

Deliverable 1.10

Design tool for graded structures with minimum distortions

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1. Introduction

Additive manufacturing (AM) is a manufacturing technology that offers a plethora of advantages compared to traditional manufacturing technologies. It enables the production of parts with complex geometries that are tailored towards specific applications and are optimised for the functionality-weight-ratio (or functionality-cost-ratio). It allows for parts with complex multi-material distributions, while at the same time material waste (during postprocessing) and production costs can be dramatically reduced.

Yet, although AM technology is steadily progressing, the approach to create the designs for AM is less advanced. Often, parts are still being designed based on the engineer's experience. This does not only often require a time-expensive trial-and-error approach, but it also limits the design efficiency for highly complex problems where non-intuitive designs might outperform conventional designs. With the effectiveness of AM depending on the corresponding design, its potential is not fully exploited yet. One approach to improve the design process is the use of computational tools. One such design tool is Topology Optimisation (TO) in combination with the Finite Element Method (FEM).

In this report, we elaborate on TO as the design tool for graded structures with minimum distortions. We will discuss critically the need and suitability of structural grading by means of a mould of GKN to produce composite parts, and present TO solutions for mono-material structures, where a grading is not of advantage. For structures where a graded multi-material solution is desirable, we will consider the B2 demonstrator – a mandrel of GKN that functions as an insert within a larger mould assembly – and demonstrate the efficiency of TO for the generation of optimised designs. To this end, we will consider the two different approaches:

- 1. Scientific approach using the TO methodology developed by UGent-MMS in this project, as presented in deliverable report D1.9
- 2. Engineering approach using the TO methodology, Tosca, implemented in the commercial software package Abaqus

The materials that are considered for this deliverable belong to the family of Fe-Ni (iron-nickel) alloys. Within this family, Invar36 is a standard grade which has a 36% Ni content and has the unique feature of a very low coefficient of thermal expansion (CTE) at low temperatures, matching the CTE of carbon fibre composites. Increasing the Ni content extends temperature range of low thermal expansion. As convenience, this report calls all Fe-Ni combinations InvarXX where XX is the corresponding Ni content (although at very high Ni content the CTE is not low anymore).

This report is structured as follows. In Section 2 we will give an overview of the benefits of topology optimisation for the creation of problem-tailored designs for Additive Manufacturing. Section 3 introduces the two use-cases (GKN mould and mandrel), including constraints and optimisation goals. In Section 4, we will introduce the design tool and elaborate on the two chosen TO approaches; requirements for and limitations of the FE model are also discussed with the focus on achieving high quality results through design optimisation. Results are presented in Section 5 for the two use-cases. In Section 6, guidelines are given for the transfer of the design tool to similar engineering problems. Lastly, conclusions follow in Section 7.



The benefit of topology optimisation for additive manufacturing

As already indicated in Section 1, TO offers the possibility to digitally generate designs that are highly suitable for Additive Manufacturing (AM) and that are tailored to specific applications. Table 1 presents an overview of the benefits of TO when used for generating AM-suitable designs.

In addition, TO offers the possibility to include (via specific mathematic formulations) manufacturing constraints such as printing direction or overhang criteria. While the most common manufacturing constraints are already included in commercial software packages (e.g., Abaqus), in-house codes can be straightforwardly extended to include the same criteria and more.

Table 1: Benefits of Topology Optimisation in relation to the benefits of Additive Manufacturing.

Benefits of Additive Manufacturing	Benefits of Topology Optimisation	
Printing of parts with complex geometries	Designs with complex geometries	
Printing of problem-tailored designs	Problem-tailored, non-intuitive designs	
Multi-material printing	Optimised, multi-material designs	
Material waste reduction and cost reduction	Material- and cost-effective designs	



3. Problem description

In this section, the two considered use-cases are presented: a full GKN mould for the production of carbon fibre composites, and the B2 demonstrator, a mandrel that functions as an insert within a larger mould assembly for the production of composite components. For both use-cases, we introduce the TO goals and the related TO constraints.

3.1. Full GKN mould

The full GKN mould, which has been the core subject for the developments within this deliverable, is illustrated in Figure 1 – here, the concept of the mould is illustrated. It consists of 4 different parts: an upper and lower mould part, each with 28 equidistant heating holes, and a back and front plate that close the design; features such as holes and inserts for the resin infusion are excluded for simplicity.

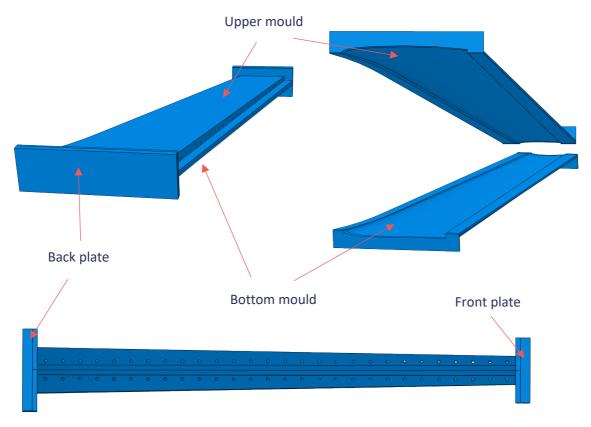


Figure 1: Illustration of the core concept for the GKN mould to produce thermoplastic composites for aerospace applications.

During the operation of the mould, a resin is inserted and combined with carbon fibre mats. The resin is then cured under high temperature and internal pressure to produce the composite. The corresponding load curves are illustrated in Figure 2.



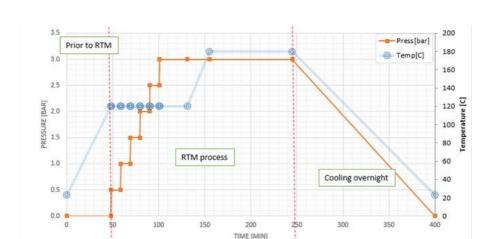


Figure 2: Thermomechanical loading applied to the mould during the production process.

To reduce the impact of the curing process on the quality of the moulded product, two production steps are of importance. The first step is the curing process itself, taking place at 180degC and 3bar. This step introduces a high thermomechanical load on the mould. Due to the resulting thermomechanical expansion of the mould, deviations in the product dimensions as compared to the target dimensions arise. The severity of the deviations depends on the distortion of the internal mould surface. The second step concerns the cooldown of the mould. If the thermal shrinkage of the mould surface differs largely from the thermal shrinkage of the composite, high stresses would be exerted on the moulded product which could damage the composite.

To ensure a high product quality, the primary goal of the TO for the GKN mould can be formulated as:

Objective 1: Generation of a mould design that minimises the thermomechanical distortions along the inner surface during the production process.

Achieving this goal will on the one hand greatly limit the deviations from the target dimensions, and on the other hand reduce (or even fully eliminate) any thermomechanical stresses on the composite during cooldown.

For the developments within this deliverable (and the creation of the mould designs), iron-nickel alloys are considered due to their low coefficient of thermal expansion (CTE). With the aim of generating a design which can be manufactured with a graded material composition (varying nickel content) through Wire Arc Additive Manufacturing (WAAM), the second goal is:

Objective 2: Find an ideal multi-material distribution using iron-nickel alloys that satisfies TO objective 1.

Last, but not least, TO is a lean tool for the generation of material-effective designs. In this context, the last goal for this use-case is:

Objective 3: Reduce the amount of material being used in the mould in consideration of TO objective 1.

At the same time, to guarantee the functionality of the mould, four design constraints are required.

<u>Constraint 1:</u> Maintain the shape of the internal surface as this defines the external shape of the final product objective 1.



<u>Constraint 2:</u> Retain sufficient material between the heating holes and the internal surface to guarantee the required heat transfer for the curing process.

Constraint 3: Retain the flanges of the individual parts for closing the mould via clamping.

Constraint 4: The mould design needs to be printable bottom-up with WAAM.

To prepare the GKN mould for TO, the core concept of the GKN mould illustrated in Figure 1 has been modified by extruding the external top and bottom surfaces of the mould as shown in Figure 3. This creates a rich design space for the TO where material will be removed where redundant.

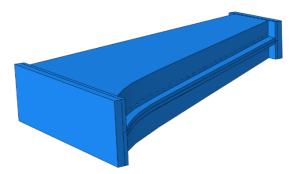


Figure 3: GKN mould prepared for TO by extruding top and bottom surface of the mould illustrated in Figure 1.

3.2. B2 demonstrator – Mandrel

The second use-case for TO in this deliverable, but of reduced extent¹, is the B2 demonstrator, the mandrel as illustrated in Figure 4. While the front and the back are free surfaces, the other sides are fully constrained by other mould parts. During operating conditions, a uniform temperature of 180degC and a surrounding pressure of 3bar on all but the free surfaces is assumed.

For this use-case, a multi-material distribution is envisaged in such a way that the mandrel is being printed (via WAAM) such that the majority is of Invar36 (blue part in Figure 4) and only a small portion (50 mm) is built with Invar55 (red part in Figure 4). The transition zone between Invar36 and Invar55 is defined as 10mm.

¹ After it has been discovered that a multi-material solution for the full GKN mould (cf. Section **Error! Reference source not found.**) is undesirable, as elaborated in deliverable report D1.9, the mandrel was defined as the B2 demonstrator. Due to limited time left in the project, only a limited amount of work could be performed for the TO of the mandrel.



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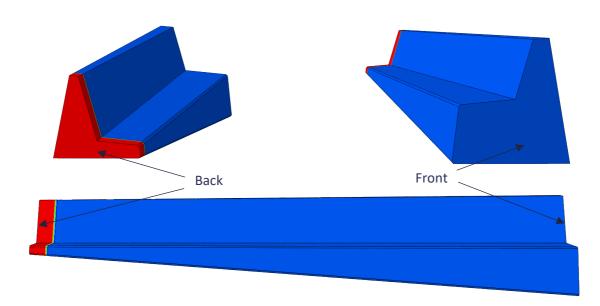


Figure 4: Illustration of the mandrel as an insert within a larger mould. Blue represents Invar36 whereas the red part is Invar55. Between both parts is a 10mm transition area of mixed composition.

The goal of the TO is:

Objective 1: Minimise the distortions on the external mandrel surface.

Objective 2: Reduce the amount of material being used in the mandrel.

To guarantee the functionality of the mould, the following design constraints are required:

Constraint 1: Maintain the shape of the external surface.

Constraint 2: The mandrel design needs to be able to withstand the thermomechanical loads.

Constraint 3: The mandrel design needs to be printable bottom-up with WAAM.



4. The design tool – Topology Optimisation approaches

In the Grade2XL project, one of the goals was to develop a design tool for graded structures with minimum distortions. To this end, two different approaches were followed. The first one is the scientific approach, that uses the TO methodology developed by UGent-MMS, as presented in deliverable report D1.9. The second approach is the engineering approach for which the TO methodology, implemented in the commercial software package Abaqus, is used. This section presents the general principle of TO, followed by the model requirements for a successful TO, and then a short overview of both approaches and their limitations.

4.1. General Principle of TO

TO is an advanced computational technique that iteratively optimises the material distribution within a given design space, for a predefined set of load conditions, TO objectives, and TO constraints, while using the principles of the FEM. At each iteration of the design cycle, the structure's response to the given load conditions is calculated via FEM in consideration of the current material distribution. Using the results of the FE analysis, the material distribution is updated based on mathematical principles in line with the TO objectives and TO constraints. The iterative design cycle continues until the TO convergence criteria has been satisfied, and the optimum design has been determined. The flowchart of the TO process is illustrated in **Error! Reference source not found.**, using the example of the TO code developed at UGent-MMS.

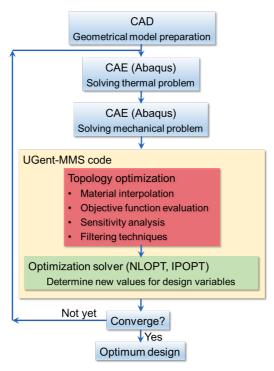


Figure 5: The flowchart of the in-house topology optimisation code developed at UGent-MMS. Copied from deliverable report D1.9.

4.2. Model Requirements

A successful TO, using the scientific approach, requires a thorough preparation of the FE model. The core requirements are the following.



Large, global design space. As already stated in Section 4.1, TO optimises the material distribution within a given design space. In this sense, it is paramount to define globally a large design space (i.e., total volume). A too limited design space may affect the final design quality, and lead to non-optimal solutions. An example of a well-defined global design space is illustrated Figure 3 at the example of the GKN mould, where the top and bottom surfaces of the initial design (Figure 1) were extruded.

Large, local design space. With TO being based on FE formalisms, the accuracy of the TO results strongly depends on the mesh size. For large elements, the design result will be coarse with less intricate details. To ensure a large, local design space it is therefore advisable to choose an element size which is in the order of the smallest printable features (as compared to AM capabilities).

Design domain vs. frozen domain. For the TO, two domains need to be defined: the design domain and the frozen domain. During the optimisation process, only within the design domain the material distribution is altered. Any material within the frozen domain sremain unchanged throughout the optimisation. Both regions are illustrated in Figure 6 by means of the GKN mould where the frozen domain is defined in accordance with constraints 1-3 (concerning the flanges, the heating holes and the internal surface) as introduced in Section 3.1.



Figure 6: Initial geometry of the GKN mould and the division into the design domain and the frozen domain as required for TO.

FE element type. The accuracy of the TO relies heavily on the accuracy of the FE analysis. The major influential factor for the accuracy of the FE analysis is the chosen element type. While linear tetrahedral elements often result in inaccuracies and should be omitted [1], quadratic tetrahedral elements (C3D10MT), linear hexagonal elements (C3D8T) and quadratic hexagonal elements (C3D20T) are the preferred elements for accurate FE results. To ensure a good balance between accuracy of the TO results and the simulation time, it is important to pay close attention to the chosen element type and the mesh size (required for a large, local design space). Often, linear hexagonal elements are an adequate, and the recommended choice.

4.3. Scientific Approach

4.3.1. Overview

For the Scientific Approach of the design tool, the TO routine developed by UGent-MMS is followed. It is a thermomechanical TO methodology for quasi-static problems, which uses sophisticated filtering techniques to prevent typical checkerboard patterns and adopts a novel formulation for multi material optimisation. This results in a unique design with a multi-material distribution that depends on the set TO objective and constraints.

The TO code is Python-based and utilises for the FE analysis the commercial software package Abaqus through its application scripting interface. The corresponding flowchart is illustrated in Figure 5.

More details on the TO methodology and the relevant mathematical formulations can be found in deliverable report D1.9 and in [2].



4.3.2. Limitations

Element type. The TO routine by UGent-MMS is currently implemented only for linear hexagonal elements. For any other element types relevant extensions and distinctions are necessary.

Thermomechanical problems. At the time of the writing, the multi-material thermomechanical TO method by UGent-MMS covers only heat conduction. Heat convection has not been considered in the project due to its intricate nature: During the optimisation process, the external surface of the design may change (unless frozen). As the external surface changes, the influence of heat convection is impacted. This necessitates a sophisticated implementation where 1) the location of the external surface is being traced and 2) the changing nature of the heat convection is included in the mathematical formulation. Such an extension will be subject of further developments after completion of the Grade2XL project.

4.3.3. Utilisation for the design tool

In delivery report D1.9, it has elaborated that with the current limitation of the excluded convection 'it is better to run the TO only for the internal pressure load case, and do the validation for thermal convection in a post-processing step.' In that spirit, the scientific approach adopts a two-stepped approach:

- 1. Perform a mechanical TO, excluding any temperature effects.
- 2. Validate the generated design with a thermomechanical analysis where conduction and convection are considered.

4.4. Engineering Approach

4.4.1. Overview

For the Engineering Approach of the design tool, the Tosca implementation within Abaqus 2022 is used. Tosca is a TO routine, which allows for an efficient and effective application of TO principles directly within the Abaqus environment, leveraging its robust FE analysis capabilities. Its ability to handle complex problems and integrate seamlessly with Abaqus makes Tosca an indispensable tool for engineers seeking to push the boundaries of design and material use.

4.4.2. Limitations

Mono-material TO. Tosca is only able to generate designs by either retaining or removing material. Although it can handle multi-material designs, it is not able to swap a material for another. An optimisation for the ideal multi-material distribution is thus not possible.

Thermomechanical problems. The Tosca implementation within Abaqus 2022 is not capable of a thermomechanical TO.

4.4.3. Utilisation for the design tool

In consideration of the limitations, the engineering approach entails the following steps:

- 1. Based on a preliminary analysis, create a set of distinct FE models with suitable multimaterial distributions as a base for the TO, where material is either removed or retained.
- 2. For each FE model perform a mechanical TO, excluding any temperature effects.
- 3. Validate the generated designs with a thermomechanical analysis where conduction and convection are considered.



5. Topology Optimisation results

5.1. Full GKN mould

As elaborated in delivery report D1.9, within the project it was discovered that for the full GKN mould (cf. Section 3.1) a mono-material structure is the desired design solution: With the goal to minimise the thermomechanical distortions along the inner surface during its operation, the ideal material solution is the one with the lowest CTE – in the present case of Fe/Ni alloys, this is Invar36. Thus, the engineering approach for the design tool collapses to merely two steps (2 and 3) – the same as for the scientific approach.

The material properties of Invar36 were to a large extent extracted from the paper of Yakout et al. [3], only the CTE was determined experimentally within this project and was already reported in [4]. For the operating temperature range of the full GKN mould, the material properties are depicted in Figure 7.

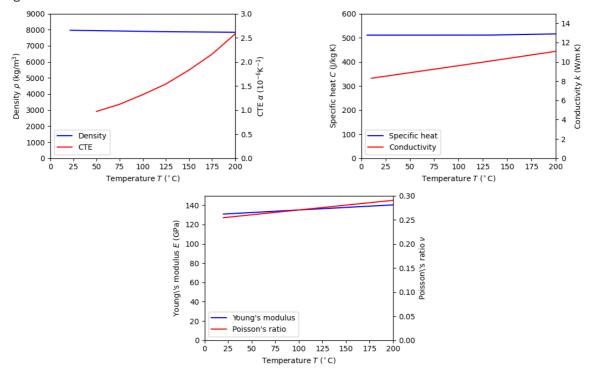


Figure 7: Material properties of Invar36 for the relevant operating temperature range of the full GKN mould.

5.1.1. Step 1 – Mechanical Topology Optimisation

In this step, to perform the TO, a purely mechanical loading is assumed, neglecting any thermal effects. Hereto, the pressure of 3 bar is being applied to the entire inner surface of the closed GKN mould. In addition, to prevent rigid body motion, displacement boundary conditions are applied as illustrated in Figure 8.



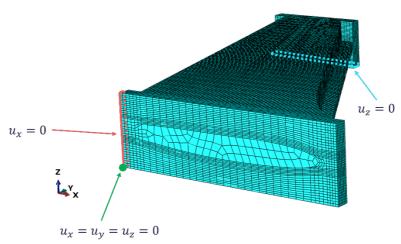


Figure 8: Displacement boundary conditions for the GKN mould.

5.1.1.1. Scientific approach

For the scientific approach, the TO for a purely mechanical loading of 3 bar pressure has successfully demonstrated in deliverable report D1.9. There, a volume reduction of 60% is enforced on the design domain (cf. Figure 6) as a TO constraint, which is equivalent to a volume reduction of 49% as compared to the full, initial GKN mould design (cf. Figure 3), excluding front and back plate. TO results are illustrated in Figure 9. A relatively homogeneous material distribution results along the length of the mould which is due to the uniform pressure application. In addition to the visible volume reduction, the TO also introduced an internal riblike cavity structure. This cavity structure is similar to the one that originates via the engineering approach, as shown later in Figure 11, and will for sake of brevity not be displayed here.

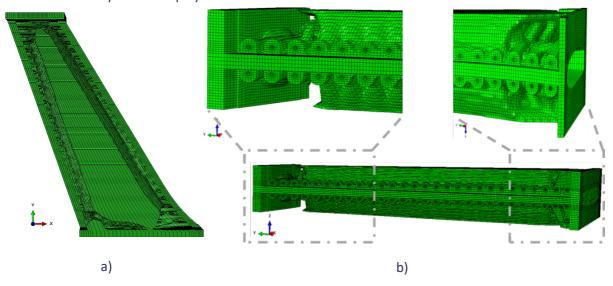


Figure 9: TO design using the scientific approach with a volume reduction of 49% as compared to the initial GKN mould design (cf. Figure 3), excluding front and back plate; only mechanical load is considered. a) Bird's-eye view, and b) side view.

5.1.1.2. Engineering approach

For the engineering approach, various volume constraints were considered in a first study, ranging between 20% and 60% volume reduction as compared to the full, initial mould design (cf. Figure 3), excluding front and back plate. Each volume constraint resulted in a design similar to the one



displayed in Figure 10 – it displays the design with a volume reduction of 40%. The different designs were analysed via thermomechanical validation, and deliberately discussed with GKN (end-user) and Ramlab (manufacturer). The TO with a volume reduction of 40% was identified as the most prospective in terms of balancing functionality and saved volume. Thus, in the following only the results for the design with a 40% volume reduction will be shown.

As for the scientific approach, the uniform pressure leads to a relatively homogeneous material distribution along the length of the mould. In addition, a riblike cavity structure is generated, which is displayed in Figure 11. It is to be noted that several small, closed cavities are present in the design. These are to be treated in a post-processing step (either opened or fully removed) to prevent air-expansion related cracking during heating of the mould.

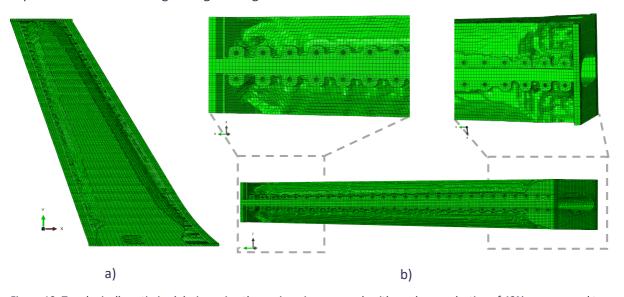


Figure 10: Topologically optimised design using the engineering approach with a volume reduction of 40% as compared to the initial GKN mould design (cf. Figure 3), excluding front and back plate; only mechanical load is considered. a) Bird's-eye view, and b) side view.

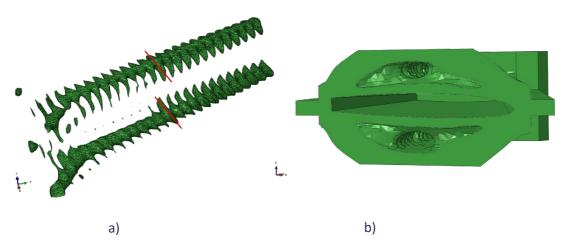


Figure 11: a) Internal cavity structure of the topologically optimised design (cf. Figure 10); the red lines indicate the location of the cross-section view. b) cross-section view of the mould illustrating the generated internal cavity design.



5.1.2. Step 2 – Thermomechanical validation

In the first step of the design tool, the TO design has been successfully generated using either the scientific or the engineering approach. During that step, only the mechanical loading has been considered. It is therefore paramount to validate the generated design(s) in a subsequent analysis through consideration of the full thermomechanical loading.

As a demonstration of this step, we will focus in the following on the design generated via the engineering approach with a volume reduction of 40%. Yet, the approach followed here is universally applicable for <u>any</u> design achieved through the engineering approach as well as the scientific approach.

In addition to the mechanical loading, that has been adopted for Step 1 (see Section 5.1.1), a thermal loading is applied in accordance with the operating conditions (cf. Figure 2): The time-dependent temperature is applied to the nodes that define the surface of the heating holes. Convective boundary conditions are applied to the external surface, assuming a convection coefficient of $h_c=15~\rm W/m^2 K$ [5]. Thermally, this leads to a non-homogeneous temperature field which is governed by the conductive and convective heat transfer phenomena. The results are illustrated in Figure 12 for $t=245~\rm min$, the end of the 180 °C temperature step, and where the highest temperatures are recorded. The comparison with the initial, non-optimised mould design (cf. Figure 3) demonstrates the non-negligible influence the TO-created cavity has on the temperature distribution, which is expected to influence in turn the thermomechanical expansion.

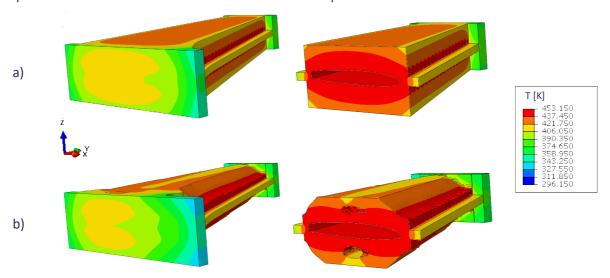


Figure 12: Temperature profile of the GKN mould at the end of the 180 $^{\circ}$ C (453.15 K) temperature step (cf. Figure 2): a) initial design (cf. Figure 3), and b) TO design (cf. Figure 10). For both mould designs, displayed are the full mould view on the left side and a cross-section view on the right side.

To validate the TO design with regard to Objective 1 (minimising the thermomechanical distortions along the inner surface), the corresponding displacement profiles are shown in Figure 13-Figure 15, comparing the initial, non-optimised mould design (cf. Figure 3) with the TO design (cf. Figure 10).



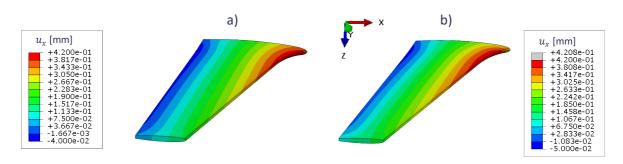


Figure 13: Displacement profile for u_x along the internal surface of the GKN mould at the end of the 180 °C (453.15 K) temperature step (cf. Figure 2): a) initial design (cf. Figure 3), and b) TO design (cf. Figure 10).

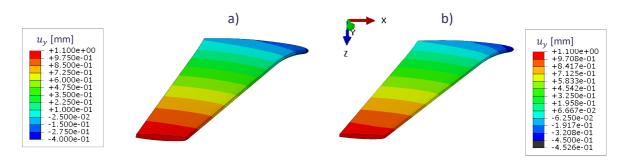


Figure 14: Displacement profile for u_y along the internal surface of the GKN mould at the end of the 180 °C (453.15 K) temperature step (cf. Figure 2): a) initial design (cf. Figure 3), and b) TO design (cf. Figure 10).

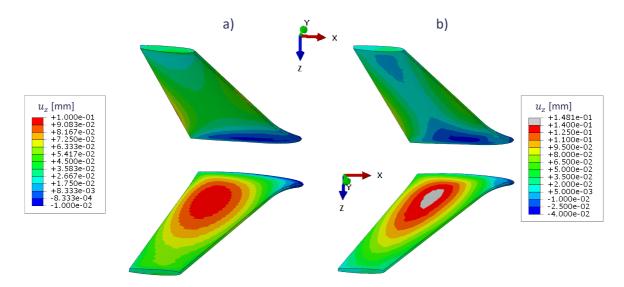


Figure 15: Displacement profile for u_z along the internal surface of the GKN mould at the end of the 180 °C (453.15 K) temperature step (cf. Figure 2): a) initial design (cf. Figure 3), and b) TO design (cf. Figure 10).

The results show that while for u_χ and u_y the change in distortion is negligible after TO, u_z slightly increases for the optimised design. The cause for the latter originates from a thermomechanical induced bending of the mould that is invoked by the temperature difference above and below the cavities in the top and bottom mould. The same phenomenon has been observed for the toy problem illustrated in Figure 9-Figure 11 of deliverable report D1.9. Yet, in face of the achieved volume reduction of 40%, the small increase of distortion along the inner mould surface can be considered as negligible.



Finally, the thermomechanical stresses at $t=245\,\mathrm{min}$, the end of the 180 °C temperature step, are displayed in Figure 16 comparing again the initial, non-optimised GKN mould and the optimised mould design. Although, stress peaks of up to ca. 240 MPa are observed for the optimised mould, those relate to sharp edges within the optimised design. These stresses are expected to drop significantly with the post-processing of the design where sharp edges will be smoothened in line with the minimum via AM printable feature size.

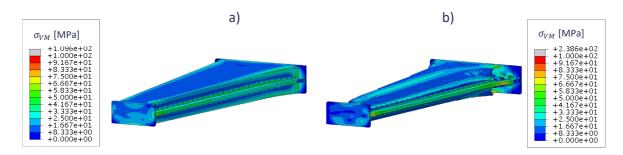


Figure 16: Von Mises stress within the GKN mould at the end of the 180 °C (453.15 K) temperature step (cf. Figure 2): a) initial design (cf. Figure 3), and b) TO design (cf. Figure 10).

5.2. B2 demonstrator – Mandrel

With the discovery that for the full GKN mould (cf. Section 3.1) a mono-material structure is the desired design solution, an alternative for the B2 demonstrator was considered for the multimaterial printing. The chosen B2 demonstrator is the mandrel as introduced in Section 3.2.

Since this switch to the new demonstrator was made towards the end of the project, only one approach for the design tool approach was followed for the mandrel. Since no TO with respect to the material composition was required (this can only be done with the scientific approach), the engineering approach was selected.

5.2.1. Transition zone

For setting up the FE model, the transition zone was modelled as a smooth transition, adopting the tanh function as illustrated in Figure 17, where the transition zone is defined to lie within the bounds $tanh(\hat{x}) = \pm 0.9$.

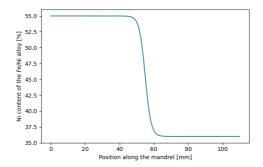


Figure 17: Tanh(x) function to describe the transition zone.

5.2.2. Material properties

For the material properties, the temperature dependent CTEs for Invar36, Invar46 and Invar49 were experimentally determined. These CTE-curves were then extrapolated and modified to estimate the temperature-CTE curve for Invar55 in resemblance with the recorded CTE-curves in Figure 28 of [6].



While for Invar36 Young's modulus and Poisson's ratio were extracted from the paper of Yakout et al. [3], the properties for Invar46, Invar49 and Invar55 had to be estimated. As a base for the estimation of the Young's moduli, the room temperature values recorded in [7] were used – either as direct values or by linear interpolation based on the two closest values. For the Poisson's ratio, the value at room temperature was assumed equal for all Invar alloys.

To obtain the variation with the temperature, the Curie temperature of each Invar alloy [8] was used. For the Young's modulus, we first assumed that the Young's modulus increases linearly from the room temperature T_{RT} up to the Curie temperature T_{C} :

$$E(T) = \frac{E(T_C) - E(T_{RT})}{T_C - T_{RT}} (T - T_C) + E(T_C)$$

To obtain the Young's moduli at T_C of Invar46, Invar49 and Invar55, a proportionality was assumed between the change of the CTE as a function of the Nickel content and the change of the Young's modulus at T_C :

$$\frac{E^{i}(T_{C}) - E^{i}(T_{RT})}{\alpha_{ref} - \alpha(T_{RT})} = const$$

with the assumption $\alpha_{ref} = 12 \cdot 10^{-6} K^{-1}$, and the superscript i representing one of the Invar alloys.

For the Poisson's ratio ν we again assumed a linear dependency:

$$\nu(T) = \frac{\nu(T_C) - \nu(T_{RT})}{T_C - T_{RT}} (T - T_C) + \nu(T_C)$$

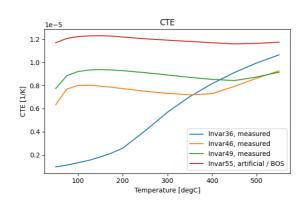
For the Poisson's ratio at $T_{\mathcal{C}}$ we assumed equality for all the different Invar alloys:

$$\nu^i(T_C^i) = const$$

	Young's modulus at RT	Curie Temperature
Invar36	131.1 GPa	260 °C
Invar46	149.7 GPa	440 °C
Invar49	153.5 GPa	480 °C
Invar55	161.3 GPa	540 °C

The corresponding temperature curves for the CTEs, Young's moduli, and Poisson's ratios are displayed in Figure 18. For any other Invar alloys within the transition zone, Abaqus interpolates those properties linearly.





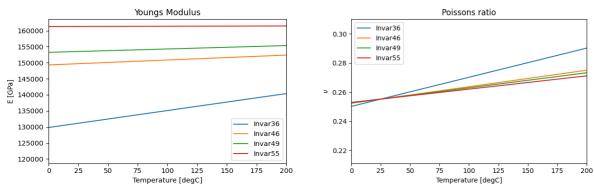


Figure 18: Adopted material properties for Invar36, Invar46, Invar49 and Invar55.

5.2.3. Load and Boundary conditions

Following the operational loads introduced in Section 3.2, a homogeneous temperature of 180 °C is set for the whole mandrel. Simultaneously, a constant pressure of 3bar is applied on all external surfaces, but the front and back face (cf. Figure 4).

For the boundary conditions, and to prevent rigid body motion during the simulation, we assumed zero displacements at the front face as illustrated in Figure 19.

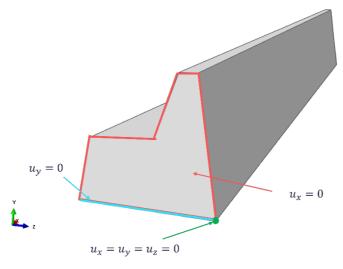


Figure 19: Displacement boundary conditions for the mandrel.



5.2.4. TO Results

Adopting the engineering approach, a purely mechanical TO (no temperature application) was performed in line with the TO objectives and constraints (cf. Section 3.2): 1) the objective function is to minimise the displacements on the external surface, 2) different volume reductions (50%-70%) as compared to a solid mandrel are considered, and 3) an overhang constraint is used [1], enforcing AM-printability from front to back face in a bottom-up fashion.

The TO results for a volume reduction of 70% is illustrated in Figure 20 where a cross-section view is depicted to visualise the internal support structure (the whole mandrel is a closed design in line with Constraint 1).

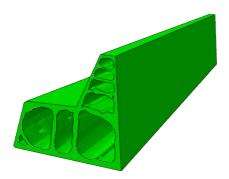


Figure 20: TO results of the mandrel for a volume reduction of 70%. Depicted is a cross-section view to illustrate the internal support structure.

The generated design was then used by GKN as an inspiration to create a new design which is optimised for the AM process. The core steps taken for the redesign were:

- Reduction of the number of supporting ribs,
- Increasing wall thickness for external and internal parts,
- Uniform rib-structure running from front to back.

The updated design is illustrated in Figure 21.

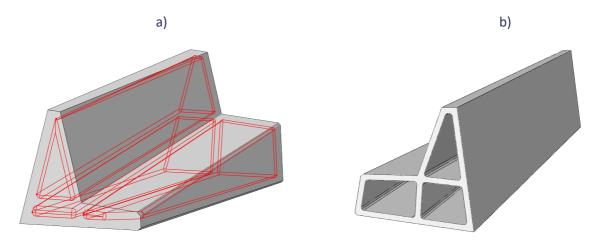


Figure 21: Mandrel redesign with an internal support structure. a) full view with the cavities highlighted in red, b) cross-section view.



5.2.5. Thermomechanical validation

For the thermomechanical validation, the TO inspired design (cf. Figure 21) was used. As before, a two-material setup (Invar36 and Invar55), with a transition zone (ref. Section 5.2.1) was considered, with the material properties introduced in Section 5.2.2. The goal of the thermomechanical validation is to ensure alignment with Constraint 2: "The mandrel design needs to be able to withstand the thermomechanical loads."

Under the application of the relevant load conditions (ref. Section 5.2.3), thermomechanical stresses are induced such as illustrated in Figure 22 by means of the von Mises stresses. Although, stress concentrations arise around the transition zone, due to the mismatch in CTE and the thereby related thermomechanical stresses to compensate for the difference in thermal expansion $\varepsilon_{th}=\alpha\Delta T$, the recorded stresses are still well below the yield stress (ca. 500 MPa). The thermomechanical analysis therefore validates the mandrel design under the according load conditions.

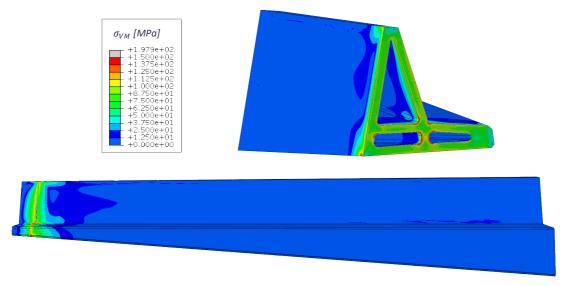


Figure 22: Von Mises stress within the mandrel due to the applied thermomechanical loads (temperature and pressure). The cross section view (top right) in the transition zone illustrates expected stress concentrations related to the mismatch in CTE.



Guidelines – methodology transfer to other engineering problems

6.1. Introduction

In order to transfer the methodology of the design tool to other engineering problems, parallels to other demonstrators within this project were sought. To this end, demonstrators B1 and B3 were studied: type and duration of the thermomechanical load, current design approach, and AM printability.

For both demonstrators it was concluded that the design tool is not applicable. The reasons hereto are the following:

- B1 demonstrator: The heating channel configuration is already optimised. For a thermomechanical TO to further optimise the heating channel configuration, the scientific approach needs to be extended towards including the convective influence of an external surface that changes during the design cycles. Yet, although this implementation, might deliver an improved design with vein-like heating channels, the printability of the design might be challenging.
- B3 demonstrator: The current design is a modular design that is based on a conventional approach. To harvest the full potential of the design tool, the current modular design approach would have to be reconsidered. The design tool could offer a multi-material design optimisation for the whole design. The biggest challenge for this demonstrator is the small cycle time of the thermomechanical loading, which requires a proper transient FE analysis. This is a time-intensive process and increases the required time effort for the TO substantially.

6.2. Guidelines

To successfully apply the design tool, it is recommended to follow our guidelines. For the sake of completeness (and future outlook), we assume that for the scientific approach, the influence of changing convection due to a changing external surface has been successfully implemented.

6.2.1. Step 0 – Availability of an FE software suite

The requirements for the design tool are the availability of an FE software suite. Only If a reliable FE programme is available, the design tool can be used.

6.2.2. Step 1 – analysis of the operational the loads

As a first step, it is important to analyse the operational loads that are relevant for the functionality of the product. What type of loads are applied? Thermal loads, mechanical loads, or a combination of both? And how are they applied? Are there other influences such as heat convection to be considered?

For the later setup of the FE model, it is important to reflect the reality as close as possible.

6.2.3. Step 2 – analysis of the geometrical constraints

Next, identify any geometrical constraints that need to be imposed. Are there any parts of the product that are important for the functionality and shall not be modified? Are there limitations on the overall shape and design of the product?



6.2.4. Step 3 – preparation of the CAD model

Following the identified geometrical constraints, create a CAD model that allows for a sufficiently large, global design space. Note that the later Topology Optimisation will only remove redundant material from this initial design; no material will be added where it has not been defined.

6.2.5. Step 4 – preparation of the FE model

To set up the FE model, fist the materials properties need to be defined according to the potentially presented multi-material combination that will be optimised for. Then, the model needs to be meshed with suitable elements (recommended are linear hexagonal elements). An element size should be chosen that is small enough to ensure a high design resolution of the TO in line with the possible/intended intricacy of the design details (as AM is capable of).

6.2.6. Step 5 – setup of the Topology Optimisation

To set up the Topology Optimisation, define first the objective function – e.g., minimisation of the thermomechanical compliance of the structure. Then, choose a desirable volume reduction. Lastly, freeze any region within the design that shall remain unaltered throughout the Topology Optimisation.

Execute the Topology Optimisation.

6.2.7. Step 6 – Analysis of the optimised design

To ensure that the Topology Optimisation has delivered reliable results, it is important to analyse the optimised design. Are the thermomechanical stresses within the required limits (e.g., below the yield point)?

Subsequently, determine a suitable AM printing setup for the generated design. 1) What is the base for printing the design? 2) What is the printing direction?

6.2.8. Step 7 – repeated Topology Optimisation(s)

Based on the gained knowledge, update the FE model, and repeat steps 5 and 6: Incorporate in Step 5 the overhang constraints to ensure printability of the design. Use varying volume reductions until a desirable, optimised design is achieved.

6.2.9. Step 8 – post-processing

After the optimised design has been generated, a post-processing step is needed. Here, any closed cavities need to be either removed or opened to prevent air-expansion related cracking during heat application. Also, the overall design needs to be smoothened to remove sharp edges which cannot be printed with AM. This step should be executed in collaboration with an AM expert.



7. Conclusions

In this deliverable report we have introduced Topology Optimisation as a design tool for the generation of AM-adequate multi-material designs. The suitability of the design tool was successfully presented for two different use-cases: 1) a mould for the production of composite parts, and 2) for the B2 demonstrator, a mandrel which is an integral part of a larger mould assembly for the production on composite components.

What concerns the design tool itself, we want to reiterate at this point two aspects. 1) Current, commercially available software suites, such as Abaqus Tosca, are incapable of both, multi-material Topology optimisation and thermomechanical Topology optimisation. To overcome these limitations, new developments are required, such as have been performed in this project. 2) The developed Topology Optimisation methodology is (at the present moment) limited for what concerns the influence of heat convection – i.e., as the Topology Optimisation may change the product's external surface during the design cycles, which in turn changes the heat convection. Although, this has not been implemented yet, adequate extensions are foreseen to be carried out in future projects.

As a closing statement for this deliverable report, we want to mention one important aspect, which the Grade2XL project has vividly demonstrated. It is the need of a strong collaboration between the FE expert, who executes the design tool, the end-user, who defines all the product requirements, and the AM expert, who setting up the printing process of the product. They all need to work together to ensure a highly optimised product design. Only then, the maximum benefits AM has to offer can be reaped.



8. References

- [1] ABAQUS, Analysis User's Manual. Version 2019, Dassault Systemes Simulia, Inc., 2019.
- [2] T. Dinh, S. Hedayatrasa, F. Bormann, M. Bosman and W. Van Paepegem, "A smooth single-variable-based interpolation function for multi-material topology optimization," *Engineering with Computers*, 2024.
- [3] M. Yakout, M. Elbestawi, S. Veldhuis and S. Nangle-Smith, "Influence of thermal properties on residual stresses in SLM of aerospace alloys," *Rapid Prototyping Journal*, vol. 26, no. 1, pp. 213-222, 2020.
- [4] A. Sood, J. Schimmel, V. Ferreira, M. Bosman, C. Goulas, V. Popovich and M. Hermans, "Directed energy deposition of Invar 36 alloy using cold wire pulsed gas tungsten arc welding: Effect of heat input on the microstructure and functional behaviour," *Journal of Materials Research and Technology*, vol. 25, pp. 6183-6197, 2023.
- [5] P. Kosky, R. Balmer, W. Keat and G. Wise, "Chapter 12 Mechanical Engineering," in *Exploring Engineering (Third Edition)*, Academic Press, 2013, pp. 259-281.
- [6] National Bureau of Standards, United States, Invar and Related Nickel Steels, U.S. Government Printing Office, 1923.
- [7] W. McCain and et al., "Mechanical and Physical Properties of Invar and Invar-type Alloys," Battelle Memorial Institute, Columbus, Ohio, 1965.
- [8] S. H. Committee, "Low-Expansion Alloys," in *Properties and Selection: Nonferrous Alloys and Special-Purpose Materials*, ASM International, 1990, pp. 889-896.

