Numerical Structural Design and Optimization of Free-Form Hydrogen Vessels in the Context of Metal-Organic Frameworks

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Abstract

Development regarding storage solutions for hydrogen is crucial to enable its widespread adoption as a sustainable energy carrier especially in the mobility and transportation sector. The application of Metal-Organic Frameworks in carbon fiber composite wound pressure vessels leads to a reduction in operating pressures and allow both a cost and CO2 footprint reduction by enabling glass fiber as a valid material choice and the exploration of free form tank designs in order to better utilize challenging design spaces in automotive vehicles. This study explores the capabilities and limitations of these tank designs using numerical multi stage optimization in LS-OPT in conjunction with LS-DYNA, BETA CAE, MATLAB and Python for the fully automated, detailed optimization of the geometry and laminate of these tanks. Encountered challenges regarding the automated creation and partitioning of design spaces and ideas for computational effective optimization by reduction of design variables are discussed. Furthermore, optimization strategies for the sizing of the composite laminate for different geometries and in compliance with required load cases are explored. Constraints by the winding manufacturing process are addressed by the development of different numerical methods for the calculation of geodesic winding paths. Some applied simplifications and methods are discussed and potential solutions provided. The results of this research confirm the functionality and modularity of the created software tool and show potential for improved design space usage for free from hydrogen tanks especially for geometrically complex design spaces.

1 Introduction

The current climate crisis accelerates the development of alternative climate neutral personal and industrial transportation options. The wide spread application of hydrogen powered cars and trucks can provide a carbon emission free approach. One of the big challenges of hydrogen powered mobility is the economic, safe and user-friendly storage of hydrogen. A new approach for hydrogen storage is the usage of Metal-Organic Frameworks [1,2]. MOFs are highly porous chemical compounds with large internal surface areas. They can be used amongst other applications to store hydrogen gas via adsorption. They promise the storage of similar amounts of hydrogen at ambient temperatures and lower pressures (60-120bars) [1] compared to conventional compressed gas storage solutions (typically 700 bars for compressed hydrogen gas). The resulting margins from the tenfold reduction in operating pressures can further benefit this storage method by either changing the tank material to a much cheaper and economical material or a better utilization of limited available space with alternative free form tanks for mobile applications in the public transportation sector. Complex tank designs can provide needed hydrogen storage volume for retrofitting of existing car design by replacing existing components of combustion engines in their challenging geometric environment.
Modern hydrogen pressure vessels are typically made of a non-permeable liner and a carbon fiber composite structural tank. Common manufacturing processes are the wet winding of rovings, which are wound onto a core material. [3]. This manufacturing process can provide necessary boundary conditions for an optimization while representing current manufacturing standards.
The possibilities of free form hydrogen tanks shall be numerically explored by optimizing the geometry of the tank designs and providing possible laminates in an automated optimization process. The feasibility of such designs regarding manufacturability, economical and functional factors shall be neglected. The study introduces the idea of free form optimization and provide guidance for the challenges encountered in the process while providing an example of the capabilities of the LS-OPT optimization tool.

2 Geometry Optimization

The free form tank optimization tool (FFTO) tool is designed with an emphasis on modularity and extendibility. LS-OPT as a platform both provides a solid foundation for the setup, communication and mathematical optimization methods for this task. The coupling with the LS-DYNA solver, programming languages and pre-processors promotes exploration of new optimization task such as this application.
It is clear that the target function of any free form tank optimization is never highest specific tank volume. Any deviation from a spherical, cylindrical or toroid shape inevitably increases weight and decreases specific tank volume. The target function therefore needs to be either the maximum tank volume for a limited design space or some volume increase at a cost of a maximum allowable weight increase. This is consistent with the use of MOFs which also do not aim to decrease the overall storage system weight but instead change functionality and environmental behavior of the pressure vessels system.

Figure 1 displays an exemplary input design space and the resulting optimized free form tank geometry with feasible laminate. In order to provide maximum freedom for possible design spaces the input requirements have been reduced to a design space that can be described by linear connected points that are grouped in multiple 2-dimensional planes parallel to each other and points need to be in clockwise order inside the planes. The extraction of these points from an arbitrary design space is currently a manual process.

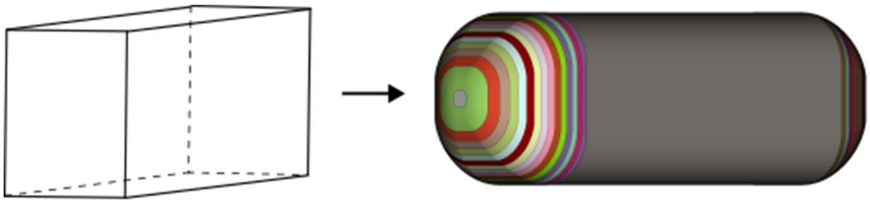

Fig.1: Concept of free form tank geometry creation

Figure 2 shows the overall workflow of the optimization, inputs, communications between stages and the output. The FFTO tool generates potential tank candidates that fit this design space or multiple sub spaces and determines a feasible laminate for each candidate. Geometry and laminate optimization are separated into two nested LS-OPT loops. In detail a MATLAB stage handles the processing of the input points, provides consistency checks, divides into subspaces and calculates geometry defining splines depending on the input settings and geometry variables. These variables can be adjusted by the optimizer and describe the shape of ellipses located at each corner of the design spaces, the geometry of the dome and other parameter describing the 3-dimensional shape of the tank. Tangency is always ensured between individual curve segments.

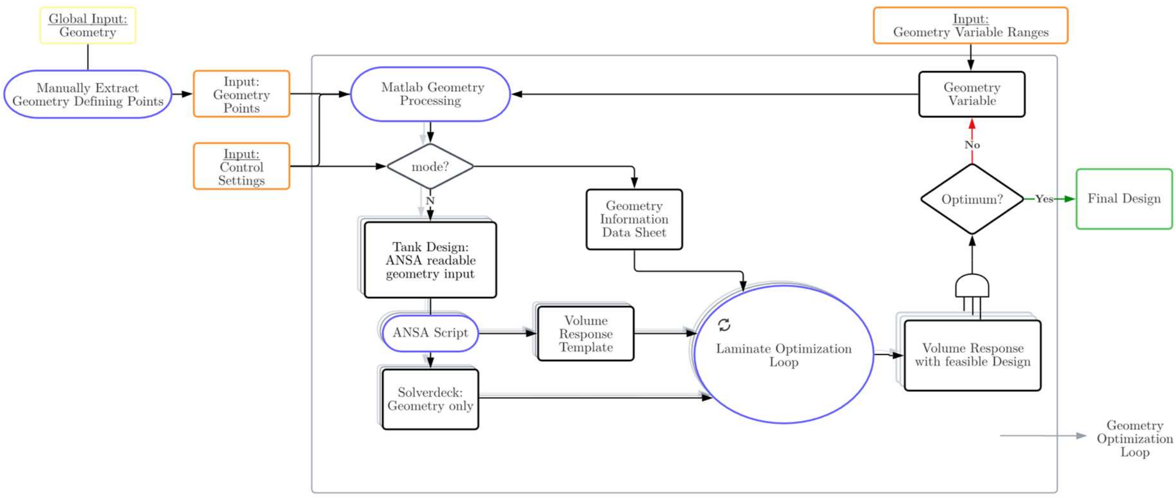

Fig.2: Workflow of the optimization loop

The splines are exported in a file and transferred to an ANSA (BETA CAE) stage. It shall be noted that the functionality of the MATLAB stage could be implemented in the Python/ANSA scripting interface. Nevertheless, it underlines the potential and beauty of the LS-OPT tool which allows for personal preference and mixing of individually powerful tools. The ANSA stage translates the information into curves and surfaces, which are meshed with shell elements and property IDs applied according to a predefined scheme and exports the LS-DYNA solver file. A template for the internal volume is created in this stage for different shell thicknesses with the ANSA tank tool. For each tank design the data is send to a nested laminate optimization LS-OPT stage.

Figure 3 provides an example for a function responsible for the geometry creation. For each of the parallel planes containing the input points a cross section is created. Since only points in clockwise order are required as an input interior angle greater than 180° need to be flagged and treated separately. For these reflex angles the corner point has to be adjusted to ensure compliance with design space borders after radius creation. After that the geometry features of all remaining corners can be generated ensuring tangency constraints between features. Logic check filter for mathematically unambiguous solutions for the tangency constraint and depending on user settings different actions are applied. Adjacent corner features that overlap each other can either result in joined curve features, a reduction in the value of the variables describing the features or, if reoccurring over multiple iterations, the creation of a singular maximum sized ellipse tank. The process is repeated for all planes and further functions treat the creation of the tank domes and auxiliary lines connecting the individual planes in the 3-dimensional space.

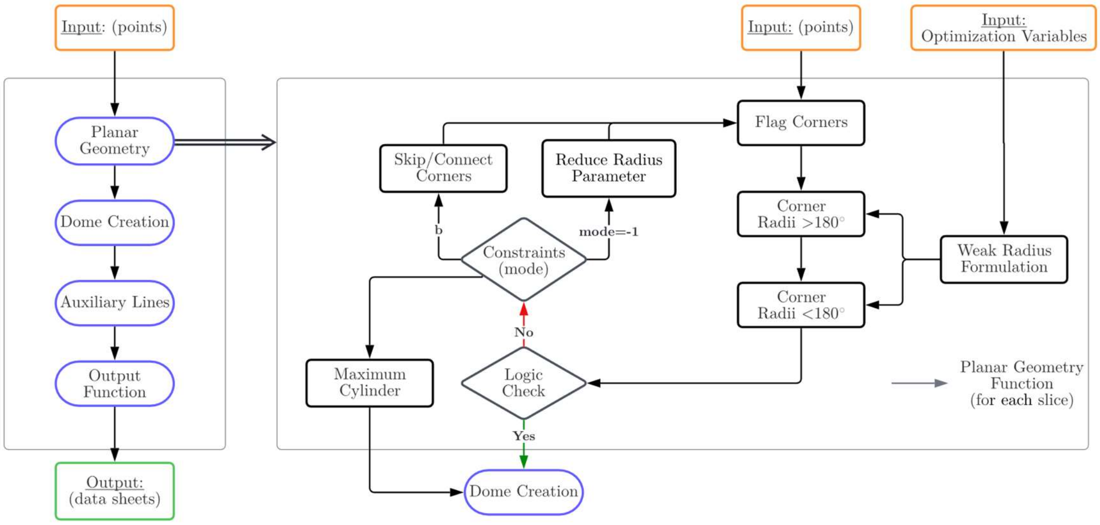

Fig.3: Schematic overview of a main function of the geometry creation code in MATLAB

3 Laminate Optimization

The laminate is optimized using a metamodel approach with variation of the laminate variable ply thickness and ply angle for multiple plies. This approach is useful in the context of the winding manufacturing method. Usually any given stress tensor of an element has one defined optimal ABD stiffness matrix. This matrix can be approximated using different combinations of plies. Considering the limitations of the chosen manufacturing method the selection of different laminates for each element is not possible since plies are wound onto the tank specimen in continuous roving resulting in one uniform coat per winding angle.

The nested LS-OPT laminate optimization takes the generated tank geometries and optimizes a feasible laminate for each design. The feasibility assessment follows an abbreviated loading requirement of the UN ECE R134 standard [4], which applies to hydrogen pressure vessels for automotive applications.It includes static minimum burst pressures of 2.25 times the normal operating pressure, fatigue tests, impact and tests at chemical and hot/wet environments. Other functional requirements can include a stiffness requirement in such way that the deformed tank at normal operating pressure complies with the design space borders. For a first approach it is reasonable to start with a simple burst pressure evaluation. Fiber failure is calculated according to the Puck failure criterion [7] with ***MAT_ENHANCED_COMPOSITE_DAMAGE**. Inter fiber failure is neglected due to a complex post initial damage behavior that cannot be displayed accurately in a linear implicit analysis of shell elements and would lead to conservative results. A follow up on different load cases and a more detailed analysis of inter fiber failure or impact is planned and the modularity of the developed code encourages these improvements.

Laminate and geometry optimization need to be coupled since the thickness of the laminate impacts the internal storage volume. The shell geometry describes the maximum allowable tank size and any shell thickness is applied inwards using the NLOC=1 option for **`*PART_COMPOSITE`**.

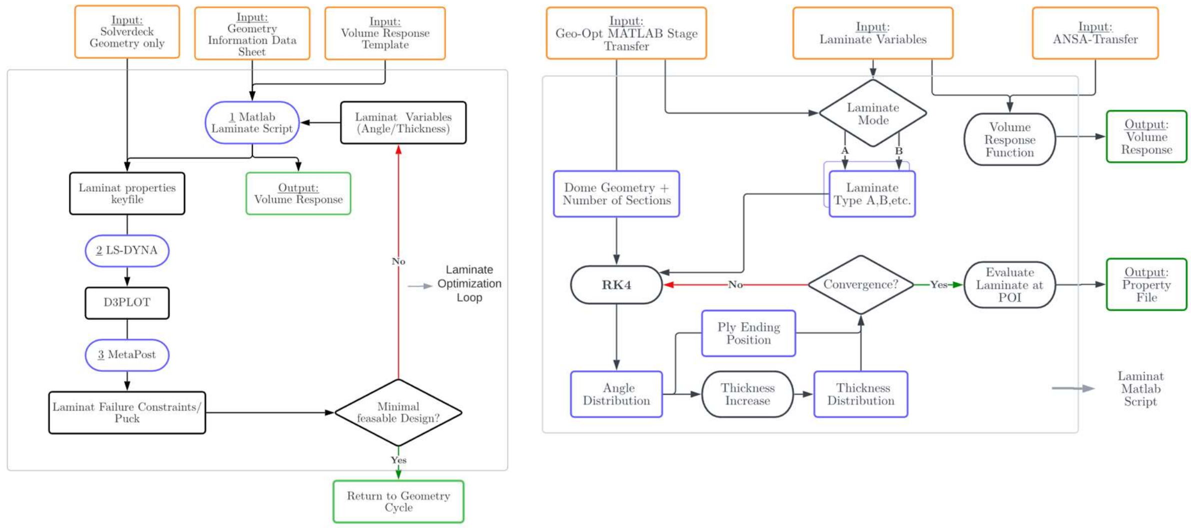

Fig.4: Workflow of the inner laminate optimization loop (left) and workflow of the MATLAB stage (right)

Figure 4 provides an overview of the laminate optimization loop and the MATLAB stage in detail. Inputs are automatically provided by the outer LS-OPT loop. The MATLAB stage translates the optimizer variables consisting of ply angles and thicknesses into a laminate that complies with manufacturing constraints such as geodesic winding over the dome area. Properties are created as an include and send to the LS-DYNA solver stage. A META (BETA CAE) stage handles post processing. Direct extraction of history variables is not possible for the selected choice of material since the information is saved as a bitflag instead of quantitative information which is preferred for metamodel creation. Iterative changes driven by the LS-OPT optimizer are made until a feasible laminate with minimum thickness is achieved. The nested loop returns volume, constraint responses and the laminate for the current design to the outer optimization loop.

Figure 4 shows the mentioned MATLAB stage on the right in more detail. The laminate variables are translated according to a predefined mode into the actual laminate that conforms to the limitations of the winding manufacturing process. This mainly refers to the discrete modelling of a single filament wound layer into two separate numerical plies with half thickness and opposing angle signs. Other adjustments such as compacting hoop (90°) plies between helical (15°-75°) plies can be automatically implemented. For deterministic reasons it is implied that any ply follows geodesic winding [5,6] constraints. Geodesic winding refers to the concept of winding a carbon fiber roving on the shortest path between two points on a curved surface. On this path the pretensioned roving only experiences forces in tension and normal to the surface of the tank. Deviations from this geodesic winding path are possible and can be compensated by friction forces counteracting the tangential forces on the roving which can lead to slippage and manufacturing defects. While this can be used to orient the anisotropic properties of the fiber to match the major axis of the stress tensor for individual areas and therefore reduce material required it also introduces strong dependency on material data calibration and difficult to handle optimization challenges. Namely ensuring continuous paths of fibers after modification of local areas especially for tanks without rotational symmetry where changes in individual roving lead to overlap and wholes in other areas. Geodesic winding paths can be calculated by solving the Clairaut differential equation [6]. Assuming rotational symmetry with an average diameter per cross section simplifies this equation and provides an unambiguous solution for all wound tank designs. The impacts of this simplification on the relevance of the solution and general implications and requirements for the manufacturability of such tank designs shall be noted and discussed at some other point in time. Geodesic winding is also preferred because it translates to a single base laminate for the whole tank that only changes with the geometry which is provided to this stage as a formatted transfer file.

The MATLAB script now calculates the average radius of cross sections and generates laminate properties according to the Clairaut equation. The calculation starts at the greatest radius to ensure at least a singular even coverage per ply at any point of the tank. With decreasing radius any ply angle converges towards 90°. In this process adjacent roving start to overlap increasingly. Helical plies can end prematurely before covering the whole tank. Ending plies change the effective geometry and

therefore according to Clairaut ply angles. Both effects (overlap and angle change) are most notably on the dome.
The Clairaut equation can be solved numerically using for example a standard Runge-Kutta method. Due to the discussed effects iterative adjustments have to be calculated until convergence is reached. The calculated winding angles are extracted at defined points of interest and converted to properties. Properties are exported as a solver deck include.

Both geometry solver deck and property includes are solved using LS-DYNA in a linear implicit analysis. It shall be noted that the simplifications of a linear analysis of a complex non-linear behavior in a carbon fiber composite pressure vessel especially close to and post damage initialization impose inaccuracies for the gathered results. Nevertheless, this type of simplification suites the premise of a rapid exploration of potential future tank designs.

4 Parametrization of Complex 3-Dimensional Spaces

For an efficient optimization of the described problem it is essential to keep the number of optimization variables in check. A trivial first step for this task is the usage of nested optimization loops to separate the geometry and laminate problems and respective variables.
The geometry description of an arbitrary tank design can ask for a large number of variables. It would be reasonable to use at least one variable to describe the radius of each edge of the design space. More variables would be needed to describe more complex features such as ellipses or splines. For the geometry description of the free form tanks a method is applied to drastically reduce the number of variables needed. A correlation between the radius of edges of a tank and the resulting stress concentration is assumed. In the premise of balancing stress concentrations to an equal level over the geometry of the tank each edge of the tank can be indirectly described by a distance and angle forming a radius. The distance can now be scaled with a function of the angle of the respective design space corner. The method could be described as a weak formulation for the radius (see figure 5a).

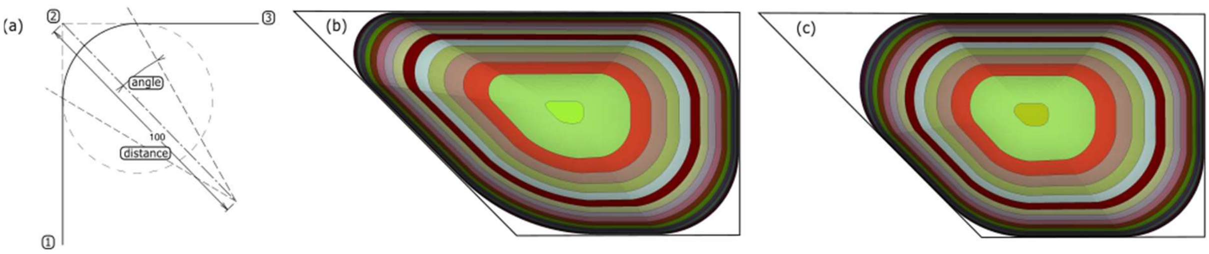

Fig.5: Weak radius formulation (a), exemplary tank with unscaled method (b), exemplary tank for an optimized scale for the weak radius formulation (c)

The function for scaling this weak radius formulation can now be optimizing to represent pressure vessel designs with an even stress distribution. Figure 5 shows the scaling effect. Stress concentrations at acute angle are avoided by increasing the radius while radii at obtuse corners can be reduced.
This method in combination with similar ones allows the generation of free form tanks based on only four variables. The weak radius angle, a parameter describing the shape of the dome, and two variables relevant for the shape of the connection between the shown 2-dimensional planar section in the 3-dimensional space. Subsequently the computational effort for exploring many possible designs has been drastically reduced.

5 Rule-based Subdivision of Design Spaces

In the premise of fully automated exploration of freeform tanks the option of dividing the initial design space into more suited subregions has to be addressed. Tests show potential performance gains with multiple smaller tanks compared to the initial design space with increased spatial complexity and sharp concave corners. This functionality is also required for an automated performance comparison of new tank designs to conventional solutions with multiple cylindrical tanks. While a manual splitting approach is certainly an option, an automated rule-based division and exploration is far more elegant and if implemented correctly provides an unbiased treatment of all options.

The challenge of this problem lies in amount of possible solutions and the numerical parametrization of valid options that in return can be optimized towards a global optimum. For preliminary exploration of tank designs it is reasonable to drastically reduce the number of options with such an algorithm. The practical procedure chosen here generates options based on rules and parameters and evaluates the options according to criteria. Criteria determine a point score for subregion pairs and ranks the options accordingly. A user defined number of top ranking options is then further evaluated according to the methods describes in chapter 2&3. The optimal solution is selected based on the target function disregarding the point score used for the preliminary evaluation of these options.

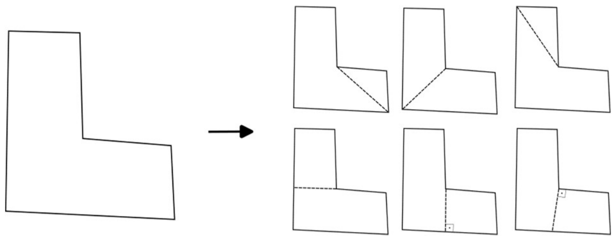

Fig.6: Incomplete, 2-dimensional example for rule-based options generation of a concave design space in L-shape.

The criteria formulated include:

- *criterion of sums of internal angles:*
  prioritizes designs with mainly obtuse interior angles over those with acute interior angles with a weighted function, sub-designs with concave corners are further penalized
- *criterion of relative size:*
  large discrepancies in tank pair sizes are penalized compared to more equal sizes
- *criterion of aspect ratio:*penalizes larger aspect ratios over more moderate ones

Both generation rules and criteria are inherently biased and need to be verified by both numerical and experimental tests. The point system provides the ability to adjust the division algorithm to validate results. The problem seems to be suited for machine learning approaches to generate data and adjust the weighted scoring systems to increase accuracy of solutions.

6 Convergence Issues for the Laminate Optimization

The optimization method described here initially proofed slow or no convergence towards an optimum. This behaviour and some improvements made to achieve better results shall be discussed.
The expected behaviour of moderately complex design spaces and their tanks without subdivision is a minimum laminate thickness for the biggest cylindrical tank possible with the smallest usage of the total volume of the design space. From there the wall thickness increases with any deviation from the cylinder and subsequent increase in total design space occupied by the tank until some optimum of the internal tank volume is reached. Additional changes to the geometry lead to an over proportional increase in laminate thickness to compensate for stress concentrations which in return leads to a decrease in the target function. Although this problem seems to be best described with a polynomial meta model second order inside the LS-OPT environment, tests show slow convergence for this metamodel approach. Other optimization strategies have been tested and also show slow convergence or entrapment in local optima. Potential reasons for this behaviour have been identified to be the following:

- Multiple implementation choices contribute to a complex correlation between stress responses and the laminate variables. The reduction in laminate defining variables and the subsequent creation of the laminate properties methods especially for the dome lead to a decoupling of laminate variables and resulting responses for the optimizer. This effect is amplified by the evaluation points of geodesic winding. Due to the convergence of ply angle towards 90° over the dome, a slight change in the ply angle variable can potentially impact the ply thickness massively in the evaluation points. This leads to both an uneven response surface for the applied composite failure criteria and local optima for the overall problem that does not represent actual material/ manufacturing behaviour. Furthermore, the pleasant simplification for the user of evaluating only maximum Puck efforts of all layers limits the options for the optimizer to match changes in optimization parameters and responses. Additionally, some numerical smoothing is required to filter either distorted elements or elements close to shell thickness and therefore stiffness discontinuities. While this prevents too

conservative results from singular bad elements it further increases the issue of parameter response correlation.
In order to achieve a reasonable convergence rate some improvements have been implemented. These include a layer-based response evaluation and revisiting numerical smoothing from a percentage threshold to a more complex outlier-based approach. Both changes did increase the likelihood of convergence at faster rates.

- The choice of shell elements for the laminate optimization is natural since fast iterative changes to the laminate properties can be made without changes the geometry of the simulation. For the application of free from tanks this simplification reaches limitations especially in the important area of the dome. Laminate defining bending stresses and interactions at ply ending cannot be modelled. While ANSA and other pre-processors provide functionality to convert laminated shell elements to solids their usefulness proofed limited for this application in regards to the implementation of correct material angles (Changing from AOPT definition in **`*PART_COMPOSITE`** to material axes per element with **`*SOLID_ORTHO`**) and the correct treatment of discontinuities of shell thicknesses and number of plies in the parent and adjacent shell elements. A custom solution via a Python script can provides required freedom in the treatment of these exceptions and directly change the solver deck into the new element formulation. First tests show significant improvements of both stability and accuracy of results compared to initial approaches at a significant cost of performance.
- The preliminary method of calculating the internal volume response was based on interpolating from a template created in the geometry optimization loop via the ANSA tank tool for possible laminate thicknesses. This method allows the calculation of the volume response without costly calling of the ANSA tool for every single laminate iteration. While it allows for a significant reduction in run time it also introduces inaccuracies. Combined with using solid elements the internal volume can be directly calculated in the process of solid element generation using basic geometric methods. Tests with the more accurate determination of the volume show discrepancies between methods of up to 2% depending on the complexity of tanks.

7 Results

Different exemplary tanks created by the optimization tool can be seen in figure 7. The features are exaggerated.

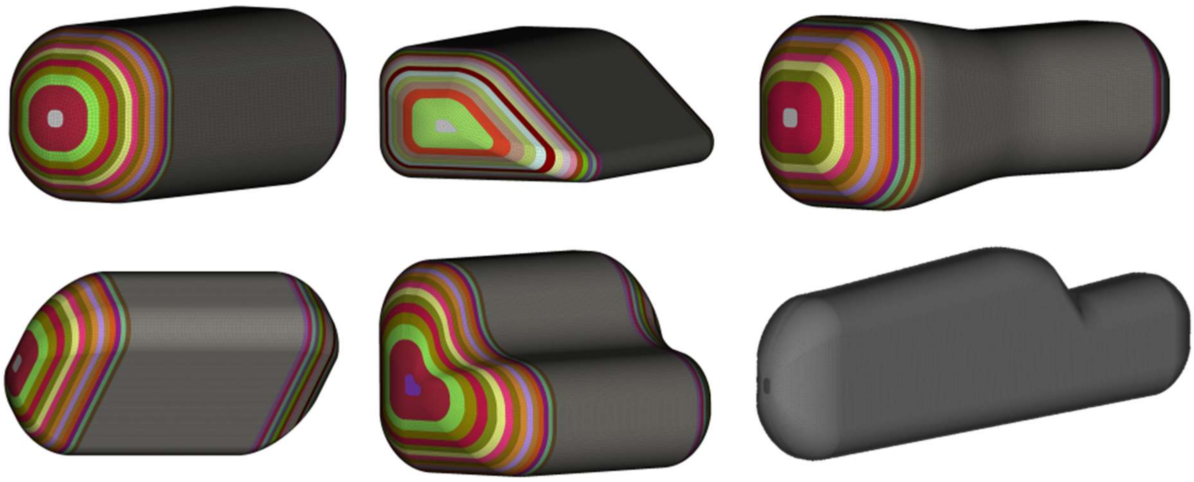

Fig.7: Demonstration of the potential to display different pressure vessel designs

Initial tests indicate the potential of these types of free form tanks to better utilize limited design spaces for the storage of hydrogen. The internal volume of these tanks show small performance increases for design spaces suited for cylindrical tanks of 5-10%. For more challenging design spaces the storage volume of these tanks can be increased by more than 50% compared to the placement of conventional cylindrical tanks.
It is important to note that the analysis performed is solely based on numerical exploration and does not reflect considerations for manufacturability, complexity and development effort required or other important factors.

8 Summary

The study presents a free form hydrogen pressure vessel optimization approach. Focus on modularity and extendibility in combination with the powerful software tool LS-OPT provide the user with an option to explore the potential of alternate tank designs. Challenges and key features are described and provide a basis for future advancements on this topic.

Initial results indicate a gain in usable hydrogen storage volumes compared to conventional tank designs at the cost of increased weight. In combination with Metal-Organic Frameworks these hydrogen storage solutions can provide substantial benefits regarding operational considerations and for applications with limited physical space.

9 Acknowledgement

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10 Literature

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