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Highlights

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- Development of a parametric, integrated simulation tool.
- Predictive Capability Maturity Model used to communicate the status of the simulation tool.
- Applications of simulation tool to the STEP Breeder Blanket Preconceptual Design Process.

Integrated Simulation for the Preconceptual Optioneering of the STEP Breeder Blanket Design

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ABSTRACT

The UK Spherical Tokamak for Energy Production (STEP) program is currently progressing the conceptual engineering design of a Spherical Tokamak-based fusion reactor. The program includes a project concerned with design of the reactor breeding blanket. The objective of this work was to develop a low fidelity, integrated simulation approach to support preconceptual optioneering and exploration of the breeder blanket technologies design space. This simulation approach allowed for parameter sweeps of different Tokamak design points to take place by varying key inputs. The objective of the simulation approach to enable designers to assess the impact of these parameters on blanket performance.

This research resulted in development of a workflow internally within the project team and externally through a design service contract. A variety of tools were integrated into a modelling framework including a bill of materials-like object orientated data structure, open-source tokamak neutronics workflow, and parametric blanket geometry tools capable of outputting material volume fractions and flow layouts. The research concluded with results produced from the integrated simulation feeding into a wider qualitative assessment of blanket technologies for chosen Tokamak design points and with further development of the workflow.

1. Introduction

The Breeder Blanket is a key technology within the fusion community that has numerous challenging requirements including the production of the Tritium fuel for a Deuterium-Tritium (D-T) Plasma, the extraction of energy from that plasma, and the shielding of components. Conceptual development of breeder blanket systems has been undertaken for decades and numerous concept designs exist at different levels of maturity. Different programs have pursued radically different technologies for the breeder blanket system as highlighted by the ITER Test Breeding Module (TBM) program [1]. The variety in concept designs in the ITER TBM program, and other blanket development activities, and the breadth of technologies [2] [3] that could be used within a blanket system demonstrates the challenge a new breeder blanket design has when optioneering. It may be possible to utilise an "off the shelf" design of breeder blanket which has been developed, however, when the Tokamak specific requirements are introduced an "off the shelf" design may not conform to them or give the optimal performance.

The project within STEP concerned with reactor breeding blanket design developed a parametric assessment tool, where possible utilising open-source packages, in order to investigate the a large blanket design parameter space and assess numerous performance parameters. The parametric tool, named the Rapid Breeder Blanket Integration Tool (RaBBIT), utilised low fidelity analysis, integrated simulation workflow to investigate the performance of different technologies. RaBBIT was not intended to capture all the considerations that should be made when considering a blanket design. Instead, the results from RaBBIT were used to feed into the STEP process for concept selection. Information about RaBBIT and the assessment modules it contains, a comparison of the RaBBIT results to an EU-DEMO design point, an assessment of RaBBIT using the Predictive Capability Maturity Model (PCMM), and examples of the application of RaBBIT within the STEP design process are given within.

2. Rapid Breeder Blanket Integration Tool (RaBBIT)

The Rapid Breeder Blanket Integration Tool (RaBBIT) was developed using a variety of packages structured to operate on a Bill of Materials representation of a STEP Tokamak design point. RaBBIT contained various modules which operated on the bill of materials. The modules that provided key input to the preconceptual design process were:

- Volume Build - Calculation of the volume fractions and thermo-hydraulic approximations of components.
- Material Generation - Nuclear materials creation and material data extraction.

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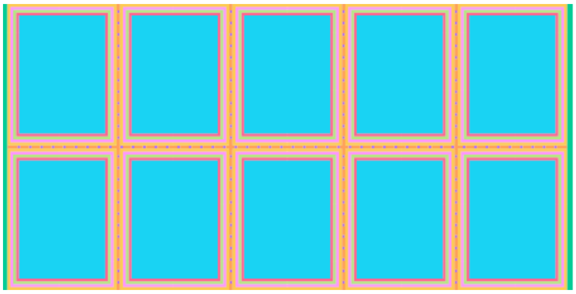

Figure 1: The parametric two-dimensional representation (with accentuated thicknesses for visualisation) of a Dual Cooled breeding zone with Sandwich Flow Channel Insert based upon the EU-DEMO DCLL [5].

- Neutronics Assessment - Calculation of heating of the system and Tritium Breeding Ratio (TBR).
- Fluids Assessment - Simplified 1D flow modeling which approximated the heat transfer coefficients (HTC) and pressure losses.
- Thermal Assessment - 1D thermal assessments of which calculated component temperatures.
- Raw Material Cost Estimate - Estimates of the raw material costs of blanket components.

2.1. Bill of Materials Analysis

At the core of RaBBIT was the representation of a Tokamak in a Bill of Materials (BOM) structure. The representation of the BOM was created using the package BOM Analysis which was created as part of this work and released to the public UKAEA Github [4]. The BOM Analysis package provided a hierarchy of materials, components, and assemblies which were operated on by different analysis packages. The Tokamak BOM was greatly simplified at the early stages of design but was capable of being expanded to include more complexity as a design matured. The motivation behind this package was to reduce the cognitive complexity of storing the data related to the Tokamak and Blanket System design.

2.2. Volume Build

The Volume Build aimed to estimate the volumes of components in the BOM for a chosen design. The analysis conducted used homogenised layers to represent the Tokamak in neutronics calculations, therefore, an estimate of the volumes of the components which the made up a homogenised volume was required. The volume calculations assumed a 2D layout extruded along a length to approximate not only the volume fractions, but information about the flow network and the layout for thermal analysis. Representations of the a Dual Cooled Design with Flow Channel Insert [5] 1, the EU-DEMO HCPB [6], and an Encapsulated Fuel Design [7] were included within RaBBIT.

2.3. Material Generation

The material data selection methods were given in the BOM Analysis package and allowed material properties to be extracted from different data sources. Additionally RaBBIT utilised an external interface to extract Temperature, Pressure, and Irradiation (where available) data from a central STEP material library. The calculation of nuclear material properties within RaBBIT took place with the open-source package Neutronics Material Maker [8], which was used to calculate the isotope composition of a homogenised body when supplied with the volume fractions from the Volume Build.

2.4. Neutronics Assessment

The neutronics assessment utilised the Paramak [9] work flow with OpenMC, DagMC, and Cubit. This workflow generated simplified geometry to represent the Tokamak in 3D using homogenised layers and with tallies for integrated heating per component, the TBR, and nuclide heating. The Parametric Plasma Source [10] was used to generate the plasma source for OpenMC with the inputs taken from an equilibrium solver. As homogenisation was used to represent complex geometry an estimation of the local heating within different components that make up the homogenised body was used. This estimate used the nuclide and photon heating heating calculated on the homogenised material and backfit the volume fractions and compositions of the sub-components to estimate the heating on these sub-components.

2.5. Fluids Assessment

A One-Dimensional fluids assessment was included based on the estimated channel dimensions, and count from the volume build and the materials parameters from the material data selection. This assessment utilised a in-house wrapper for OpenModellica with additional Tokamak relevant correlations for pressure losses. The tool approximated the HTC and change in pressure within the system alongside an approximation of the required pumping power.

2.6. Thermal Assessment

The One-Dimensional thermal assessment module took geometry calculated within the Volume Build and an thermal path, and created a resistor network assuming a linear or cylindrical layout. Boundary conditions such as an assumed first wall heat flux or the HTC calculated by the fluids assessment were then applied to the resistor network. The resistor network was then solved with the open-source Tool Thermpy1D [11] to estimate the temperatures in each of the components of the assembly.

2.7. Raw Material Cost Estimate

As the volumes of the components were calculated within RaBBIT for neutronics analysis, the masses of the materials were easily estimated. Using the mass of components, the raw material costs were modelled, including the cost of enrichment of Lithium-6. The raw material costs were highly uncertain and did not represent the full cost of the blanket system but provided a method for feeding information on competing parameters into the qualitative

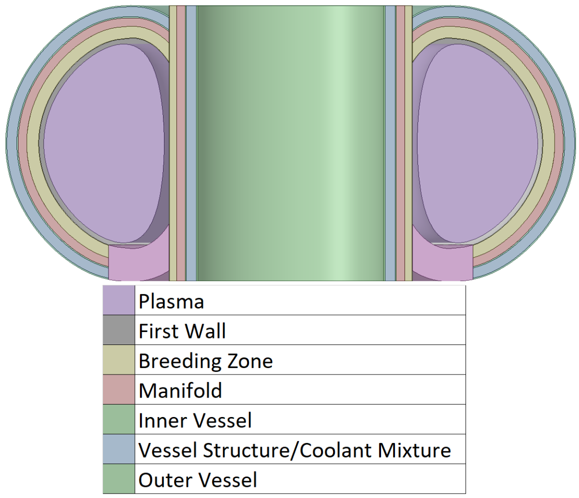

Figure 2: EU-DEMO Tokamak Representation in RaBBIT with Paramak

Table 1
Results of Comparison of RaBBIT Workflow against EU-DEMO Publication

Parameter	Ref. HCPB	Calc. HCPB	Ref. MLCB	Calc. MLCB
TBR	1.18	1.132 ± 0.000	1.15	1.138 ± 0.001
Blanket Heating (MW)	1,931	1,953 ± 1	1,646	1,648 ± 1
Vessel Heating (MW)	49	26 ± 0	77	26 ± 0
Divertor Heating (MW)	170	158 ± 0	197	184 ± 0
Total Heating (MW)	2,150	2,137 ± 1	1,920	1,858 ± 1

assessment and for investigating sensitivity to changes in material costs.

3. Comparison of RaBBIT Workflow against EU-DEMO Publication

To improve confidence in the use of RaBBIT, a comparison between the results of an EU-DEMO publication [12] to the results of a RaBBIT workflow with inputs from the publication was made.

3.1. Model Setup

The geometry of the EU-DEMO Tokamak is represented by the Layered Ball reactor in Paramak [9]. The homogenised layers were calculated using the Volume Build module of RaBBIT based on the local geometry supplied in [12].

The major components that were expected to have a significant impact the analysis were captured in the geometry shown in 2. From the plasma out, these were:

- The first wall with representative square channel first wall volume fractions 3.
- The breeding zone with representative hexagonal pin volume fractions 3.
- The manifold with a simplified two channel manifold volume fractions 3.
- A layer of stainless steel for the inner vessel structural material.
- A layer of water representing the inner vessel coolant.
- A layer of stainless steel for the outer vessel structural material.

Additionally, the divertor was included and represented by the a homogenised body with a water/Eurofer mixture.

The material and geometries of the components such as thicknesses of vessel, plasma shape, and pin spacing were taken from [12]. The following remaining parameters that were required for the RaBBIT analysis and were not included in the reference paper were:

- The gaps between the first wall and the plasma taken from the scrape off layer thicknesses given in [13].
- The plasma parameters were taken by the the parametric plasma source reference paper [14].
- The divertor radial thickness was taken as the minor radius of the plasma based on an estimate from the geometry plots given in [12].

3.2. Results of Comparison

The results of the comparison between the publication and the RaBBIT workflow are given in 3.

While an exact match between the results is unlikely due to the assumptions made within the model, the difference between the RaBBIT workflow and the higher fidelity reference analysis helps to build confidence in the applicability of the RaBBIT workflow for the pre-conceptual analysis of blanket designs. It is worth noting that [12] reported an increase in TBR of 0.02 when a homogenised first wall and breeding zone were used which has been included in 3.

4. Verification and Validation

The Predictive Capability Maturity Model (PCMM) [15] was used to assess and communicate the maturity of the analysis of a preconceptual blanket design in RaBBIT and to identify areas for improvement. The PCMM results were from a typical the blanket analysis performed using RaBBIT within the STEP design process and are given in 2 along with a discussion on the supporting evidence in this section.

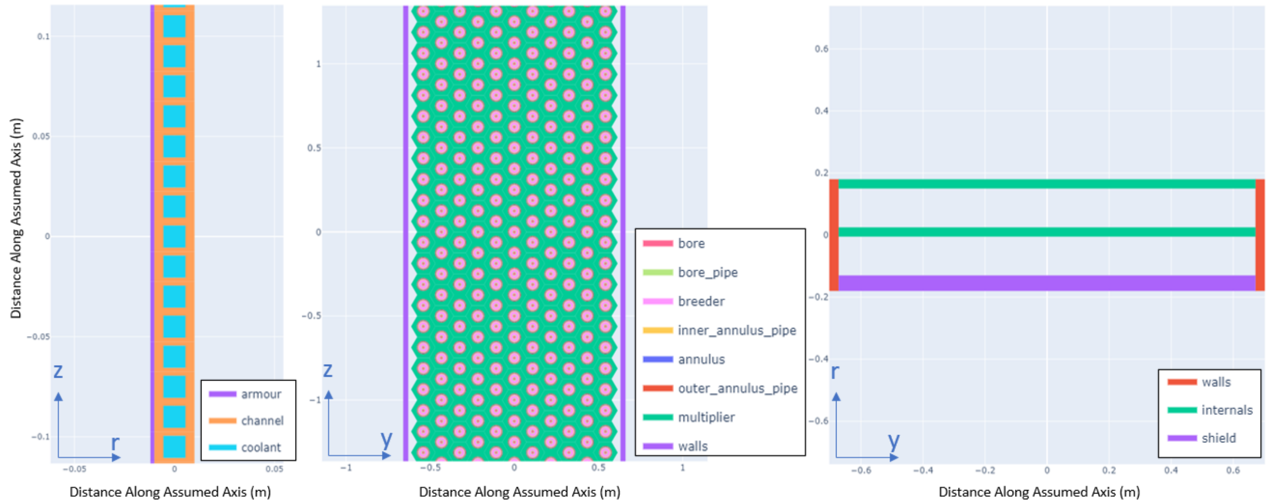

Figure 3: 2D Representations of Geometry from Volume Build. Square Channel First Wall (Left), Hexagonal Pin Breeding Zone (Centre), Two Channel Manifold (Right)

Maturity / Element	Level 0	Level 1	Level 2	Level 3
Representation and Geometric Fidelity		Assessed Required		
Physics and Material Model Fidelity		Assessed Required		
Code Verification		Assessed Required		
Solution Verification		Assessed Required		
Model Validation	Assessed Required			
Uncertainty Quantification and Sensitivity Analysis	Assessed	Required		

Table 2
PCMM Assessment of workflow used to support the STEP design with RaBBIT

4.1. Representation and Geometric Fidelity

As shown in 3, significant geometric simplifications were made when compared with more detailed parametric geometry from tools such as [16]. The geometry, however, captured the major components related to the various assessments made, the key parameters which govern the geometry, and approximated the sub-components of the blanket system.

The homogenisation of the geometry for neutronics analysis reduced the fidelity of the analysis but in doing so allowed the run time to be reduced. Within the workflow, the homogenised materials fractions were based on the Volume Build 2D geometric representation of the geometry which were then used for thermo-fluid analysis. These simplifications did not replicate the geometric fidelity of the components but did describe the major components of the system. For this reason, the Representation and Geometric Fidelity was given a Maturity Level 1.

4.2. Physics and Material Model Fidelity

One of the primary drivers for RaBBIT was the low-fidelity coupling of different physics that act within the system. Significant important physics (such as a detailed first wall heat flux model) were not captured within the system due to the level of fidelity of the analysis and a more mature design being required to capture such physics.

The major physics models which impact the performance parameters assessed using the workflow were captured with one-way and sequential coupling. The material models used for the neutronics were taken from established libraries, ENDGB-7.1-NNDC [17], which are based on experiment. The material data was taken from published data but the workflow typically applied to the STEP blanket design process did not include the change in properties with to irradiation due to lack of data. As the major physics models were coupled and the material data was based on experiment the Physics and Material Model Fidelity is given a Maturity Level 1.

4.3. Code Verification

RaBBIT was implemented and managed following formal Software Quality Engineering practices. RaBBIT used repository management software and included continuous integration for testing, deployment of documentation, static analysis of code with quality gates, and code formatting.

RaBBIT included unit and regression testing with a coverage of over 80%. Where external code were used to calculate the performance parameters assessed (such as [11]) additional tests were included within RaBBIT to check the implementation and results. The test suite also compared the results of a number of benchmarks against an expected uncertainty. For example, the areas and volumes of the CAD generated by Paramak were extracted and compared with the

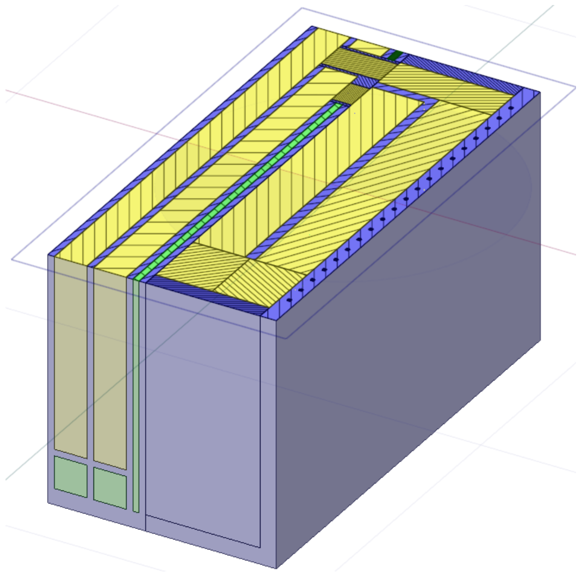

Figure 4: Parablank Representation of a Dual Cooled Blanket Design used for Comparison to volumes calculated by Volume Build module. Liquid Metal is shown in Yellow, Structural Material is shown in Blue, Gas Coolant is shown in Green.

values measured in a CAD tool and the Thermal Assessment were compared with both a 1D and 2D representation in a Finite Element Analysis model.

The majority of the RaBBIT modules did not include a formal peer review process (although the external repositories such as Paramak may), therefore, the analyses were given Code Verification Maturity Level 1.

4.4. Solution Verification

The standard deviations of the OpenMC Monte Carlo neutronics results were reported alongside the calculated values of integrated heating and TBR within the workflow. The numerical error of the different RaBBIT modules were calculated for a number of specific cases. For example, a parametric blanket heterogeneous geometry generation tool, Parablank, was used to to generate a number of different design points of higher fidelity geometry. These design points were compared to the volume predictions by the Volume Build module and an error between the methods was found (less than 20% difference in volumes). Additionally, the difference between heterogeneous and homogeneous neutronics was oerformed using Parablank, varying with with geometry and type of design. An example of the Parablank geometry that is compared with 1 is given in 4. Parablank will be the subject of future publication.

In addition, the impact of parameters such as merge and faceting tolerance within the Paramak workflow were assessed for their impact on TBR and integrated heating. The workflows applied to the STEP Blanket design utilised tolerancing parameters which the results were relatively insensitive to. As sensitivity studies of the solution and the errors associated with different modules within RaBBIT were understood the Solution Verification was given Maturity Level 1.

4.5. Model Validation

The results of the workflows were not compared with experimental data due to the lack of experiments which represent the workflow, therefore, the Model Validation was given a Maturity Level 0.

4.6. Uncertainty Quantification and Sensitivity Analysis

The majority of the results produced for the preconceptual optioneering focused on a form of sensitivity assessement, for example, investigations looked at the impact of Tokamak parameters on TBR or the sensitivity of enrichment and breeder to multiplier ratio on the cost of blanket. However, the combination of uncertainties within the analysis was not investigated. As shown in 3 the results were compared with higher fidelity models where possible to understand the uncertainty within the analysis, however, a comparison of the entire workflow to an external higher fidelity model could not be done due to lack of data.

One area of significant uncertainty that was not investigated was the changes in the nuclear material properties. While possible to include different material libraries within RaBBIT, the current workflow utilised does not account for sensitivity in material data, therefore, Uncertainty Quantification and Sensitivity Analysis was given a Maturity Level 0.

4.7. Required Maturity Level

The level of maturities required within the PCMM are dependent on the risk tolerance of the decision makers and the use of the modelling and simulation being performed. The maturity levels required for the preconceptual optioneering of the blanket system were set by the authors as the use of the data was of moderate consequence and sat between scoping studies and design support. The data produced was not intended to be the sole factor in driving design decisions and instead was used to inform wider qualitative studies. As the STEP design matures, it is expected that the required maturity level for all analysis conducted on blankets increases.

The required Maturity Level of all elements was set to 1 with the exception of Model Validation due to the lack of experimental data available.

5. Role of RaBBIT within the Preconceptual Design Process

The analysis methods within RaBBIT were low-fidelity they introduced significant uncertainty into the analysis 4. In addition to the uncertainty, numerous blanket system performance parameters were not captured by RaBBIT such as tritium recovery rate and the structural performance of different designs. The project could not investigate multiple different designs of blanket systems to the high level of fidelity required to fully understand the uncertainty introduced or assess the different performance parameters that

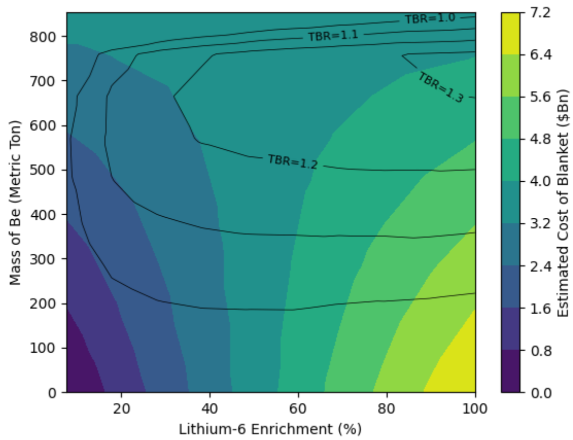

Figure 5: Variation on estimated Li and Be cost and TBR with in Li-6 Enrichment and Beryllium mass.

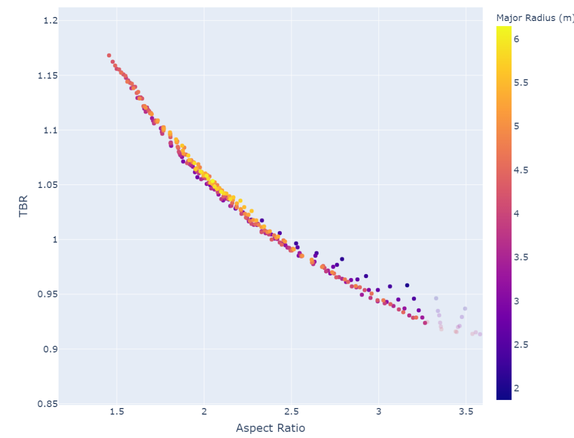

Figure 6: Relationship between TBR and Aspect Ratio for a fixed structural, breeder and multiplier content, and fixed Lithium-6 enrichment

are required to compare designs quantitatively. Instead, the analysis produced fed into qualitative assessments for the optioneering of the blanket system. The aim of qualitative assessments was to select a concept or concepts for higher-fidelity analysis. Despite the wide scope of concepts that can undergo low-fidelity assessment in RaBBIT, where data is known comparison to higher fidelity design points was included within RaBBIT as part of the testing suite 4.

6. Applications of RaBBIT within the STEP Design Process

In addition to informing the STEP optioneering process, the information produced by RaBBIT helped improve the understanding of breeder blanket systems. A selection of applications of RaBBIT used within the STEP program has been included to highlight the benefits a low-fidelity, intergrated analysis approach can bring to a program.

6.1. The Optimisation of Blanket Parameter for Raw Material Cost

In order to develop understanding of the possible relationship between fractions of breeders and multipliers, and varying Lithium-6 enrichments the costs of different design points were modelled. An example of the results of this type of analysis are given in 5 which included a thick blanket and 10 percent structural content within the breeding zone. This analysis used a linear cost-enrichment model but different relationships for Lithium-6 enrichment have been proposed [18]. The results of the analysis had a significant degree of uncertainty particularly due to the assumed material costs and, as such, the absolute values of raw material cost in 5 were not considered valuable to the design process. Instead, the value in performing this analysis at an early stage was that it highlighted the complex relationship between enrichment and multiplier content.

6.2. Investigation into the Impact of Aspect Ratio on TBR

The aspect ratio of the Tokamak is a key parameter of a design and impacts the TBR. Understanding the impact of aspect ratio on TBR was an important input to the selection of a Tokamak major and minor radius and RaBBIT was used to perform a sweep of different major and minor radii 6 for a specific blanket design. These results showed the expected relationship between the assessed parameters with variations at larger aspect ratios due to geometric artifacts.

6.3. Investigation into the Maximum Breeding Zone Structural Content for Different Technologies

At early stages in the design process, value was found in estimating the maximum structural content within the breeding zone that can achieve the TBR requirements for different enrichments, materials and fractions of materials. An example of the results for a particular Tokamak design point (aspect ratio, divertor configuration, blanket thickness etc.) is given in 7. These results were obtained from RaBBIT by running an optimisation of the enrichment with the objective of maximising the structural content of EUROFER97 in a 83Pb-17Li design. The results were then be compared to the different designs of blankets within the fusion community and against the results of different blanket technologies to inform the quantitative optioneering.

6.4. First Wall Temperature Limits

An investigation into the capability of coolants to handle different heat fluxes was conducted to inform the layout and choice of first wall coolant. This was investigated within RaBBIT by using the Fluids and Thermal assessment modules to calculate estimated flow conditions, HTC, and temperature in the first wall. The backfitting of the integrated heating onto the components which made up the homogensied first wall assessed by the neutronics allowed

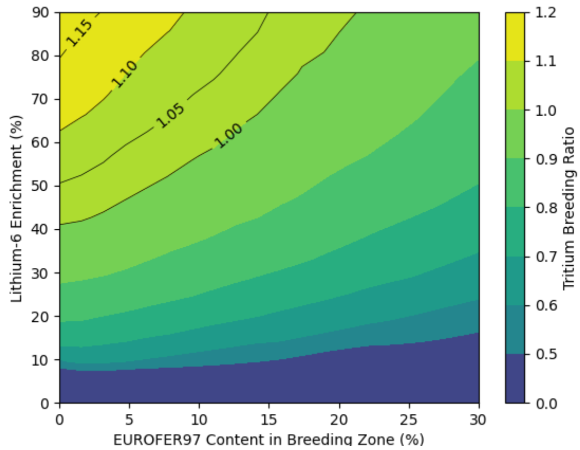

Figure 7: Relationship between the Lithium Enrichment, Structural Content, and TBR for a Tokamak Design Point using 83Pb-17Li

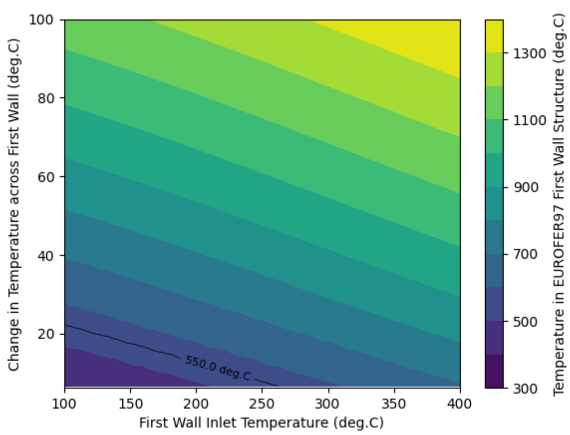

Figure 8: First Wall EUROFER97 structural material temperature variation with flow temperatures

for a better estimate of the component temperatures. For a heat flux of 1MW/m**2 first wall heat flux 8, maintaining the EUROFER97 below an assumed temperature limit was challenging for first wall geometry modelled in this sweep. This method allowed different geometries and first wall flow parameters to be investigated.

7. Conclusion

A low fidelity, integrated simulation workflow named RaBBIT was developed which supported the STEP breeder blanket system optioneering. A summary of the modules which made up RaBBIT was given which highlighted the capabilities of the workflow and, where possible, provided information about the open source tools used. A comparison of the results of a RaBBIT sweep to a EU-DEMO publication showed similar results for TBR and heating which builds confidence in RaBBIT but without more detailed information about the EU-DEMO analysis it is not possible to conclude the on an absolute difference between the approaches. The Predictive Capability Maturity Model was used to assess RaBBIT with both the scoring and justification for that scoring given within. The PCMM model was found to be a very powerful tool for communicating the status of analysis completed with RaBBIT and identifying areas to improved the predictive capability. Examples of the application of RaBBIT within the blanket optioneering approach on STEP were given in order to demonstrate the value of a low fidelity, integrated workflow at early stages of blanket design. As a blanket design progresses, the level of fidelity of tools will increase but, given the often completing requirements and desire for higher maturity levels in the PCMM model, benefits will exist in using parametric, coupled workflows, with the integration of parametric geometry tools such as Parablank and multiphysics analysis tools.

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