and the comparison among the contour of the topologies is shown in Fig. 9.
Fig. 6. Optimized topologies for high Reynolds RANS–SA model with different optimization constants: Case 1 (first column), Case 2 (second column), Case 3 (third column).
The functional values are shown in Table 6. It can be noticed that this problem has multiple local minima, which can be achieved by changing the optimization constant’s value. The final topologies of cases 1 and 2 obtained with the RANS–SA model perform better in both evaluations than the topologies obtained with NS. However, the case 3 setup still presents lower functional values than the other cases. Furthermore, the behavior of case 3 is more intuitive, given that the best performance occurs when the same model is used for both the design and evaluation, i.e., the NS design shows an energy dissipation value around 12% lower when evaluated with the NS equations, while the RANS–SA design has a value around 16% better when evaluated with the RANS–SA model. Thus, the extra computational time required by the complete model (RANS–SA) is justified.

5.2. $\beta_{geo}$ analysis

This section presents a brief analysis of the algorithm behavior under changes in the $\beta_{geo}$ value. The setup used is the same as previously presented for Case 3 (Table 3). Fig. 10 displays the viscous dissipation value and topologies for different geometry angles. It can be observed that the optimized topologies for angles lower than 140° have the tendency to form only one channel and to keep the outlet at the left bound of the domain. As the domain angle goes beyond 180° the algorithm finds a local minimum and the solution stays around the split channel topology. Thus, the 180° domain has the best ratio between functional value and domain size.

5.3. Rotational speed analysis

Here, an analysis of the algorithm behavior under changes in the rotational speed value is shown. The setup used is the same as previously presented for Case 3 (Table 3). Fig. 11 shows the viscous dissipation value and
Fig. 8. Post-processed topologies for high Reynolds RANS–SA model with different optimization constants: Case 1 (first column), Case 2 (second column), Case 3 (third column).
topologies for different rotations. The viscous dissipation value increases almost linearly with the increase in the rotational speed. The optimized topology obtained at 5,000 [rpm] starts the transition from the single-channel to the split channel. Thus, the algorithm chooses to split the flow in smaller channels as the rotation increases.

6. Conclusion

The concept of topology optimization is applied to design optimized topologies of turbulent flow in rotational domains with the improved Spalart–Allmaras model with rotation correction. First, the methodology is evaluated on the design of high Reynolds flows for different optimization constants. Then, several cases are analyzed by changing the domain geometry and the rotational speed.

The study of the effect of the optimization constants in the algorithm shows that the topology is highly influenced by the choice of the constants. The best functional values are achieved with the third case setup, which presents high values for $\kappa_{max}$ and $q$. The Case 3 setup shows objective function values around 31% lower than the remaining setups.

The effect of post-processing the results by removing the effect of the material model is analyzed. The functional values increase in the post-processed topologies, given that the gray areas on the topology contour are removed and
no infiltration is present. These gray areas usually smooth the velocity increase near the wall, and consequently, reduce the velocity gradients.

The study on the domain angle shows that the algorithm achieves the best local minimum for the 180° geometry. Also, the algorithm holds this minimum even for higher angular values. This domain is analyzed for different rotational velocities, and it shows that the viscous dissipation value increases almost linearly with the increase in the angular velocity for the respective optimized topology.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix. Sensitivity verification via finite differences

This section shows the finite difference verification of the automatic differentiated sensitivities calculated with the pyadjoint library. The central finite difference is used, which is given by:

$$\frac{\partial J}{\partial \alpha} = \frac{J(\alpha + h) - J(\alpha - h)}{2h}$$

where the perturbation used is $h = 1 \cdot 10^{-6}$.

This verification considers the domain shown in Fig. 5 with $\beta_{geo} = 180^\circ$ and a uniform design variable distribution of $\alpha = 0.5$. The chosen trial points are presented in Fig. A.12. Table A.7 shows the sensitivity comparison between the value calculated with pyadjoint and the value obtained with finite differences. It can be observed that the sensitivities are in good agreement, and the highest discrepancy occurs for the small values, such as for trial point 6 which presents a difference of 0.74%.
Table A.7
Sensitivity verification for FD and adjoint approaches.

<table>
<thead>
<tr>
<th>Trial point</th>
<th>X</th>
<th>Y</th>
<th>Central diff</th>
<th>Adjoint</th>
<th>Difference %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.60</td>
<td>0.00</td>
<td>−1.421</td>
<td>−1.416</td>
<td>−0.41</td>
</tr>
<tr>
<td>2</td>
<td>0.52</td>
<td>0.30</td>
<td>−177.679</td>
<td>−177.681</td>
<td>0.00</td>
</tr>
<tr>
<td>3</td>
<td>0.30</td>
<td>0.52</td>
<td>−382.298</td>
<td>−382.299</td>
<td>0.00</td>
</tr>
<tr>
<td>4</td>
<td>0.00</td>
<td>0.60</td>
<td>−249.450</td>
<td>−249.451</td>
<td>0.00</td>
</tr>
<tr>
<td>5</td>
<td>−0.30</td>
<td>0.52</td>
<td>−39.435</td>
<td>−39.434</td>
<td>0.00</td>
</tr>
<tr>
<td>6</td>
<td>−0.52</td>
<td>0.30</td>
<td>−11.400</td>
<td>−11.397</td>
<td>−0.03</td>
</tr>
<tr>
<td>7</td>
<td>−0.60</td>
<td>0.00</td>
<td>−0.225</td>
<td>−0.227</td>
<td>0.74</td>
</tr>
<tr>
<td>8</td>
<td>0.90</td>
<td>0.00</td>
<td>−0.767</td>
<td>−0.767</td>
<td>0.00</td>
</tr>
<tr>
<td>9</td>
<td>0.78</td>
<td>0.45</td>
<td>−20.859</td>
<td>−20.855</td>
<td>−0.02</td>
</tr>
<tr>
<td>10</td>
<td>0.45</td>
<td>0.78</td>
<td>−22.778</td>
<td>−22.769</td>
<td>−0.04</td>
</tr>
<tr>
<td>11</td>
<td>0.00</td>
<td>0.90</td>
<td>−19.386</td>
<td>−19.391</td>
<td>0.03</td>
</tr>
<tr>
<td>12</td>
<td>−0.45</td>
<td>0.78</td>
<td>−6.103</td>
<td>−6.105</td>
<td>0.02</td>
</tr>
<tr>
<td>13</td>
<td>−0.78</td>
<td>0.45</td>
<td>−4.200</td>
<td>−4.199</td>
<td>−0.02</td>
</tr>
<tr>
<td>14</td>
<td>−0.90</td>
<td>0.00</td>
<td>−1.882</td>
<td>−1.883</td>
<td>0.04</td>
</tr>
</tbody>
</table>

References


