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Multi-physics Topology Optimization with Application to Molten Salt Fast Reactor

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ABSTRACT

In the last decades, topology optimisation is playing an increasingly important role in the industrial design approach for different applications, including structural mechanics, civil engineering, architecture and fluid mechanics. This work aims at improving the studies regarding multiphysics topology optimisation of systems governed by fluid flow and heat transfer, including an application to the Molten Salt Fast Reactor (MSFR), investigating two different approaches. At first, this work assesses the well-established gradient-based algorithms using 2D benchmarks using COMSOL Multi-physics. These results represent the starting point for developing an adjoint-based open-source optimisation solver in OpenFOAM for non-adiabatic flows. This method, defined by a Lagrangian formalism of the sensitivity analysis, led to promising results, with lower computational cost but higher residuals, which underlined the need for further tests. Finally, this work considers the topology optimisation of the EVOL geometry of the MSFR, aimed at minimising the temperature gradient and pressure drops inside the reactor. The results showed impressive improvements regarding the system operative conditions.

1 INTRODUCTION

Design optimisation is an old field of research that was subjected to deep mathematical theories and inspired numerous industrial and engineering applications [1, 2, 3]. In the last decades, the rise of computational power led to the development of several advanced programming methods to achieve the optimum shape of engineering structures in numerous scientific fields under different constraints such as stress, displacement and kinematic stability. The generic optimisation problem is characterised by a function $J(\mathbf{x}) : \Omega \to \mathbb{R}^n$ called objective function [4]. The vector of state variables $\mathbf{x}$ represents the degrees of freedom of the problem, and Ω is the feasible space defined by the constraints, equalities or inequalities, that $\mathbf{x}$ must satisfy. The problem is aimed at determining $\mathbf{x}_0 \in \Omega$ such that $J(\mathbf{x}_0) < J(\mathbf{x})\, \forall \mathbf{x} \in \Omega$.

The present work focuses on the topology approach to optimisation. This method relies on discretising the overall domain through a control variable γ associated with a fictitious material.

By interpolating the control variable between 0 and 1, it is possible to solve the primary equation in the case of γ = 1 and the equation associated with the fictitious material in the case of γ = 0. The final fictitious material field defines the optimum topology of the problem, leading to the minimisation of the cost function. Considering the Finite Element discretization, the topology optimisation problem is defined as:

$$\begin{cases} \min\limits_{\gamma} : J = J(\mathbf{u}(\gamma), \gamma) = \sum\limits_{i} \int_{\Omega_i} f(\mathbf{u}(\gamma_i), \gamma_i) dV, \\ \text{subject to} : G_0(\gamma) = \sum\limits_{i} u_i \cdot \gamma_i - V_0 \leq 0, \\ \qquad\qquad : G_i(\mathbf{u}(\gamma), \gamma) \leq 0, j = 1, ..., M, \\ \qquad\qquad : \gamma_{\min} \leq \gamma_i \leq 1, i = 1, ..., N, \end{cases} \tag{1}$$

which reads: determine the material distribution which minimises the cost function J subjected to the volume constrain $G_0(\gamma)$ and to the M other possible constraints, where $\mathbf{u}$ is the state variable vector satisfying the primary equations. In the present work, the topology optimisation of a multiphysics system follows two different approaches. First, this work considers the gradient-based optimisation algorithms using COMSOL Multi-physics, using 2D benchmarks of problems already discussed in literature [5] to achieve a complete knowledge of the optimisation approach. The results obtained represent the starting point for developing an open-source optimisation solver in OpenFOAM based on the adjoint approach for fluid flow and heat transfer systems. Finally, the topology optimisation approach is applied to the EVOL geometry of the Molten Salt Fast Reactor to minimise the temperature gradient identifying the best reactor core shape. For brevity, this work only shows preliminary results, extended in [6].

2 OPTIMISATION THEORY

Three 2D benchmarks are considered for the topology optimisation with both the gradient-based and the adjoint method. First, a pure heat conduction problem is studied aiming at the definition of the optimal conduction path to remove heat inside the domain. A 2D square with 100 mm edges is subjected to uniform heat generation of 3 W/m^3 in a pure heat conduction domain. The temperature in the central portion of the left edge is set equal to 293 K and represented the heat sink while adiabatic boundary conditions are imposed on the other edges. The second test instead deals with a pure fluid flow optimisation problem with the purpose of pressure loss reduction in a piping system: the inlet velocity of 0.0266 m/s and zero pressure boundary condition at the outlet are imposed. Then, a Multi-physics and multi-objective problem is considered [7]. In this last case, a cooling system governed by fluid flow and heat transfer is subjected to optimisation of both pressure losses and temperature gradient: a central square domain is subjected to uniform heat generation of 100 W/m^3 and connected to the inlet on the left side with a fixed temperature of 293 K.

2.1 Gradient Based Topology Optimisation - COMSOL

The first benchmark, dealing with steady state pure heat conduction optimisation, is governed by the Fourier's law:

$$-\nabla(k(\gamma)\nabla T) = Q. \tag{2}$$

In this case, each element was associated to a value of the design variable γ that was related to the thermal conductivity through the SIMP interpolation scheme:

$$\gamma_p = \gamma_{min} + (1 - \gamma_{min})\gamma^{psimp}, \tag{3}$$

where γ is the control design variable, γ_p is the penalised variable, $psimp$ is the penalisation coefficient and γ_{min} is defined as 0.001. With the preceding interpolation scheme the thermal conductivity was defined as:

$$k(\gamma) = k_{max}\gamma_p, \tag{4}$$

where k_{max} is defined as 1 W/mK. The objective function J of this optimisation problem was defined as the dissipation of heat transport potential capacity

$$J = \int_\Omega (k\nabla T)^2 dV. \tag{5}$$

In the second benchmark the fluid dynamics was modeled with 2D Navier-Stokes equations and continuity equation under the assumptions of stationary laminar flow and incompressible fluid:

$$\begin{cases} \rho_{fl} \cdot (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \mu(\nabla^2 \mathbf{u}) + \alpha(\gamma) \cdot \mathbf{u}, \\ \rho_{fl}(\nabla \cdot \mathbf{u}) = 0, \end{cases} \tag{6}$$

where α is the inverse permeability of porous medium and was defined with the Darcy interpolation scheme as a function of the design variable $\gamma : \Omega \to [0, 1]$:

$$\alpha = \alpha_{max} \cdot \frac{q(1 - \gamma}{q + \gamma}, \tag{7}$$

where q is the penalisation factor. The objective function was defined as the difference between the average pressure at the inlet and the outlet of the duct:

$$J = \bar{p}_{inlet} - \bar{p}_{outlet}. \tag{8}$$

In the last benchmark, the optimisation of a 2D three-terminal heat sink cooling performance was investigated through a topology optimisation process. The problem was defined by a central square domain subjected to uniform heat generation of 100 kW/m^3 connected to the inlet on the left side with fixed temperature of 293 K. The fluid dynamics was modelled under the assumptions of stationary laminar flow and incompressible fluid with 2D Navier-Stokes equations and continuity equation. The heat transfer in the fluid was modelled with the steady-state convection-diffusion equation:

$$\rho C(\mathbf{u} \cdot \nabla T) = \nabla \cdot (k\nabla T) + Q, \tag{9}$$

where C is the heat capacity, k is the thermal conductivity of the fluid and Q is the uniform heat generation. In this optimisation, a dual objective function was adopted for the optimisation of both heat transfer and fluid flow. The global objective function is defined as:

$$A = \omega_1 B + \omega_2 C, \tag{10}$$

where B and C were defined as follows:

$$\begin{aligned} B &= \int_\Omega (T - T_{in})^2 d\Omega, \\ C &= \int_\Omega \left[\frac{1}{2}\eta \sum_{i,j} \left(\frac{\partial u_i}{\partial x_j} + \frac{partial u_j}{\partial x_i} \right) + \sum_i \alpha(\gamma) u_i^2 \right]^2 d\Omega. \end{aligned} \tag{11}$$

The thermal objective function B is related to the difference between the mean temperature of the design domain and an objective temperature, in this case, the inlet temperature of the fluid flow. The second objective function is proportional to the total flow power dissipated in the fluid system and it is related to the total pressure drop in the system; ω_1 and ω_2 are weighting factors of the two objective functions used to calibrate the convergence of the optimisation toward the minimisation of the fluid power dissipation or the mean temperature.

2.2 Adjoint Topology Optimisation - OpenFOAM

The results obtained with the benchmarks previously exposed represent the starting point for the development of an OpenFOAM optimisation code based on the adjoint approach [8]. This method implements, through a Lagrangian formalism, a sensitivity analysis independent from the number of control variables adding a set of auxiliary equations named adjoint equations. The Lagrangian approach allows to define the following Lagrangian function for the optimisation problem of a fluid system with heat transfer [5]:

$$L = J + \int_{\Omega} (\mathbf{u}, q, T_a) R(\mathbf{v}, p, T) d\Omega, \tag{12}$$

where J is the objective function, $(\mathbf{u}, q, T_a)$ is the vector of Lagrangian multipliers constituted by the state variables of the adjoint equations and $R(\mathbf{v}, p, T)$ is the set of primary governing equations. The adjoint optimisation problem is defined as: find $(\mathbf{y}, \lambda, \gamma)$ such that $\nabla L(\mathbf{y}, \lambda, \gamma)$ = 0, where $\mathbf{y}$ is the state variable vector, λ is the adjoint variable vector and γ is the control variable. The adjoint equations and the corresponding boundary conditions are obtained from the evaluation of the Lagrangian function gradient. The sensitivity analysis is calculated performing the derivative of the Lagrangian function with respect to the control variable:

$$\partial_\gamma L[\delta\gamma] = \int_{\Omega} J'(\gamma)\delta\gamma. \tag{13}$$

The adjoint equations for the fluid flow optimisation benchmark and the corresponding boundary conditions were formulated following the mathematical procedure previously shown and defining a cost function equal the pressure drop between the inlet and the outlet of the system similarly to the previous case:

$$\begin{cases} -2D(\mathbf{u})\mathbf{v} = -\nabla q + \nabla \cdot (2vD(\mathbf{u})) - \alpha\mathbf{u} \\ \nabla \cdot \mathbf{u} = 0. \end{cases} \tag{14}$$

For the adjoint optimisation of the pure heat conduction problem, the objective function includes the thermal component and the volumetric constrain through the Augmented Lagrangian Multipliers method [9] as follows:

$$J = \int_{\Omega} (T - T^*)^2 d\Omega - \lambda_k c_k + \omega c_k^2, \tag{15}$$

where λ_k is the k-th Lagrangian multiplier, ω a scalar weight factor and c_k was defined as follows:

$$c_k = \left[\frac{\int_{\Omega} \gamma d\Omega}{\int_{\Omega} d\Omega} - V_{target} \right]^2. \tag{16}$$

In this way the adjoint equation for the pure heat conduction problem is:

$$\nabla \cdot (k(\gamma)\nabla T_a) = -(T - T^*). \tag{17}$$

In the Multi-physics and multi-objective optimisation problem, the cost function is defined as the sum of two contributions to optimise both the heat transfer and fluid flow:

$$J = J_f + J_t = \omega_1 \left(\int_{inlet} pd\Gamma - \int_{outlet} pd\Gamma \right) + \omega_2 \int_{\Omega} (T - T_{in}^2 d\Omega. \tag{18}$$

Carrying out the accounts, the final form of the adjoint equations for this problem is:

$$\begin{cases} -(\nabla \mathbf{u})\mathbf{v} - (\mathbf{v} \cdot \nabla)\mathbf{u} - \nabla \cdot (2vD(\mathbf{u})) + \nabla q + \alpha(\gamma)\mathbf{u} + T_a \nabla T = 0, \\ \nabla \cdot \mathbf{u} = 0, \\ -\mathbf{v} \cdot \nabla T_a - \nabla \cdot (K \nabla T_a) + T - T_{in} = 0. \end{cases} \tag{19}$$

2.3 MSFR Topology Optimisation

The Molten Salt Fast Reactor model (Figure 1) is constituted by a cylindrical core connected to the heat exchanger, linked to the secondary loop and the pump through the hot leg and the cold leg of the reactor [10]. Fixed temperature values are imposed on the heat exchanger walls and the pump was modelled with a volume force. In the cylindrical core, homogeneous heat production of about 3000 MW is imposed [11]. The reactor core is discretized by a design variable γ which interpolates, through a proper interpolating scheme, a porous media introducing a volumetric force in the steady-state Navier-Stokes equations for incompressible fluids as in equation 6. The difference between average inlet pressure in the heat exchanger and the average outlet pressure from the pump system results to be the most effective objective function to reduce the recirculating areas.

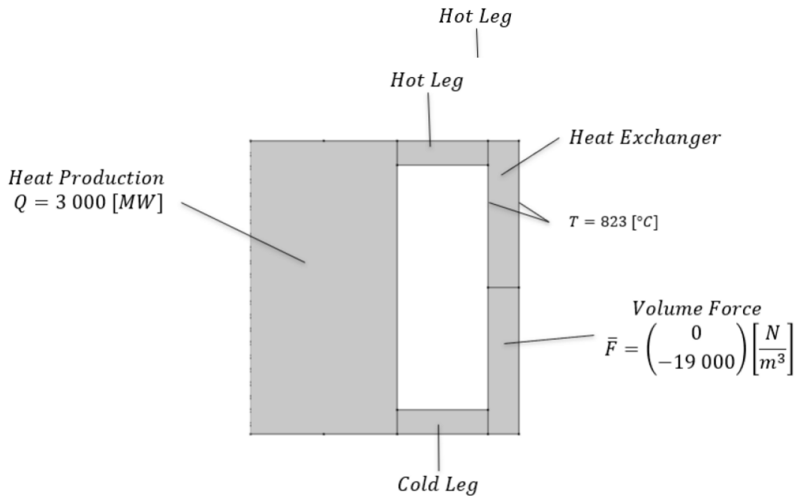
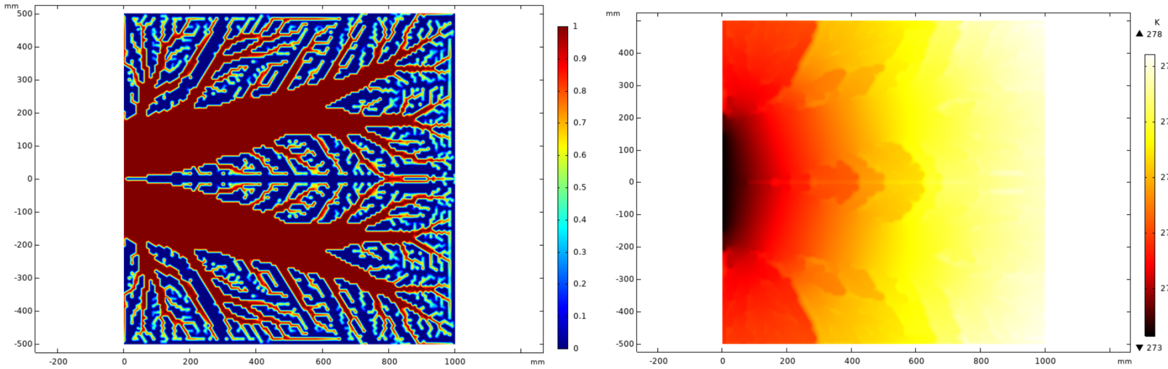


Figure 1: MSFR initial geometry and boundary conditions

3 RESULTS AND DISCUSSION

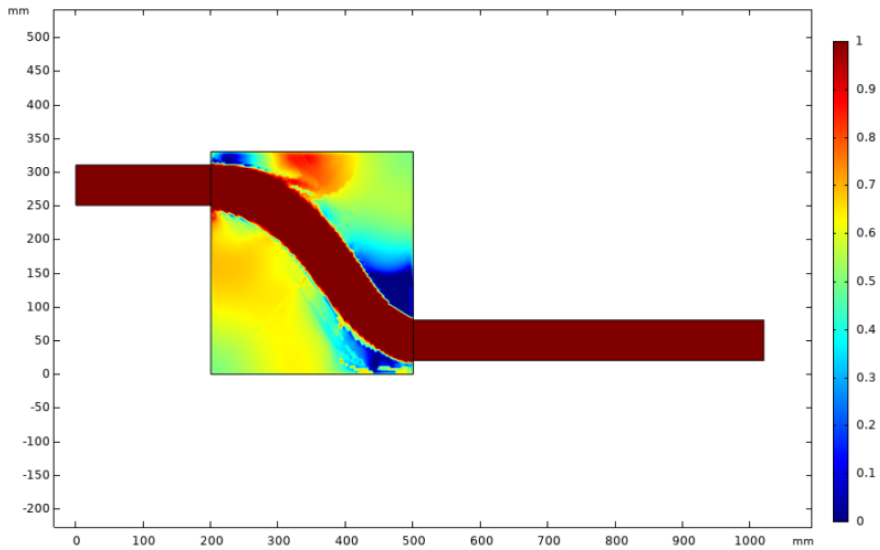
3.1 Gradient Based Optimisation Results

For the pure heat conduction optimisation problem, imposing volume constraints for the volume occupied by the more conductive material, the following topology and temperature results (Figure 2) are obtained. The more conducive material domain shows a dendrite shape (red areas) according to the previous works [4]. In the pure laminar flow problem, the optimisation algorithm succeeded in defining an S-bend shape for the duct (Figure 3) able to reduce the pressure drop from 0.729 to 0.335 Pa.



(a) Topology Optimisation (b) Temperature

Figure 2: Topology optimisation and temperature field (V_{target} = 0.5).



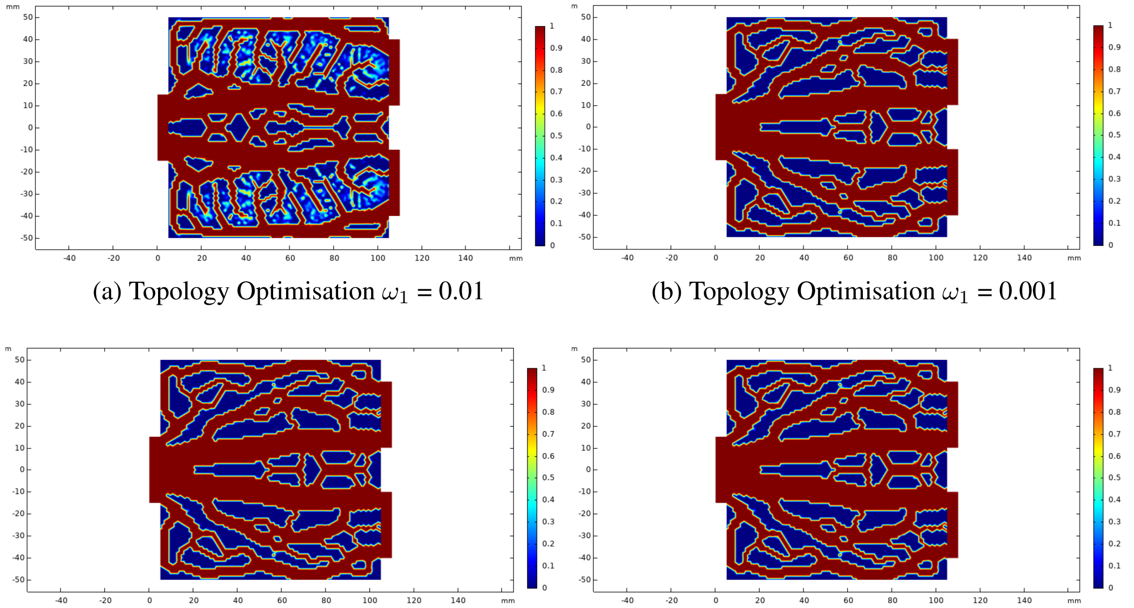
(a)

Figure 3: Topology optimisation results

In the Multi-physics and multi-objective benchmark, the topology results shown in Figure 4 are obtained varying the weighting coefficient ω_1 related to the thermal component of the cost function. Increasing ω_1 the free flow areas, identified by the red colour (γ = 1), tend to occupy the marginal regions of the domain succeeding to decrease the thermal excursion of about 28 K to the not optimised case. In the case of pure fluid flow optimisation (ω_1 = 0), the thermal excursion reaches a value of 81 K but decreasing the pressure drop of about 91%.

3.2 Adjoint Optimisation Results

In this section, the results obtained with The OpenFOAM optimisation solvers are shown. Again, the topology optimisation succeeded in defining an optimised free flow path for the pure



(a) Topology Optimisation ω_1 = 0.01 (b) Topology Optimisation ω_1 = 0.001

(c) Topology Optimisation ω_1 = 0.0001 (d) Topology Optimisation ω_1 = 0

Figure 4: Topology optimisation and temperature field (V_{target} = 0.5).

laminar flow problem able to reduce the pressure drop (Figure 5). In Figure 6 the pure heat conduction optimisation results show a conductive material path similar to the one obtained with the gradient-based method.

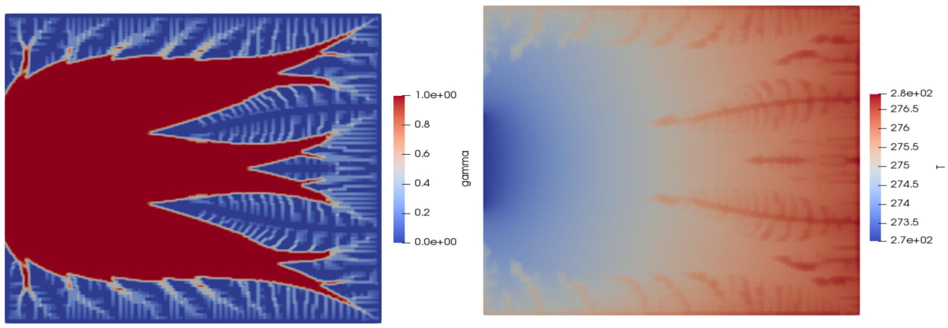
(a)

Figure 5: Topology optimisation results

Considering the multi-physics and multi-objective optimisation, the adjoint approach was able to define free flow paths (red areas in Figure 7) able to reduce the pressure drop and temperature gradient in the domain as a function of the weighting coefficients in the objective function: a higher value of the coefficient related to the thermal component of the cost function results in a coolant free path able to reduce the average temperature in the system.

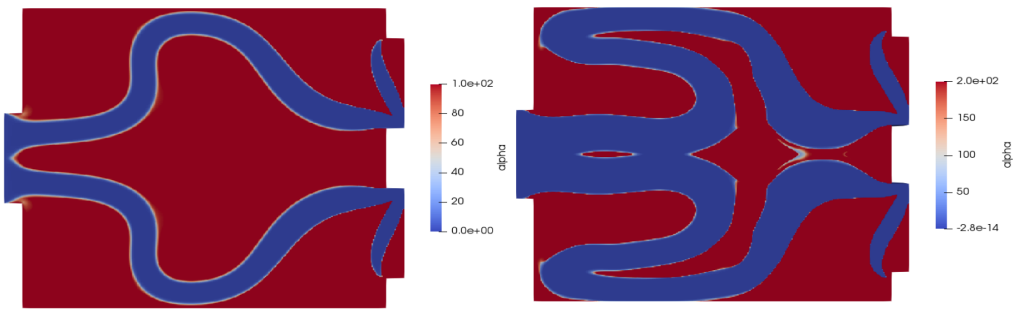
3.3 MSFR Optimisation Results

The gradient-based method was applied to the EVOL geometry of the MSFR with the software COMSOL Multi-physics. The optimised geometry, shown in Figure 8, was subjected to a validation test. The velocity and temperature fields of the base case and optimised geometry are shown in Figures 9 and 10. The topology optimisation was able to reduce the maximum



(a) Topology Optimisation (b) Temperature

Figure 6: Topology optimisation and temperature field (V_{target} = 0.5).



(a) Topology Optimisation ω = 0.1 (b) Topology Optimisation ω = 0.5

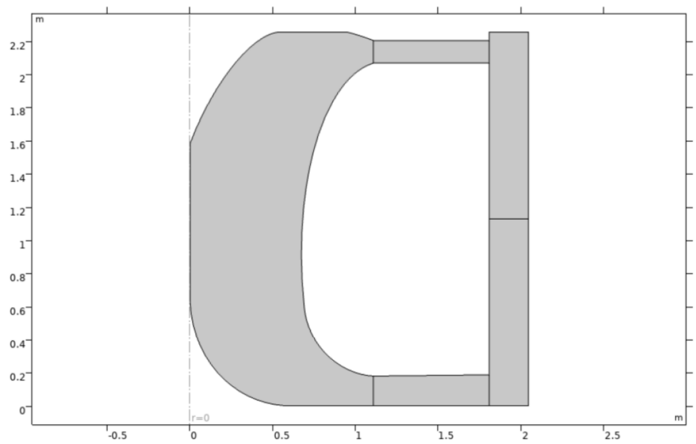
Figure 7: Multi-physics Topology Optimisation Results.

temperature in the core from 1739 K to 1130 K and the average temperature from 1137 K to 991 K. Nevertheless, the average temperature in the hot leg increased by 3% leading to possible improvements in the thermal yield of the power plant.

4 CONCLUSIONS

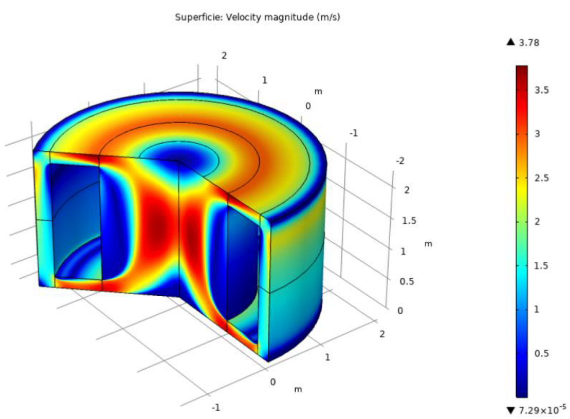
The gradient-based algorithms gave promising results regarding fluid flow and heat transfer optimisation. These methods, even if are not limited by fluid flow instabilities with the increasing of Reynolds number, are characterised by high computational cost. This makes them an important tool for the optimisation of 2D problems. In the second part, a multiphysics optimisation solver based on the adjoint approach was implemented in OpenFOAM. The adjoint optimisation was tested with the same 2D benchmarks of the previous section. The comparison between the results obtained with the two software was limited by the fact that the adjoint algorithm implemented the "one-shot" approach which involved a sensitivity analysis calculated with only partially converged quantities and resulted in numerical tests with high residual values. Nonetheless, the adjoint optimisation showed remarkable results characterised by low computational cost. For these reasons, it represents a promising tool for further three-dimensional studies regarding thermal-hydraulic problems of engineering interest. However, it induces high residual values which introduces the need for further validation tests and the computational instabilities induced by turbulence limit its applicability to low Reynolds numbers.

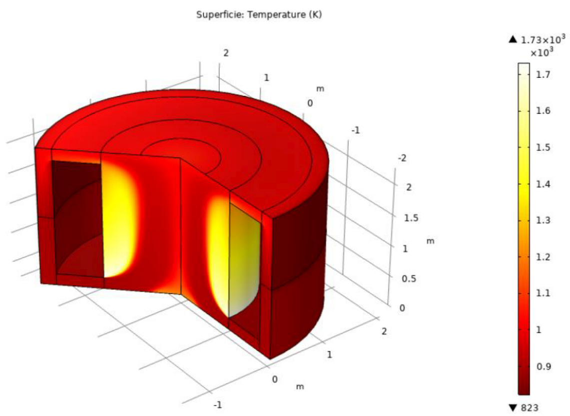
In the final part, the topology optimisation was applied to the MSFR. The promising thermal-hydraulic optimisation results obtained can be extended to more complex systems. In



(a)

Figure 8: MSFR optimised geometry





(a) EVOL Velocity Field (b) EVOL Temperature Field

Figure 9: EVOL geometry base case results.

particular, the stability of the COMSOL gradient-based algorithms represents a promising starting point for multi-physics optimisations including the neutronic economy in the reactor defining an additional contribution in the cost function aimed at minimising the neutron leakages from the core.

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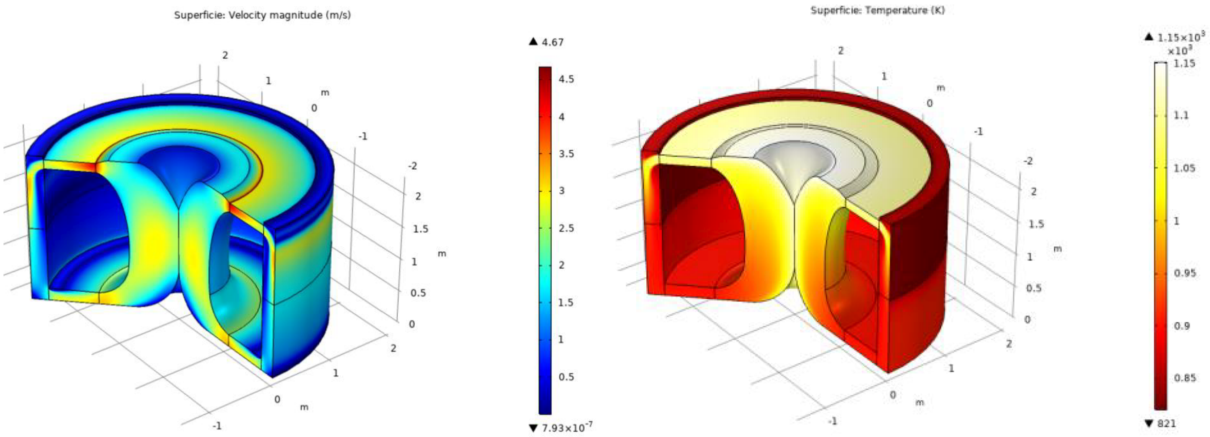

(a) Optimised Velocity Field

(b) Optimised Temperature Field

Figure 10: Multi-physics topology optimisation results.

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