

Project FORTE - Nuclear Thermal Hydraulics Research & Development

Specification Supporting a UK Nuclear Thermal Hydraulic Modelling Capability





SYSTEMS AND ENGINEERING TECHNOLOGY

An introduction to Project FORTE

The Department for Business, Energy and Industrial Strategy (BEIS) has tasked Frazer-Nash Consultancy and its partner organisations to deliver the first phase of a programme of nuclear thermal hydraulics research and development.

Phase 1 of the programme comprises two parts:

- The specification and development of innovative thermal hydraulic modelling methods and tools; and
- ▶ The specification of a new United Kingdom thermal hydraulics test facility.

The work is intended to consider all future reactor technologies including Gen III+, small modular reactors and advanced reactor technologies.

Our project partners

The team is led by Frazer-Nash Consultancy and includes:













For more information, visit www.innovationfornuclear.co.uk/nuclearthermalhydraulics.html



Executive Summary

Control of 'thermal hydraulics' (encompassing all of fluid flow and heat transfer) is key to all current and future nuclear reactor designs, underpinning both reactor performance and safety. Therefore, a thorough understanding of thermal hydraulic effects, the capability to simulate them accurately and validate the prediction methodologies experimentally, is essential for efficient design and safe operation through life. This was recognised in the outputs from the Nuclear Innovation and Research Advisory Board (NIRAB) in the form of two recommendations:

- The development of a major new UK Nuclear Thermal Hydraulic Test Facility; and
- The development of new Nuclear Thermal Hydraulic Modelling techniques and tools.

These recommendations were then developed into tasks under the BEIS 'Digital Reactor Design' programme of work. This specification document (part of the deliverables for Project FORTE) is focused on the development of the UK thermal hydraulic modelling capability. The primary objectives are to:

- Specify future UK thermal hydraulic modelling R&D work that it is focused on addressing industry requirements and government objectives; and
- Identify and communicate how this R&D enables the development of UK capability in digital reactor design.

This document describes the systematic approach that has been used to progress the 'user requirements' captured in Reference 5 into a set of 34 research and development proposals. In addition to a workshop enabling UK experts to develop proposed solutions to the modelling challenges, the approach has included: exploring and defining what is meant by a nuclear thermal hydraulic modelling capability; considering the UK in an international context; and identifying the synergies with other industry sectors.

The outputs include activities focused on: developing, supporting and maximising the overarching aspects of what makes a capability successful; work to enable the use of advanced existing methods in a UK industrial context; and research to advance the state-of-the-art.

The total volume of research and development included in this specification far exceeds the total expected budget for Phase 2 of this work. It is therefore recommended that the outputs are used to 'build' a programme of work to meet a particular aim or focus; three examples are included to illustrate this process. However, two projects were universally considered to be of value regardless of future technology decisions and are therefore strongly recommended for Phase 2:

- Maximising UK Collaboration and Collective Learning aims to establish a framework for collaborative working in nuclear thermal hydraulic modelling, developing and sharing good practice and lessons learned.
- Increased Participation in Benchmarking aims to re-engage the UK in international benchmarking activities thereby promoting international collaboration and enabling improved confidence in and understanding of nuclear thermal hydraulics modelling tools.

Further recommendations include that the:

- UK should adopt the use of international tools and help to build on them, rather than re-inventing our own;
- Thermal hydraulics model development work-stream should continue to integrate, where possible, with the Virtual Engineering work-stream; and
- Availability of high performance computing to UK industry is explored and, if necessary, expanded.

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1 Introduction

1.1 Project Context

The UK Government's 2013 Nuclear Industrial Strategy described significant ambitions for the UK to grow our nuclear capability; with the key aim of becoming a preferred nation state partner of the global nuclear technology industry. To help fulfil the strategy's initial objectives, the Nuclear Innovation and Research Advisory Board (NIRAB) was established in 2014. NIRAB comprised experts from both industry and academia with the objective of advising Government on the approach to and coordination of nuclear innovation, research and development in the UK. NIRAB existed from January 2014 until December 2016, publishing annual reports and companion documents that analysed and described the civil nuclear Research and Development (R&D) landscape. In March 2016, a set of recommendations for innovation and research programmes was published (Reference 1), with the recommendations being prioritised in a subsequent, November 2016 report (Reference 2).

In October 2015, the Government set aside £250m for civil nuclear R&D activities "...to re-ignite the nuclear industry in the UK". Approximately half of that budget was to be used for activities relating to the development of specific reactors (i.e. Advanced Modular Reactors (AMRs)); the remainder was to be applied to more general civil nuclear R&D. Control of a large part of that budget was inherited by the Department for Business, Energy and Industrial Strategy (BEIS) from its antecedent, The Department of Energy and Climate Change (DECC). This funding is currently being used specifically to address NIRAB's high priority recommendations.

'Thermal hydraulics' (encompassing all of fluid flow and heat transfer) is key to all current and future nuclear reactor designs, underpinning both reactor performance and safety. A thorough understanding of thermal hydraulic phenomena and the capability to simulate them and validate the prediction methodologies experimentally, are essential for the efficient design of advanced reactors and their safe operation through life.

Historically the UK has had a strong capability in thermal hydraulic science and engineering, which was derived from and can be applied across many industries. The majority of the most successful Computational Fluid Dynamics (CFD) codes have their origins within UK research institutions, notably Harwell and Imperial College. There remains considerable UK-based expertise and impetus in the development of thermal hydraulic modelling tools and techniques to service the needs of other industries. However, the lull in activity in the UK civil nuclear industry since Sizewell B was commissioned in 1995 is also evident in nuclear thermal hydraulic research. The UK currently has no major civil nuclear thermal hydraulic test facilities and activity in modelling R&D has been constrained by the limited funding or other stimulus, from either the UK industrial base or government.

In order to begin to reverse this trend, and within the overall aim of allowing nuclear energy to play a significant role in the UK's future energy mix, two of the NIRAB recommendations relate to nuclear thermal hydraulics:

- The development of a major new UK Nuclear Thermal Hydraulic Test Facility; and
- The development of new Nuclear Thermal Hydraulic Modelling techniques and tools.

These recommendations have been developed into tasks under the BEIS 'Digital Reactor Design' programme of work. Project FORTE is Frazer-Nash's designation for the BEIS Research and Development Phase 1 project on UK nuclear thermal hydraulic engineering.

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1.2 Programme Goals

The overall aims of the four-year Nuclear Innovation Programme are:

- By 2020, establish the UK as a partner engaged in collaborative design projects for new reactors (Generation IV and SMR), building on its existing and growing design expertise;
- By 2030, maturing R&D results in deployment of new plant with significant UK design content and manufactured parts;
- By 2050, R&D has facilitated UK industry to be a significant partner in the global deployment of Gen III+, Gen IV and SMR technologies.

The specific benefits of the programme are expected to be:

- Enhanced designs, increased productivity and a step change in the way that nuclear design, development and construction programmes are delivered;
- Increased and widespread uptake of modern digital engineering practices within the UK nuclear industry;
- Improved understanding and safety of through life performance of reactor components;
- A greater predictive modelling capability and understanding of passive safety arguments;
- A highly-skilled workforce able to drive design improvements and underpin operations and regulation of future reactors; and
- Leverage to facilitate extended UK participation in associated international activities.

All of these aims and benefits cannot be met by nuclear thermal hydraulic research alone, however, all activities and outputs from this project have been considered in the light of whether they make progress towards achieving these aims as well as whether they achieve the specific project deliverables.

1.3 Report Structure and Objectives

This specification document (part of the deliverables for Project FORTE) is focused on the development of the UK thermal hydraulic modelling capability. The primary objectives are to:

- Specify future UK thermal hydraulic modelling R&D work that it is focused on addressing industry requirements and government objectives; and
- Identify and communicate how this R&D enables the development of UK capability in digital reactor design.

This work builds on previous Project Forte work to perform a critical review of the state-of-theart in nuclear thermal hydraulic modelling tools/techniques reported in Reference 6 and the user requirements gathered from stakeholder engagement activities reported in Reference 5, which are not duplicated here. The remainder of this document is structured as follows:

- Section 2 provides a definition of what is understood by a Nuclear Thermal Hydraulic Modelling Capability and its component parts;
- Section 3 describes the approach that has been taken to develop the user requirements captured in Reference 5 into research recommendations;
- Section 4 considers both relevant international programmes and current UK skills in the context of world-wide capability and activity;
- Section 5 presents identified opportunities for tools/methods from other industry sectors with the potential to add value in Nuclear Thermal Hydraulic Modelling; and
- Section 6 discusses recommendations for the way forward for nuclear thermal hydraulic modelling R&D in the UK with reference to potential R&D projects included in Annex A.

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2 A UK Thermal Hydraulics Modelling Capability

Computational modelling techniques are established as integrated processes throughout modern engineering, science and technology. They are used in a diverse range of applications to produce useful datasets, develop real-world understanding, inform design processes and facilitate organisational decision-making. Nuclear thermal hydraulic engineering is no exception, with modelling used at all stages of the planning, design and justification of nuclear facilities.

The capability to perform thermal hydraulic modelling is therefore important in enabling cost efficient and effective reactor design and operation. This section describes the concept of a nuclear thermal hydraulics modelling capability (Section 2.1), the development of the current UK capability (Sections 2.2 and 2.3) and considers the possible future requirements (Section 2.4).

2.1 Characterising "Capability"

The modelling capability considered by this report consists of the specification, coding and execution of mathematical models in order to simulate plant performance or investigate fluid flow and heat transfer in a civil nuclear context. This definition has been developed in-line with the BEIS ITT for this work, and, drawing on this, the project has been primarily focussed around the development of methods and tools, and in specifying the research that might support them. However, a 'nuclear thermal hydraulic modelling capability' must be broader than just the methods and tools employed - there are other aspects of capability that are equally important in delivering a solution that is industrially useful and acceptable to regulators.

There is significant value in taking a 'whole system' view of this capability. For example, including the enabling and supporting elements, both technical and non-technical, gives a more complete understanding of what it takes to deliver a modelling solution. Figure 1 presents the structure graphically, illustrating the features required by a UK Thermal Hydraulics Modelling Capability and how those features interrelate to enable a whole capability. In order to develop as comprehensive a picture as possible, this structure has been developed with academic and industry stakeholders and used to classify all of the research and development project proposals created (Section 6).

Presenting capability as a structured whole means that it is easy to identify where a weakness in one area may compromise the overall capability. Similarly it serves as a reminder that there is little point in conducting extensive research and development to improve an area which is limited by some other factor. Mapping the whole capability allows the demonstration of all of the ways in which a specific package of research and development enhances the UK's capability (Table 2 in Section 6).

In reference to Figure 1, experimental testing is a vital part of developing a modelling capability. Experimental data is often associated with validation and uncertainty reduction of a model in the later stages of its development, but testing is also often needed to identify phenomena, develop physical understanding and provide input data. Test data is, therefore, used throughout the development of a modelling solution, and hence, access to the facilities and the funds necessary to perform experiments is key to a successful capability.

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Design and Safety Case Development

Providing a modelling capability to facilitate the thermal hydraulic aspects of reactor design, operation and safety assurance

Personnel

Appropriately trained and experienced thermal hydraulic engineers in both research and industry environments.

Engineers with experience of reactor design and operation.

Hardware/Infrastructure

Computing hardware for the use of modelling tools.

Access to test facilities for the investigation of thermal hydraulic effects and the provision of validation data.

Modelling Methodology and Software Solution

The tools necessary to provide the thermal hydraulic information needed for relevant aspects of reactor design and safety assurance.

Concepts and Doctrine

Best practice for the use of thermal hydraulic modelling in design and safety assurance.

A clear and common understanding of the expectations of the UK regulator with regard to the thermal hydraulic information needed to support new and existing reactor design and operation.

A strategy for collaboration and interoperability.

Physical Understanding

Understanding of fundamental/generic fluid flow and heat transfer.

Understanding of the complex phenomena relevant to specific nuclear reactor designs.

Knowledge and understanding of nuclear reactor design and operation.

Physical/Empirical Mathematical Models

High fidelity physical and empirical mathematical models (typically, for CFD) to simulate thermal hydraulic phenomena or combinations of phenomena.

Low fidelity models/correlations (typically for system/sub-channel codes) for process/components predictions

Numerical methods to enable accurate, efficient & stable computational solutions.

Mathematical methods to enable automation of aspects of model build and

solution.

Modelling Tools

Tools to provide thermal hydraulic information to support reactor design including both overall performance and detailed component optimisation.

Tools to provide thermal hydraulic information suitable for providing supporting evidence for the assurance of nuclear safety.

Tools to enable automation of model build/set-up.

Thermal hydraulic modules for reactor simulators.

Platforms for physical/mathematical model research and testing and validation.

Tools for the visualisation and communication of results.

Inputs

Material properties data.

Design specific geometry and performance data.

Environmental conditions.

Data for the development of empirical mathematical models.

Development of required outputs (incl. accuracy); i.e. a clear understanding of the question you are trying to answer.

Verification and Validation

Clear methodology for reducing the risk of unforeseen error in modelling, including uncertainty quantification

Access to existing validation

Access to test facilities to generate new validation data.

Advanced simulations (DNS/LES) to provide validation for lower fidelity models.

Thermal Hydraulic Modelling Capability

<u>Digital Reactor Simulation</u> <u>Platform (WP1)</u>

Economic and Cost Models

Integrated Design and Analysis Tools

Integrated Engineering Solutions

Multiphysics Models

Safety Case Methodology

Figure 1: UK Thermal Hydraulic Modelling Capability

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2.2 The Evolution of the UK Capability

The current UK civil nuclear power generation capability comprises 14 AGRs (Advanced Gascooled Reactors) and 1 PWR (Pressurised Water Reactor). These reactors were designed and built from the 1960s to early 1990s, building on continuous reactor research, design and operation stretching back to the 1940s. Activity in UK civil nuclear reactor design largely stopped after the completion of Sizewell B and the cancellation of the Dounreay fast reactor programme¹. From that time (until 2013), the UK civil nuclear industry has been focused on reactor operation, plant life extension, decommissioning and waste management, and research focus shifted toward nuclear fusion as a promising longer term prospect for power generation.

Without a civil nuclear fission reactor design and development programme, there was little incentive for innovation in the UK's capability. The level and type of analysis work that is needed to support operation is not the same as that required to develop and substantiate a new design. In such a highly regulated industry, the burden of demonstrating that a specific tool or method is fit-for-purpose is significant. Therefore, once a method is established as suitable for a task, there is less incentive to change it, even if a newer method can offer advantages. Therefore, the development or adoption of new thermal hydraulics modelling tools is driven by the need to simulate new designs comprising new flow features, components or working fluids. Therefore, with no development programme, the drive in the UK civil nuclear industry has been low, with a significant proportion of UK capability still associated with the tool set developed to support the safety assurance of the existing UK reactor fleet (such as the MACE and PANTHER codes employed by EDF Energy). The UK's research efforts have continued to progress, but with a diminishing community of researchers. The application of advanced modelling methods to new and existing international reactor designs is well within the experience and skills of a number of UK researchers. However, without a UK based reactor programme or a consistent or predictable source of funding, UK activities and involvement in international programmes has become fragmented and sporadic.

Historical experience of some Gen IV reactor technologies has been all but lost, as the engineers involved in the UK programmes have retired. More recent experience has been gained by some specific individuals in academia, through involvement in international programmes. In addition, organisations developing both a Molten Salt Reactor and a High Temperature Gas Reactor have completed at least some of their early concept design work in the UK. However, as with all Gen IV reactors, further development will likely be based where there is a significant body of expertise in that specific technology and, critically, the availability of substantial further investment and opportunities for deployment. On the basis of these two factors, the UK lags behind other countries in attractiveness for Gen IV reactor developers.

In modern, international nuclear codes, such as those listed in Section 3.4.2, the UK civil nuclear industry does not hold widespread expertise. The majority of these codes are developed and validated for Light Water Reactor (LWR) use and, because the UK only operates one such plant, the need for UK skills in this area has been low.

In contrast, in modern, more general purpose fluid modelling tools, such as CFD, there remains considerable UK-based expertise and impetus in their development to service the needs of other industries. Section 5 of this document discusses the modern modelling practice in automotive, aerospace, defence and other industries to highlight any that may be applicable.

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¹ Note that this comment relates to civil reactor design only, capability in reactor design for defence purposes is not considered by this programme. In some component areas, such as pumps, UK industry has continued to develop and support international reactor design.



2.3 The Current UK Capability Picture

Considering the current UK nuclear thermal hydraulics modelling capability in the context of Figure 1 requires taking a multi-dimensional view. For example, in the modelling of aspects of the current reactor fleet relevant to continued operation, the UK has a well-developed and 'fit for purpose' capability already (although 'state-of-the-art' approaches are not regularly employed). In the thermal hydraulic modelling of molten salt reactors, the UK capability (and indeed the world capability) is far less well developed. Even within a single reactor technology the picture is complicated as some phenomena are better understood than others and some methods are well understood in an academic context, but less so in an industrial one. It is therefore not possible to represent the 'UK capability' easily on a diagram or map it onto Figure 1.

The hardware needed to support the use of advanced thermal hydraulic modelling methods and (to a large extent) the concepts and doctrine are common across all reactor types. These areas are not the main focus of this project, but development in both would need to run alongside developments in thermal hydraulic modelling to deliver a complete capability.

The specific knowledge and skills needed by personnel and the modelling methodology and software applied are dependent on the type of thermal hydraulic problem at hand. It is important to understand that, in thermal hydraulics (arguably) more than in any other technical discipline, the specific reactor technology under consideration matters, as one of the defining differences between technologies is their primary circuit working fluid (coolant). These aspects of the UK capability are summarised in Sections 2.3.1 to 2.3.3. A fuller description of the state-of-the-art in thermal hydraulic modelling capability is included in Reference 6.

It is worth noting the important distinction between the level of maturity of a reactor design and the level of maturity of the thermal hydraulic modelling capability that supports it. For example:

- HTGRs and VHTGRs are categorised as Gen IV reactors, but the thermal hydraulic modelling of single phase gases has the highest thermal hydraulic modelling TRL of any reactor primary circuit fluid.
- LWRs are an established technology with many operational plants throughout the world, but the thermal hydraulic modelling of the two-phase flow present under many conditions is still an area of significant empiricism and uncertainty.

2.3.1 Gas Reactors

In the context of this section 'gas reactors' are defined as any reactor where the primary circuit fluid is a gas, which includes GFR and VHTR.

The UK capability in the thermal hydraulic modelling of gas flows and heat transfer is at least as good as the rest of the world. UK industry has a good physical understanding of the phenomena and fluid material properties and access to a good range of appropriate state-of-the-art modelling tools. Due to the extensive need to model gases in other industries, there is also a reasonable number of skilled personnel who could transfer their skills to the nuclear industry with only a modest amount of training.

As with all thermal hydraulic modelling, the UK has a good capability in general purpose tools like CFD and in the physical and empirical models embodied within them. The civil nuclear industry currently lags behind some other industries in the use of state-of-the-art tools, especially for licensing purposes, and there is a great deal to be gained by a wider application of extant CFD modelling capabilities to nuclear thermal hydraulics. The main barrier being the demonstration of confidence and validation of the methods in a civil nuclear context (this observation is echoed in Section 6.2).

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UK engineers have significant experience with the current fleet of gas reactor (AGR) system modelling tools. Although it is unlikely that these specific tools will be used to model new reactor designs, a good understanding of the phenomena of importance and the underlying methods used will stand UK engineers in good stead in developing modern equivalents. A pebble bed core design (rather than a prismatic core) will require the development of new methods or the use of new international thermal hydraulic system tools, but this is likely within UK capability.

The ability to generate civil nuclear validation data within the UK has been limited by a lack of facilities, but there is a good capability to design and operate test rigs investigating the flow of gases in other industries. There is also a better body of international test data available for gases than for more unusual fluids, although it is not as extensive, in a nuclear context, as that for LWR.

The areas where UK capability would need to be developed for modelling gas reactors are consistent with world capability gaps identified in Reference 5.

2.3.2 Light Water Reactors

Light water reactors encompass both large and small reactors using light water as a primary circuit fluid (BWRs and PWRs).

The thermal hydraulic modelling capability required to operate an existing PWR already exists in the UK. However, a number of the methods employed would now be considered out-of-date in countries with a more extensive LWR fleet or significant design activity. UK physical understanding of phenomena of importance in PWRs is good (although in industry it is vested in a relatively small number of organisations). As the UK does not currently operate a BWR, this understanding is lacking in much of industry.

Specific UK organisations have experience of small PWR design for defence purposes which includes both thermal hydraulic modelling and testing. Although it is not possible for UK civil nuclear industry to benefit from any specific IP relating to defence applications, relevant thermal hydraulic knowledge and experience exists within a number of organisations.

UK academic institutions are already performing research to advance (a reasonably good) capability in CFD modelling of the two-phase water flow relevant to LWR design, funded via EPSRC and industry contributions. The main challenge (in common with the rest of the world) is that this capability is still not at a TRL where it can be used to model the complex conditions seen during the faults of most interest to reactor designers to a sufficient level of confidence to support nuclear safety.

Much of UK industry does not have a good level of knowledge and experience with international 'nuclear codes', i.e. system and sub-channel codes, beyond those used for Sizewell B. In particular, UK industry knowledge and experience of BWR specific codes is low. As discussed in Reference 6, there are a large number of international tools available with the most widely used system and sub-channel codes typically being the product of a single nation or large corporation. Where there has been significant investment in such tools, there are often political and commercial barriers to UK industry gaining access to them for the purposes of reactor design.

2.3.3 Liquid Metal and Molten Salt Reactors

Reactors that employ a liquid metal (including sodium, lead and lead-bismuth eutectic) or a molten salt as the primary circuit fluid introduce additional challenges from a thermal hydraulic perspective. These fluids are less commonly used in other industries and therefore less widely understood.

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The UK (and the world) capability in the thermal hydraulic modelling of these fluids is significantly less than for gases and water. The majority of the recent expertise with these fluids in the UK resides within academic institutions. There is one UK organisation currently developing a molten salt reactor design where industry expertise is being grown. There is also a body of UK based knowledge dating from the historic fast reactor programme (including thermal hydraulic aspects), some of which has been captured by this project and the 'Fast Reactor Knowledge Capture' project within the Nuclear Innovation Programme.

In common with the rest of the world, the UK lacks capability across all areas of thermal hydraulic modelling of liquid metals and molten salts and there is the need for further R&D to address pertinent issues. For example, the high thermal conductivity of liquid metals makes a significant number of the methods employed for water and gases unsuitable. New methods are under development internationally, but lack the maturity and user base of LWR tools.

2.4 Future UK Capability

The nature of a future UK Nuclear Thermal Hydraulic Modelling Capability will primarily depend on choices that are made within the UK policy and funding landscape and market forces. The emphasis, extent and nature of the future capability will be defined by the reactor technologies that the UK decides to invest in and the role that the UK decides to pursue within the global nuclear industry. Key questions to enable the definition of this role are currently unanswered; without this clarity, objective down-selection of research and development proposals is impossible or counter-productive. This difficulty arises because it is not possible to define specific propositions that will make both a significant short-term impact and provide benefit across the range of possible future scenarios.

However, the structure of a UK nuclear thermal hydraulic modelling capability that has been developed (Figure 1) fits a variety of possible futures and is useful for examining, comparing and checking the comprehensiveness of research and development proposals. Strengthening the enabling elements of the structure (Personnel, Hardware and Infrastructure, Concepts and Doctrine) is likely to provide benefits regardless of the core Modelling Methodology and Software Solutions needed to support technology choices. For example, access to High Performance Computing (HPC), i.e. supercomputers, is key for the exploitation of advanced modelling methods. There is a need for access to HPC now, and this will only increase with increased uptake of these methods. The development of diverse commercial and organisational approaches to allow better utilisation of the UK's existing HPC facilities is outside the remit of this project, but would be an enhancement of the enabling elements.

It is important to acknowledge that it is not possible or desirable to separate the UK capability from the world capability. This is particularly apparent in the thermal hydraulic modelling tools currently available. The most widespread CFD tools are truly global in their use and their wide range of applicability across a range of industries gives them an extensive user base both within the UK and internationally. System and sub-channel codes are less universal, with differences in the preferred toolset between countries. As previously discussed in Section 2.3.2, these modelling tools are not necessarily comprehensive for new reactor designs and not all are freely available within the UK. However, due to the significant cost and time implications of duplicating the existing toolset, it is strongly recommended that the UK develop its capability by adopting tools and building on world capability rather than attempting to develop a completely independent set.

This project and the other recommendations made by the NIRAB committee have been developed on the premise that the UK will be directly involved in future reactor design. Indeed the title of the programme under which Project FORTE falls is 'Digital Reactor Design'. When

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considering the capability that the UK may need in the future, therefore, the enabling and support of reactor design activities (rather than imported reactor operation or the sale of technical software or services) has been taken as the most important consideration. However, achieving this vision will take time and on-going investment beyond just nuclear thermal hydraulics. It is important to set realistic, shorter term goals that fulfil the UKs short term needs as well as working towards the longer term vision.

Following the timeline laid out by the Nuclear Innovation Programme aims, and considering an example possible evolution of the UK's technology aspirations towards this goal, the following timeline for capability development is postulated.

2.4.1 Short Term (2020 horizon)

"By 2020, establish the UK as a partner engaged in collaborative design projects for new reactors (Generation IV and SMR), building on its existing and growing design expertise"

The current Nuclear Innovation Programme is scheduled to complete in March 2021. This short term horizon is consistent with the programme and therefore the capability development identified can be connected with the project proposals within this document (described in Section 6 and Annex A).

The currently envisaged new build projects in the UK are all based around LWR technologies. Therefore, in the short term, it is likely that UK industry will want to focus on the thermal hydraulic modelling necessary to regulate and operate these imported designs. Furthermore, it is likely that most of the first SMR reactors to be ready for deployment will be based on light water technologies. International state-of-the-art codes have been created and customised to support a wide range of LWR reactor systems. For industry, using such (international) system and sub-channel codes that are available and beginning to build a sustainable user base is overwhelmingly the most cost effective initial approach and likely the only pragmatic option in the short term. This is already starting to happen, but progress is slow. Due to the need to keep costs down, a lack of UK-based experience and for the protection of IP, the majority of the thermal hydraulics work on current new build projects is being performed outside of the UK.

Despite the relatively mature nature of LWR technologies, research and development activities over his timescale are needed to building capability in areas where the current modelling tools are weak². The need to reduce costs is perhaps the single most pressing requirement for the civil nuclear industry. Currently used predictive capabilities for LWR embody considerable uncertainties, and in a nuclear context the natural and necessary response is to design plants with large margins, to ensure unsafe conditions are not approached. This imposes considerable economic penalties on the plants which could be reduced by improvements in predictive techniques. In addition, events such as Fukushima Daiichi accident, coupled to the desire to simplify and reduce the costs of plants, have increased reliance upon passive safety.

Prediction of thermal hydraulics performance under passive, natural circulation conditions is particularly difficult, increasing the importance of further developments in capability in this area. This is reflected in the number of project proposals in Annex A relating to natural convection and the improved prediction of heat transfer. In the less mature Gen IV technologies, the tools are less well developed and there is the potential to grow the UK involvement in the future of these tools. However, whilst some initial steps down this path would be possible, it is unlikely that much could be achieved by 2020. The focus would need to be on initial 'engagement' with

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² Whether this process should be a candidate for government investment, or should be paid for by operators is a matter of active debate (see Section 7).



one or two projects, likely in a niche area, to develop UK R&D capacity and gain a 'foot in the door' of reactor development programmes (a number of suitable options are given in Section 6).

The highly regulated nature of the nuclear industry means that any new or novel methods/tools would need to be subject to rigorous code verification and application specific experimental validation of results before they would be appropriate for use. Guidance on such activities has been documented under initiatives co-ordinated by the OECD NEA Committee on the Safety of Nuclear Installations (CSNI³). This time consuming and expensive process can be a significant barrier to the use of more generally applicable methods by the civil nuclear industry. Research and development activities over the next two years can play an important role in breaking down the barriers by demonstrating the value of methods, even without achieving any specific scientific advancement (noted in Section 6.2).

2.4.2 Medium Term (2030 horizon)

"By 2030, maturing R&D results in deployment of new plant with significant UK design content and manufactured parts"

Expanding the UK's role to be more than an operator of imported designs requires evolving the modelling capability from that required to support regulation and operation of reactor technologies to being able to deploy a full lifecycle design and safety substantiation toolset. Depending on the short term choices made, the predominant need would likely remain a light water modelling capability. By 2030, it is envisaged that this would include tools incorporating UK developed, innovative capability and a significantly increased pool of skilled personnel.

By 2030, considerable development in the UK's involvement in Gen IV reactor technologies could be achieved via appropriate collaborations and direct involvement in international programmes. However, it is not sensible for the UK to be a contributor to all of the possible Gen IV technologies; endeavouring to support too many technologies is almost certain to leave sources of research funding stretched too thin to make meaningful contributions to any. Nuclear thermal hydraulic modelling is required for all technologies to progress, but the magnitude and precise details of the capability required is different. Therefore the congregation of the capability around one or two Gen IV technologies is both likely and desirable. This down-selection could be via either direct intervention in policy and government funding (e.g. the Advanced Modular Reactors (AMR) Competition) or may occur via market forces.

It is worth noting that the embodiment of a nuclear thermal hydraulic modelling tool set will likely differ in the UK from that currently seen elsewhere in the world. Some of the most successful nuclear specific international tools are (or have been) owned, maintained, licenced and distributed by a national body, rather than a private commercial organisation or a specific academic institution. These tools are used in conjunction with vendor specific tools (and data) and commercial generic modelling methods to form a complete solution. In the absence of such a body (and considerable amount of sustained funding) it is hard to visualise a future with 'UK' reactor tools. Rather, it seems more likely that each reactor vendor will acquire and/or develop their own thermal hydraulic modelling solution (with the support of their supply chain, including commercial software vendors). The key for successful R&D may therefore be in providing the foundation and focus on which to build a UK capability and foster national collaboration, rather concentrating on providing the tools themselves.

Whilst adopting and adapting currently available 'nuclear' modelling tools is all that can be expected by 2020, by 2030 UK vendors may arrive at conditions where an increasing

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³ https://www.oecd-nea.org/nsd/csni/cfd



percentage of 'indigenous' tools is preferable. This can arise by the motive to apply the latest scientific and computational methods, but also for security of provision⁴.

Public funding in nuclear thermal hydraulic research and development is likely to be required to achieve the 2030 aims by supporting:

- Academic research to maintain the UK at the cutting edge of new innovation and to ensure a pipeline of skilled individuals for a growing industry;
- Industry and academic engagement in international collaborative activities; and
- Development required for future reactor design activities where the timescales for return on the investment is too long (or too uncertain) for solely industry investment.

2.4.3 Long term (2050 horizon)

"By 2050, R&D has facilitated UK industry to be a significant partner in the global deployment of Gen III+, Gen IV and SMR technologies"

The current BEIS nuclear innovation programme (in all areas) takes only the first steps towards this future and a sustained programme of reactor development and associated research, focused on specific technologies and designs, would be needed to achieve it. Therefore looking this far into the future does not, currently, identify any factors that need urgent action. The reactor designs to be pursued are not defined, and computing, modelling and regulatory developments cannot be sensibly anticipated.

Developing a modelling toolset, as identified as a medium term goal, is not a short activity - approximately ten years from concept to validated maturity is needed for a piece of complex, high performance simulation software. Therefore, there is currently sufficient time to pursue the 'adopt and adapt' strategy outlined in Section 2.4.1 to satisfy immediate needs, and create tools when appropriate for the medium to long term goals. This will only be successful, however, if there is a:

- Sustained period of funded (by independent vendors, or government, or a combination of both) activity in both UK reactor design and associated research;
- Consistent pipeline for the generation and retention of suitably qualified and experienced engineers and scientists to both employ and advance the tools; and,
- Periodic reassessment of the UK and international position, and re-steering of the R&D activities by, for example, undertaking an update of this document every five years.

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⁴ There is a sense in which having one's own toolset is part of "being in the club" i.e. considered a first-class nuclear nation, and serious partner, able to lead, own, develop and innovate in technology programmes.



3 The UK in an International Context

UK nuclear R&D funding compared to international peers, and the UK's capability landscape are well described in the February 2017 NIRAB survey (Reference 3). Similarly, publically available information shows that the research into advanced reactors and the building of new Gen III reactors is led by Canada, China, EU (plus Switzerland), France, India, Japan, Russia, South Korea, USA. Sources include:

- ► IAEA Advanced Reactor Information System⁵ (ARIS);
- ► IAEA Power Reactor Information System⁶ (PRIS);
- Gen IV forum⁷; and
- World Nuclear Association Small Nuclear Power Reactors Review8.

Although the UK has previously not been an 'active' participant in Gen IV forum development programmes, the UK has recently re-joined as an active member. UK investment budgets in civil nuclear R&D are small in comparison to the countries above.

In this context, there are a large number of ongoing international thermal hydraulic research programmes, and sets of modelling tools are in existence world-wide that have been continuously refined over decades. This, along with the expected international aspects of new reactor designs, creates a strong incentive to not attempt to initially duplicate or re-invent these efforts, but instead to collaborate with other tool users and contribute to their development. While the UK is part of some of these programmes, the contributions are small and limited to a small range of individuals or institutions. The UK has strong skills that are relevant to these programmes, which could make a significant contribution given appropriate funding and high-level engagement.

This section provides an overview of the current international research and toolsets, focussing on Europe and the USA.

3.1 IAEA Coordinated Research Activities

IAEA's Coordinated Research Activities (CRAs) aim to stimulate and coordinate the research activities of member countries in selected nuclear fields. These are carried out through Coordinated Research Projects⁹ (CRPs), which bring together scientific institutes from different member countries to work on problems of common interest. It has a total budget of €7 million with a UK contribution of €331,000 in 2014. A number of active CRPs deal with thermal hydraulics for Gen IV reactors, SMRs and application of CFD to Nuclear Power Plant Design:

- High Temperature Gas-cooled Reactor (HTGR) Physics, Thermal Hydraulics and Depletion Uncertainty Analysis (no UK participation);
- Modular High Temperature Gas-cooled Reactor Safety Design (the UK is a participant);
- Understanding and Prediction of Thermal Hydraulics Phenomena Relevant to Supercritical Water-cooled Reactors (SCWR) (UK participation from the University of Sheffield, working on computational predictions of supercritical phenomena);

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⁵ https://aris.iaea.org

⁶ https://www.iaea.org/PRIS

⁷ https://www.gen-4.org

⁸ http://www.world-nuclear.org/information-library/nuclear-fuel-cycle/nuclear-power-reactors/small-nuclear-power-reactors.aspx

^{9 &}lt;u>http://cra.iaea.org/cra/index.html</u>



- Sodium Properties and Safe Operation of Experimental Facilities in Support of the Development and Deployment of Sodium-cooled Fast Reactors (SFR) (NAPRO) (no UK participation);
- Design and Performance Assessment of Passive Engineered Safety Features in Advanced Small Modular Reactors (no UK participation); and
- Application of Computational Fluid Dynamics (CFD) Codes for Nuclear Power Plant Design (no UK participation).

The advantage of participating in a CRP is in the sharing of resources and data as the group work towards a common goal. Although the CRPs are co-ordinated by the IAEA, participants are expected to self-fund their activities.

3.2 Current and Recent Thermal Hydraulic Research in Europe

The EU 7th Framework Programme funded NURISP (NUclear Reactor Integrated Simulation, 2009 to 2012, €10.3M¹0, UK participation from Imperial College London, which was funded €44,581) and NURESAFE¹¹ (NUclear Reactor Safety Simulation Platform, 2013 to 2016, €9.3M, UK participation from Imperial College London, which was funded €53,937), which continued from the 6th Framework NURESIM project.

NURESAFE's subprojects included:

- Multiphysics applications involving core physics.
- Multiscale analysis of core thermal hydraulics, from DNS to sub-channel modelling.
- Multiscale and multiphysics applications of thermal hydraulics (LOCA, PTS and BWR issues such as dry-out and modelling of the suppression pool).

The objective of NURESAFE is to deliver to European stakeholders a reliable software capacity usable for safety analysis and to develop a high level of expertise in the proper use of the most recent simulation tools. Integration of simulation tools was achieved using the NURESIM simulation platform¹². The NURESAFE programme intends to provide a more accurate representation of physical phenomena by developing and incorporating the latest advances in core physics, two-phase thermal hydraulics and fuel modelling into best estimate codes. This involved developing significant capacities for multiscale and multiphysics calculations, and for deterministic and statistical sensitivity and uncertainty analysis, and facilitating their use in a generic environment.

The EU 7th Framework Programme also funded THINS¹³ (Thermal Hydraulics of Innovative Nuclear Systems, €10.5M, 2010 to 2015, UK participation from Imperial College London and Computational Dynamics (now Siemens PLM) who were funded €66,977 and €64,000 respectively to perform research into the computational modelling of pebble bed reactors). The project topics included:

- Advanced reactor core thermal hydraulics;
- Single phase mixed convection;
- Single phase turbulence;
- Multiphase flow; and
- Numerical code coupling and qualification.

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¹⁰ https://www.cordis.europa.eu, the budgets stated are the "total costs", not just the EU contribution.

¹¹ http://www.nuresafe.eu

¹² http://www.nuresafe.eu/docs/NURESIM-flyer_v2.pdf

¹³ http://www.ifrt.kit.edu/thins



The project aimed to establish an experimental database and develop new and more accurate physical models and numerical simulation tools. Twelve experimental facilities were included in the project, and the project generated substantial new data. New correlations for models were developed for heat transfer and pressure drops. They were (partially) validated, based on the established test data and also implemented in numerical codes.

Currently, there are a number of consortia in Gen IV reactor technologies supported through Horizon 2020, including SESAME, MYRTE and SAMOFAR, all running between 2015 and 2019. The former two are concerned with liquid metal cooled reactors (including both SFR and LFR), whereas the latter is concerned with Molten Salt Reactors (MSR).

The SESAME (Simulations and Experiments for the Safety Assessment of MEtal cooled reactors, €6.6M, no UK participation) is solely concerned with thermal hydraulics, focusing on fundamental, safety-related, generic challenges. The complementary MYRTE (MYRRHA Research and Transmutation Endeavour, €12M, no UK participation) project focuses on the further development of the MYRRHA reactor in Belgium, with a large part devoted to thermal hydraulics. The two projects work closely together and identified the following key areas of development:

- Liquid metal heat transfer;
- Fuel assemblies; and
- Plenum and system thermal hydraulics.

The projects aim to validate analytical and simulation methods with reference data. The projects recognise that there are significant limitations and difficulties with physical experiments with (opaque) liquid metals given the difficulty of the accessibility of instrumentation to the regions of flow of interest and level of fidelity that experiments can provide. High fidelity simulation data, typically Direct Numerical Simulations (DNS) or Large Eddy Simulations (LES), are to be used to generate data to complement or replace experimental data for model validation.

The SAMOFAR (Safety Assessment of the MOlten salt FAst Reactor¹⁴, €5.2M, no UK participation) project aims to achieve a number of objectives, including:

- To deliver experimental proof of concept of the safety features of the MSFR;
- To provide a complete safety assessment of the MSFR and chemical plant; and
- To update the conceptual design of the MSFR with all input gathered during the project.

In the area of thermal hydraulics, the project aims to develop experimental facilities to produce data on heat transfer and flow/loop instability, as well as develop leading-edge multiphysics codes, including uncertainty propagation for transient calculations.

3.3 Current and Recent Thermal Hydraulic Research in USA

There are two major ongoing national R&D projects in nuclear modelling and simulations in the US: CASL and NEAMS funded by the Office of Nuclear Energy and previously CESAR, funded by the Office of Science of the DoE.

The Consortium for Advanced Simulation of Light Water Reactors¹⁵ (CASL) aims to deliver solutions to industry-defined challenges for current LWR technologies. It is funded by the US Department of Energy, receiving \$30 million in 2018 and due to receive \$27.8 million in 2019. It is a consortium between US industry, national labs and universities with a vision to provide leading edge modelling and simulation capabilities to deploy within the US nuclear energy industry to

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¹⁴ http://samofar.eu

¹⁵ https://www.casl.gov



improve LWR operational performance. One of its key outputs is to develop and validate the Virtual Environment for Reactor Applications¹⁶ (VERA). The thermal hydraulic analysis is based on a coupled approach between the system/sub-channel codes and CFD. The UK has some involvement in the project: Rolls-Royce sits on one of the advisory bodies; UK personnel from Siemens PLM contributing in the area of CFD modelling; and NNL contributes in the chemistry of CRUD formation.

The Nuclear Energy Advanced Modelling and Simulation Program¹⁷ (NEAMS) develops and validates predictive analytic computer methods for the analysis and design of advanced reactor and fuel cycle systems including Gen IV reactors (SFR and HTGRs) and SMRs. The vision of the NEAMS Pellet-to-Plant Toolkit (a high performance computing solution for nuclear performance and safety) is to provide insights that cannot be achieved through experimentation alone. Consequently, high fidelity simulation is the focus of the methodology that is being developed.

The Centre for Exascale Simulation of Advanced Reactors¹⁸ (CESAR) focussed on the two key components of reactor core modelling physics - computational fluid dynamics and neutron transport - with particular focus on parameter regimes required for robust, coupled reactor core modelling. The program received \$4 million a year for 5 years from the Office of Science to enable exascale reactor simulations, which will fundamentally change how nuclear reactors are built, tested and operated. This was expressed as a two-fold goal:

- To drive the design of future hardware architecture, system software and applications based on the algorithmic requirements of nuclear engineering applications; and
- To develop a new generation of underlying algorithms which successfully exploit exascale computing to solve significant reactor simulation problems.

Nek5000, the CFD code, central to NEAMS, was a key component of CESAR.

3.4 Modelling Toolsets

Modelling tools for thermal hydraulics are complex, difficult and expensive to develop to a level of maturity to be reliable for design, and particularly for safety justification. High quality verification and validation evidence is needed for the wide range of components and physical phenomena. This is difficult and expensive for nuclear thermal hydraulics on its own, even without accounting for the (necessary) coupled tools, incorporating neutronics for example. Therefore, the availability, functionality and application of complete modelling tools is closely linked to national and international R&D and reactor build programmes.

There are no toolsets available that are able to be openly obtained that are qualified *a-priori* to be used and accepted by a regulator for safety analysis of a new reactor design (although a reactor developer is free to use them for design studies, at their own (commercial) risk). This is because they require reactor specific Verification and Validation (V&V) evidence to support their use for a particular purpose.

Thermal hydraulic modelling tools for nuclear applications can be broadly split into two categories

- General purpose simulation codes (Section 3.4.1).
- System and sub-channel 'nuclear' codes (Section 3.4.2).

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¹⁶ https://www.casl.gov/vera

¹⁷ https://neams.inl.gov

¹⁸ https://cesar.mcs.anl.gov/content/about-cesar



3.4.1 General Purpose Physics Simulations

This primarily means CFD codes, which are in many instances available from a commercial vendor (such as ANSYS FLUENT and CFX, or Siemens PLM STAR-CCM+, all of which were substantially developed in the UK), or are open-source (Code_Saturne (France), OpenFOAM (UK) or Nek5000 (US)). Some nuclear domain codes are developed and owned by national bodies e.g. NEPTUNE_CFD (EDF, France), TRIO_U (CAE, France) or Hydra-TH (Los Alamos, US).

CFD codes are potentially applicable to any reactor type, can provide a detailed 3D calculation of flow field and represent much of the physics explicitly (the UK is a world-leader in the use and development of CFD codes and models). However, the use of CFD models in nuclear thermal hydraulic prediction is not without its challenges. The general purpose and flexible nature of the tools mean that the results are often sensitive to the decisions of each user and, despite the considerable physical basis for the models, CFD codes still embody many empiricisms. This leads to uncertainty in the predictions and extensive validation, focused on the class of problem being tackled, is needed, especially for safety and licensing purposes. Suitable validation data can be expensive or difficult to obtain, either because dedicated experimental facilities with appropriate measurement capability are needed, or extant data is not made openly available by reactor developers or national organisations.

In addition, despite recent advances in computing, it is still too numerically intensive to perform large-scale design and safety CFD analysis on a whole core or a whole primary circuit.

3.4.2 System and Sub-channel Codes

Unlike CFD, these codes do not solve the fundamental 3D continuum mechanics equations, but use a simplified equation set and coarser geometrical representation of the system. In essence, "systems codes", model flows in one-dimensional piping networks. For any system that can reasonably be modelled as such, systems codes (after decades of development) present a powerful and relatively cheap-to-run modelling tool.

The one-dimensional conservation equations are supplemented by 'closures' relating, for example, heat transfer or pressure drop to local flow conditions. Such closures need to be derived based on extensive experimental measurements and their applicability is often limited to specific designs and ranges of conditions. The models, therefore, need considerable experimental data to develop the inputs as well as for validation. Additionally, all reactor designs have regions which are not well represented by a 1D approach, which introduces uncertainty into the model predictions.

System codes (such as ATHLET (Germany) CATHARE (France), RELAP or TRACE (both US)) represent the transient response of the entire primary circuit of a reactor, while sub-channel codes (such as COBRA-TF/CTF (US), FLICA (France) or VIPRE (US)) provide more detail (typically) on an individual fuel channel. There also exist a large range of nuclear industry specific codes that typically perform analysis of a specific piece of plant, for example, GOTHIC (US), which is used to analyse containment conditions during accidents.

These tools were typically developed for LWR technologies, and are most widely validated for them, but can be applied to any reactor technology. The UK civil nuclear industry lags the international community in the extensive use and development of these codes, because it

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predominantly owns and uses only the tools needed to analyse and operate AGRs (for example MACE, PANTHER and FEAT), and not those for the more common BWRs and PWRs¹⁹.

In addition to simulating LWRs, some system codes have been adapted to simulate other coolants. For example, TRACE has been used to simulate the Phenix SFR end-of-life natural circulation experiments²⁰. In addition, some system codes have been developed specifically for other coolant types, such SAS4A/SASSYS-1²¹, developed since the 1960s by Argonne National Laboratories for liquid metal reactors.

3.5 Outlook

The assessment of the UK's positon relative to the nuclear industries worldwide inevitably leads to an assessment and comparison of tools, because they become the repository for, and embodiment of, much of a reactor technology programme's knowledge.

System and sub-channel codes are usually the property of reactor developers or national organisations, but access can be obtained or negotiated. However, in all cases, an analyst will require reactor specific closure data to make accurate predictions that are acceptable to a regulator. That is difficult or expensive to obtain, requiring significant experimental data, or other high quality inputs, potentially obtained by CFD. The closure data embodied by system and subchannel codes represents the output of the huge investments made in the 1980s and 1990s.

Therefore, a modelling capability that is to be employed by the UK in the short term will, in all likelihood, require access to either these tools, as developed and used by international peers, or access to validation data that they hold. Making good use of these tools also requires significant training and experience, and so contact and collaboration with their developers is highly beneficial. Several of the project proposals that have been developed for this report make propositions to collaborate with the developers and users of these tools.

A number of the project proposals make specific suggestions regarding international tools and research, which include:

- Joining the international efforts to benchmark thermal hydraulic 'tools' is proposed by project P2_A.
- The "UK LWR predictive modelling validation centre" hosted in Bangor proposed by project P2_D requires obtaining and gaining competence in international tools for comparison.
- Professor Shuisheng He (University of Sheffield) is the UK representative on the current IAEA CRP related to SCWR, as progressed by project P5_G.
- Selecting international tools to adopt is the emphasis of project P6_A.
- The adoption and coupling of modern internationally used tools for BWR fuel modelling is proposed by project P6_C.
- Obtaining, applying and improving the US CASL CRUD modelling tools is proposed by project P6_D.

However, these project proposals were derived 'organically' by exploring the existing knowledge of the UK stakeholders who contributed to them. Because of the UK's prolonged absence from many activities, there may be opportunities that were not proposed due to lack of contacts and

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¹⁹ However, Sizewell B uses legacy versions of US tools such as RELAP, COBRA and LOFT-5 as well as UK developed PANTHER for PWRs.

²⁰ https://doi.org/10.1016/j.nucengdes.2018.02.038

²¹ https://www.ne.anl.gov/codes/sas4a-sassys-1



experience. It is recommended that all projects carried out under this programme consider the potential for international collaboration at regular intervals.

It is also noted that there exist other possible (or necessary) motivations for joining specific international efforts, chosen based on factors much broader than just thermal hydraulics. For example, if a need was identified for a specific fuel cycle to use or dispose of plutonium, this would influence a reactor technology choice and thereby the programmes that would be of most value. Furthermore, major UK participation in some international initiatives would require strategic and high-level industrial, governmental or regulator coordinated actions.

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4 Development Approach

The key purpose of this document is to define areas of focus, where packages of research and development effort could be used to enhance the UK nuclear thermal hydraulic modelling 'capability' (Section 2).

To specify these areas of focus, industry has been engaged to capture 'statements of need' in areas of thermal hydraulic modelling and testing. Our engagement involved nearly 60 UK and international organisations and covered Gen III, Gen III+ and Gen IV reactor technologies as well as current UK operational experience. Reference 5 formally records the process that has been used to capture, manage and refine this information into a series of modelling 'user requirements'.

As a first stage in defining potential capability improvements, a coherent understanding of the modelling shortfall is needed. This should be developed from an in-depth understanding of both the important thermal hydraulic phenomena and the capability of current modelling techniques. Identifying the shortfalls allows the 'user requirements' drawn from industry engagement to progress into 'modelling requirements' and from there to propose research and development work to deliver them.

This section describes the systematic approach that has been used to progress the 'user requirements' captured in Reference 5 into the research proposals discussed in Section 6 and presented in detail in Annex A.

4.1 Approach

Reference 5 records 80 modelling user requirements. These vary in scope, from those that are exclusive to a particular reactor design or technology, to those that are more generally applicable. They also represent a wide range of topics, encompassing modelling tools, approaches, philosophy and personnel.

Some of the requirements are the result of modelling challenges that have existed for a long time. Entire careers have been dedicated to moving the state-of-the-art forward but still the problems are not completely solved. It is therefore not possible or reasonable to try and completely address them all. Therefore, in order to make recommendations which are Specific, Measurable, Attainable, Relevant and Timely (SMART), it is necessary to analyse and potentially down-select the requirements. In the absence of a technology focus or a well-defined UK strategy, there is no obvious way of down-selecting the requirements. The approach that has been adopted is systematic and pragmatic for down-selection within the timescale and budgetary constraints of this project, but it is acknowledged that this approach is not the only method that could have been used. Figure 2 illustrates how the user requirements have been progressed through to proposed research by:

- 1. Investigating methods of grouping the requirements to identify areas of common ground and important differences;
- Assessing each of the requirements in terms of whether addressing them furthers the UK ambitions in the context of the BEIS medium term aims (Section 1.2);
- 3. Developing the requirements into a number of 'topics' linked to less specific user 'challenges' to promote creative thinking;
- 4. Facilitating a workshop involving the major stakeholder organisations, either UK based or with interests in UK new-build, to discuss the challenges, consider the modelling

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- deficiencies relating to the challenge, potential improvements that would be needed to address them and to recommend ways forward;
- 5. Developing the output from the workshop into a number of specific research and development project proposals;
- 6. Linking the project proposals back to the original user requirements to assess the extent to which the requirements will be addressed by carrying out the proposed work; and
- 7. Linking the project proposals back to the BEIS medium term aims (Section 1.2) to assess how carrying out the work addresses the ambitions of the UK.

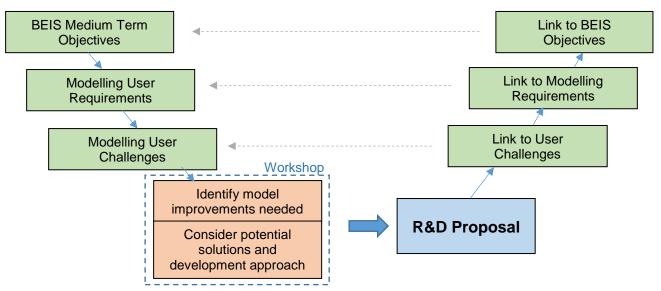


Figure 2: Approach to the Development of Research Proposals

The analysis of the requirements and the resulting modelling challenges are presented in Section 4.2. A description of the development of recommendations via a workshop is included in Section 4.3. The individual R&D project proposals are included in Annex A along with clarification of the linking to the user requirements.

4.2 Analysis of requirements

The first step in the requirements analysis was to characterise and group the requirements according to areas of commonality. A large number of possible groups were investigated; the most useful groupings were found to be:

- 1. Consideration of the requirements in terms of the most important types of thermal hydraulic phenomena that need to be modelled. It was necessary to use quite a high level approach at this stage; many cases involve the interaction of multiple phenomena, in some cases the precise phenomena of greatest importance are not yet known.
- 2. Characterising the area of the reactor that the requirement relates to e.g. is the requirement most relevant to the fuel, heat exchangers, or plenums?
- Characterising the reactor technology or technologies to which the requirement is relevant.
 Some requirements are only relevant to one technology, some are common across a range of technologies.
- 4. Consideration of the 'type' of capability development (see Section 2.1) needed to address the requirement i.e. is the most likely way forward a tool improvement, a development of

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underlying understanding, improved use of the models or improved training in particular techniques?

The second step built on the grouped results and considered the BEIS medium term objectives to develop a set of criteria against which to judge the potential benefit addressing each requirement. The benefit criteria applied were:

- 1. How important are improvements in this area to reactor design, operation and safety?
- 2. How widely applicable is this requirement to the design and operation of different types of reactor?
- 3. How likely is R&D in this area to result in a successful improvement?
- 4. Can a measureable benefit be achieved in the 3-year timescale of Phase 2?
- 5. How strong is the UK capability in delivery of R&D in this area?
- 6. How extensively is this requirement being addressed internationally?
- 7. How well does addressing this requirement meet the overall aims of the BEIS programme?

It should be noted that because the 'scoring' of the requirements against such criteria is highly subjective, a quantitative approach to scoring was not considered suitable. In addition, meeting each criterion is not a simple positive or negative attribute. For example, for Criterion 6, significant international activity presents both opportunities for collaboration and also introduces the risk of the UK repeating work that has already been done elsewhere and failing to make an impact. Despite these limitations, applying a consistent set of criteria to every requirement helped to understand how the resulting research might be delivered and exploited for the benefit of the UK.

Through processing the requirements in this way, the potential development landscape was partitioned into eight 'topics' (Table 1). Four of the topic titles refer directly to relevant types of thermal hydraulic phenomena; Boiling and Condensation, Large-Scale Multiphase Flow, Turbulent Flow, Turbulent Heat Transfer. The 'Advanced Fluids^{22'} topic is focused on Gen IV reactor technologies using an unusual primary circuit fluid. The 'Multiphysics' topic examined the potential for combining thermal hydraulic modelling with the modelling of other physics. Two of the topics capture the higher level requirements around the use of modelling tools; Multi-fidelity and Best Practice and Uncertainty Evaluation.

The topics are described in more detail in the workshop briefing pack in Annex B and the requirements which can be linked to them, are summarised in Table 1. Although in some cases the requirements are assigned to a single topic only; this has generally not been possible in such a complex information environment, so there remains a 'many-to-many' mapping between topics and requirements. In addition, some requirements can be evaluated from a number of perspectives, so have been deliberately assigned to several topics. The numbered requirements are defined in Reference 5 and are therefore not reproduced in this document.

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²² The term 'advanced fluids' is used throughout this report to refer to liquid metals, molten salts and supercritical fluids used in many advanced modular reactor designs.



Topic	Linked User Requirements (Reference 5)
1: Multi-fidelity: The combined use of modelling methods across the full range of fidelities and scales (from DNS to system codes).	AGR_M_02, AGR_M_03, AGR_M_08, AGR_M_09, HTGR_M_04, LMFR_M_01, LMFR_M_03, LMFR_M_06, LMFR_M_07, LMFR_M_08, LMFR_M_10, PWR_M_06, SCWR_M_01
2: Best practice and uncertainty evaluation: Improving the confidence in and quality of model predictions.	AGR_M_05, LMFR_M_06, PWR_M_20, PWR_M_21, SCWR_M_01, SCWR_M_06
3: Boiling and condensation: The use of mechanistic modelling to improve predictions.	BWR_M_01, BWR_M_02, BWR_M_03, BWR_M_06, BWR_M_07, LMFR_M_05, PWR_M_01, PWR_M_03, PWR_M_09, PWR_M_10, PWR_M_11
4: Large-scale multi-phase flows: The prediction of the effects of complex, transient multi-phase flows.	BWR_M_04, BWR_M_05, BWR_M_08, BWR_M_09, PWR_M_01, PWR_M_02, PWR_M_04, PWR_M_08, PWR_M_16, PWR_M_17, PWR_M_22
5: Advanced fluids: The additional challenges of molten metals, molten salts and supercritical water.	LMFR_M_01, LMFR_M_02, LMFR_M_04, LMFR_M_05, LMFR_M_07, LMFR_M_08, LMFR_M_09, LMFR_M_13, LMFR_M_16, LMFR_M_17, MSR_M_03, MSR_M_04, MSR_M_05, MSR_M_06, MSR_M_07, SCWR_M_02, SCWR_M_03, SCWR_M_05, SCWR_M_06
6: Multiphysics: The coupling of thermal hydraulics modelling with neutronics and chemistry.	BWR_M_04, BWR_M_09, HTGR_M_05, HTGR_M_06, HTGR_M_07, HTGR_M_08, HTGR_M_09, HTGR_M_10, MSR_M_01, MSR_M_02, PWR_M_11, PWR_M_12, PWR_M_14, PWR_M_19, PWR_M_22
7: Turbulent flow: The prediction of pressure drops, mixing and buoyancy driven circulation.	AGR_M_01, AGR_M_04, AGR_M_06, HTGR_M_01, HTGR_M_02, LMFR_M_04, LMFR_M_07, LMFR_M_08, LMFR_M_09, LMFR_M_10, LMFR_M_11, LMFR_M_12, MSR_M_03, MSR_M_07, PWR_M_05, PWR_M_07, PWR_M_08, PWR_M_12, PWR_M_15, SCWR_M_02, SCWR_M_04
8: Turbulent heat transfer: The prediction of surface heat transfer and buoyancy influenced convection.	AGR_M_01, AGR_M_06, HTGR_M_03, LMFR_M_01, LMFR_M_07, LMFR_M_08, LMFR_M_09, LMFR_M_12, LMFR_M_15, PWR_M_05, SCWR_M_02

Table 1: Linking of Topics to Requirements

Processing of the requirements resulted in 4 'unlinked' requirements (AGR_M_07, LMFR_M_14, PWR_M_13 and PWR_M_18). Despite not being clearly linked to a topic, PWR_M_13 and PWR_M_18 are each indirectly progressed by at least one of the projects proposed in Annex A.

AGR_M_07 relates to access to HPC facilities and was omitted from the development of challenges because research into the further development of high speed computing capability is in the remit of computer scientists and beyond the scope of this project. The availability of HPC facilities in the UK is a matter of capital expenditure and infrastructure rather than innovation.

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However, increased use of advanced thermal hydraulic modelling tools will result in an increased need for HPC facilities as discussed in Section 2.4.

LMFR_M_14 relates to reactor coolant pumps and the broader topic of 'pumps'. The development of pumps (for a variety of applications) is a specialist area in itself. It is worth noting that the UK already has an established industry in the design and manufacture of nuclear and turbine island pumps which has endured despite the lack of UK based nuclear new build. Pumps have therefore been excluded from the current work on the basis that:

- A programme to 're-ignite' a dormant industry is quite different from a programme to expand and support an already very successful industry; and
- Considering pumps in appropriate detail would require another programme of not dissimilar scale as this one.

4.3 Development of Research Proposals

From the definition of the eight topics and their supporting information and requirements, a structured 2-day workshop was the primary method used to mature and develop the research and development recommendations. This approach maximised the involvement of the UK thermal hydraulic modelling community beyond the core team; engaging the wider community in this way had a number of key advantages:

- The nuclear thermal hydraulic modelling expertise in the UK is sparse with little duplication of experience between organisations. Therefore, to capture all of the available expertise, it was important to involve organisations outside the core team.
- The resulting R&D work is to be carried out by the UK community, for the UK community. To maximise the potential for exploitation and to ensure that all projects are practical and sensibly specified it was important to involve both those who will potentially be performing the research and those who will be using it.
- The workshop enabled a natural process of down-selection, as the community would be more inclined to focus on the areas of greatest need, and where the UK is well placed to deliver valuable work.
- The workshop gave an opportunity for the UK nuclear thermal hydraulics modelling community to come together for a common purpose. Opportunities to do this have been scarce over recent years.
- The workshop enabled dissemination of the work to date and both consolidated involvement in the project for those who chose to contribute to the requirements, and gave an additional opportunity for involvement for those who did not contribute at an earlier stage.

The workshop participants were selected and invited based on our previous stakeholder engagement activity. The intention was to maximise participation of the different types of users and Table 2 of Reference 5 demonstrates that all user groups were represented.

Annex B of this document provides further details on the workshop; it presents the briefing pack provided to stakeholders prior to the workshop along with the agenda for the days and a list of workshop participants. Stakeholders were engaged in advance of the workshop and given an opportunity to indicate which of the topic areas were of most interest to them.

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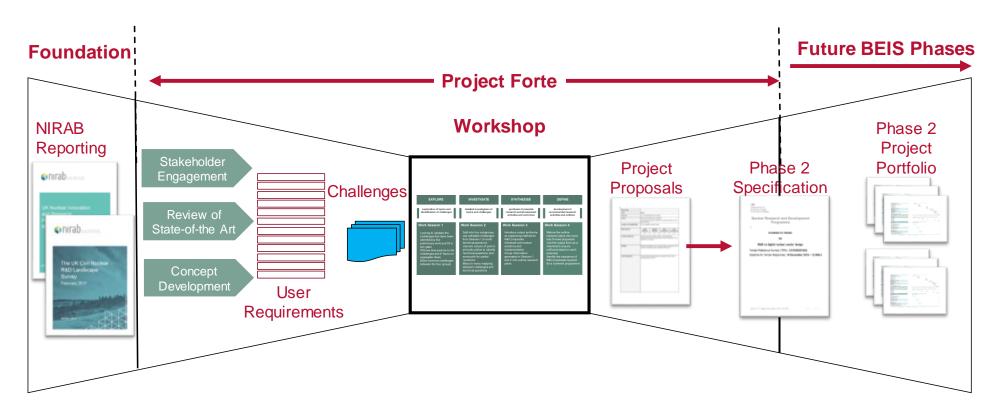


Figure 3: Workshop Information Flow

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Figure 3 shows the information flow for the workshop along with the eight topics, the input to the workshop was around 50 'user challenges'. These were developed from the linked user requirements and endeavoured to present the issues in a simpler, more succinct form. The challenges were carefully phrased to avoid specification of a solution approach or steering the workshop participants and to maximise the potential for innovative ideas. The challenges enabled the value of the previous work to be presented to the participants, although the participants were also given the opportunity to present additional challenges and the original user requirements were available to provide further information where required.

The workshop comprised four work sessions, which are summarised in Figure 4.

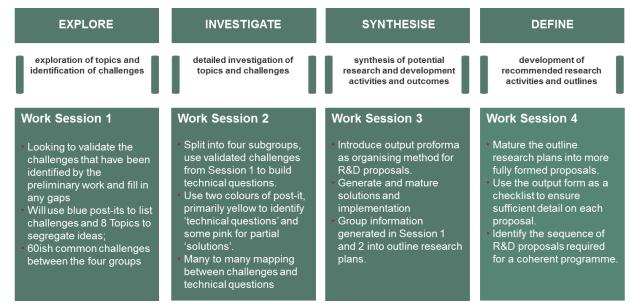


Figure 4: Workshop Approach

The first two sessions examined the initial challenges to ascertain the specific modelling deficiencies that related to that challenge. The second two sessions then considered and developed ways forward to address those deficiencies and therefore propose solutions to the challenges. Output from the workshop was used to develop the majority of the R&D proposals presented in Annex A.

Although the workshop was the primary source of the project proposals, in some cases a key individual was unable to attend the workshop and contributed a proposal separately. Additionally, a number of proposals were developed by the Project FORTE core team based on the initial Phase 1 research work or the previous experience and knowledge of the team. Each R&D proposal specification records its source for traceability.

The project proposals were then developed and reviewed by the core team and are presented in a consistent format in Annex A and discussed further in Section 6.

Not all of the challenges presented yielded a project proposal to address them. There were a variety of reasons for this, including:

- Stakeholder agreement that the area was already being well progressed internationally and that the UK would struggle to make a valuable contribution;
- The workshop participants did not know enough about the challenge to suggest a suitable way forward;

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- The challenge was extremely complex and it would be infeasible or too extensive to scope a project that resulted in an exploitable outcome in reasonable timescales; and
- Stakeholders considered the challenge to be of lower priority compared to the other challenges and therefore less workshop time was given to its development.

Following the workshop, the project team reviewed all of the project proposals against the initial set of challenges to check that nothing obvious had been missed. However, in the absence of any objective down-selection criteria, and based on the breadth of qualifications and experience that the stakeholders had, the 'natural selection' process that the workshop presented was considered a pragmatic method of down-selecting research and development ideas.

The resulting project proposals represent enough potential solutions and development approaches to occupy the available budgets several times over and will ensure a substantial feedstock of ideas for the planning and specification of Phase 2.

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5 Cross Industry Transfer

Nuclear thermal hydraulics involves consideration of a diverse range of phenomena relating to numerous components, but few aspects are entirely unique to it as a discipline. A wide range of industries exist that design and operate complex systems in a high value, high integrity and often regulated environment, and they encounter and are required to solve a related set of thermal and flow problems. Despite these similarities, and the potential for mutual benefit, it is not uncommon for particular tools or techniques to be predominantly used or even completely limited to a specific industry, often for historical reasons.

This section considers approaches to thermal hydraulic (and related) modelling used across a range of industries and identifies those with a possible overlap with, or a potential application to, the civil nuclear industry. Section 5.3 explains how these commonalities might be exploited and indicates where the investigation of specific opportunities for cross-over have been incorporated into the project proposals in Annex A.

5.1 Identification Approach

A working group of senior Frazer-Nash technical staff was assembled (including engineers and physicists), with an average experience of more than 15 years in industry and research, across a wide range of sectors. The group assessed what opportunities exist to transfer methods and approaches from other industries, by considering:

- What is done well in a given industry what is novel, highly effective or highly regarded?
- Where is there common-ground or shared challenges to allow bi-directional transfer?

The industries considered were:

- Transport (Aerospace, Automotive and Marine);
- Oil and Gas, Chemical and Process;
- Gas Turbines;
- Defence and Security;
- Conventional Power and Renewables;
- Nuclear Decommissioning; and
- Software and Modelling.

The working group identified a range of candidate technologies under each topic, which are briefly described below. While there are many items identified that are already activities performed in nuclear thermal hydraulics research and reactor development and analysis, it was the view of the group that many technologies identified are rapidly evolving, particularly given advances in computing power, and so may be able to supplement or supersede normal nuclear industry approaches. Similarly, the identification of commonality provides an indication of a diverse source of possible skilled engineers (of whom there is currently a shortage and will be necessary in the development of advanced nuclear technologies) and indicates where a disruptive or innovative perspective can be sought.

In order to exploit the identified technologies, a suitable engineering partnership would need to be found for the source technology and the nuclear application, and a technology transfer or collaboration project defined, in a similar manner to the project proposals defined in this specification.

In some cases what was identified were approaches and ideas that are not, of themselves, 'hard' transferrable methods, but are concepts noted to provide an inspiration from other fields.

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The candidate technologies state what is now considered possible or routine, and so can induce innovation, alter a mind-set or preconception, or they can reinforce a view that modelling and simulation is becoming ever more widely applicable. For example, methods and activities that were considered restricted to an academic or early stage R&D setting, say 10 years ago, are now, in some instances, part of routine design and analysis processes.

5.2 Candidate Technologies

5.2.1 Transport

From a thermodynamics and fluid mechanics perspective, the transport sector typically concerns itself with aerodynamic performance (drag and stability) and thermal management (e.g. within engine spaces).

- In the roadcar and racecar industries, the use of HPC CFD analysis in the inner design loop for aerodynamics and thermal management is now routine. This includes the resolved turbulence simulations of the transient flow behaviour that strongly influences the lift and stability of the roadcar.
- 2. The design of civil aircraft makes significant use of optimisation and adjoint methods to improve performance and quantify trade-offs.
- 3. The use of uncertainty quantification during design evaluation processes is strongly embedded in civil aerospace.
- The aerospace industry led the way in terms of standards and processes for V&V of numerical models.
- The concept of computer based 'digital twins' is well advanced in the automotive industry
 particularly to facilitate efficient manufacturing, assembly and maintenance scheduling, but
 also incorporating engineering analysis.
- Aerospace performs industry-wide benchmarking of simulation tools for, say, lift and drag
 and the performance or turbulence models. As part of this there are open access and
 standard representative, non-proprietary geometry and configurations available for use by
 the R&D community.
- High fidelity, unsteady resolved turbulence (LES) CFD is now common for aircraft
 components such as flaps and landing gear to predict, for example, stall behaviour or noise
 generation.
- 8. Assessment of aerospace standards and recommended practices to adopt mature best practice. Specifically:
 - NASA-STD-7009A 2016 STANDARD FOR MODELS AND SIMULATIONS, whose purpose is "... to reduce the risks associated with M&S-influenced decisions by ensuring the complete communication of the credibility of M&S results. ... [it] achieves this by establishing a minimum set of requirements for the key elements related to M&S, including development, maintenance, operation, results analysis, training, credibility assessment, and reporting." The parallel with decision making based on nuclear thermal hydraulics modelling and simulation is clear.
 - SAE ARP 4754A Guidelines for Development of Civil Aircraft and Systems. This standard deals with the role of whole system architecture in the allocation and distribution of safety critical functionality amongst diverse system elements and the consideration of the safe system design throughout the whole range of operating states. Components whose behaviour is dominated by thermal hydraulic

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phenomena contribute strongly to overall nuclear reactor safety in an analogous way.

5.2.2 Oil and Gas, Chemical and Process

The oil and gas, chemical and process industries share with the nuclear industry the potential for low probability accidents that can produce substantial environmental contamination, damage assets, and cause reputation damage for operators and the industry as a whole.

- 1. Quantitative Risk Assessment (QRA), specifically for fire, blast and pollutant dispersion.
- 2. Extensive and sophisticated multiphase flow simulation tools.
- 3. Huge validation datasets for multiphase flows at a range of flow regimes and components.
- 4. A culture of decision making that values "pedigree" in analysis code choice, and does not always choose the latest or more advanced tools. This is a feature common to nuclear thermal hydraulics and could be addressed with a common approach.
- 5. Issues regarding scaling of test and laboratory to operational conditions. This is an oil and gas requirement that may benefit from the rigour applied in nuclear thermal hydraulic scaling analysis.
- Recent interest and developments in data driven analysis and machine learning.
- 7. Experience in analysing the behaviour of systems and components with unusual and highly varying fluid properties.
- 8. Methods for performing simulations that involve long transients, including heat transfer to and within solid components.
- 9. There is a need for passive cooling and natural convection prediction tools, which is currently not that well done. This could be an opportunity for common development or transfer from nuclear thermal hydraulics.
- 10. The processes of fouling, particle transport, sedimentation, separation occur frequently and are well studied.

5.2.3 Gas Turbines

Gas turbines are used both for aerospace and marine propulsion and also for stationary power generation. They have been categorised separately to their application area because they represent a highly complex engineering discipline of their own. Of particular relevance to nuclear thermal hydraulics is the importance of heat transfer in gas turbines.

- The adoption of "digital twin" and service based life/condition assessment of components, which accounts for the operational history of components and transients that it has experienced. This includes the handling and interpretation of large datasets of measurements from a large installed base of common assets.
- 2. Gas turbine blade cooling passages include heat transfer processes and enhancement techniques with strong similarities to those seen in NPP.
- Systematic and quantifiable decision making to allow the reduction of conservatism and lowering of margins to improve performance and the economy of devices.
- 4. Coupled modelling methods, relating materials, structural, thermal and aerodynamic performance.
- 5. High fidelity CFD models that are used to capture the details of blade or combustor flows.
- 6. Benchmarking activities for simulation tools, for example for combustors.

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5.2.4 Defence and Security

While the defence industry has a different culture and goal to civil nuclear power generation, it considers the integrity of whole systems with multi-decade lifecycles, multi-layered protection and redundancy and the performance of equipment under extreme conditions or in a degraded state.

- Enterprise architecture meta-modelling or Model Based Systems Engineering (MBSE) where the interaction of the requirements of the system are elucidated across its whole life
 cycle from concept to decommissioning and the costs modelled, dependencies captured
 and trade-offs identified.
- 2. Noise and vibration, particularly flow and acoustic induced vibration in pipework systems.
- 3. Machine learning techniques (e.g. intelligence algorithms).
- 4. Shock, blast, fire, dispersion and evacuation modelling.
- 5. Simulation of free surface flows and cavitation for naval applications.
- 6. High integrity and high fidelity simulators and training tools (e.g. for submarines or helicopters), including mathematical models capable of predicting the response of the 'platform' to operator actions in real-time.

5.2.5 Conventional Power and Renewables

Coal generation and Combined Cycle Gas Turbine (CCGT) thermal plants share many of the same performance issues as nuclear generation. However, they have a dissimilar culture for the consequences of failure of components, where failure causes economic damage, but does not have the nuclear safety consequences.

- 1. Modern coal power plants use supercritical steam power cycles. This experience of design and analysis is directly transferrable to SCWR design.
- Conventional thermal power plants as well as molten salt thermal storage for solar power plants are considering supercritical CO₂ power cycles. These are an attractive option for high temperature advanced reactors too.
- 3. Analysis of high temperature heat exchangers (i.e. boilers or steam generators), including depositions, fouling, corrosion and erosion of tubes.
- 4. Flow and acoustic induced vibrations and the associated fatigue damage of components. In some cases this will relate to very similar components to those found in reactor circuits.
- 5. Multiphase flows including boiling, sprays and droplet flows.

5.2.6 Nuclear Decommissioning

While still part of the nuclear industry, decommissioning often involves organisations that are not necessarily well connected to the developers of advanced reactor technologies, and focusses on other aspects of thermal hydraulics that are not primarily to do with reactor core or primary circuit operation.

- 1. Fouling, particle transport and sedimentation.
- 2. Nuclear ventilation and containment including natural ventilation and passive cooling.
- 3. Cask and flask modelling for fuel transport and storage, particularly passive cooling of these items and their fire-worthiness.

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5.2.7 Software and Modelling

Software and modelling is not an industry of itself, but there are advanced methods and tools that practitioners are able to apply to any industry with complex systems, nuclear thermal hydraulics being no exception.

- Probabilistic approaches to uncertainty quantification analysis, including the incorporation of sparse measurements into predictive models to increase their accuracy by a known amount.
- The application of data reduction, machine learning and model fitting to synthesise the
 results of large numbers of highly detailed simulations to an emulator (e.g. a response
 surface) able to be used in rapid design assessments or as a sub-component of larger
 simulations.
- 3. Development and use of HPC facilities enabling the industrial use of advanced modelling, data processing, digital twins, machine learning and AI (Artificial Intelligence).
- 4. Using cloud computing to dynamically scale the resources available to run intensive modelling campaigns, such as large scale Multi-disciplinary Design Optimisation (MDO).
- 5. Handling, processing and visualisation of very large datasets.
- The use of high level systems engineering definitions of complex systems to drive and define the requirements for, and conclusions needed from, nuclear thermal hydraulics models.

5.3 Exploitation of Technologies

The difficulty of, and route to, incorporating and exploiting the identified technologies in nuclear thermal hydraulics R&D varies from the straight-forward (where a service or skill can be bought/contracted openly and is prevalent in the UK) to the difficult (where a change in culture, regulatory approach or to standards is required). In general, the transferable skills are vested in the engineers and organisations delivering capabilities into each sector, and so any transfer is likely to be most effectively achieved by partnering agreements.

Despite potential difficulties, it is recommended that the potential of cross-industry transfer to deliver shorter timescales and reduced costs is specifically promoted for all aspects of the Nuclear Innovation Programme. To this end, several of the identified technologies relating to thermal hydraulics already constitute part of the project proposals defined in Annex A:

- Several of the projects aim to increase the use of resolved turbulence CFD in the nuclear thermal hydraulics design and analysis process. The automotive and aerospace sectors have already incorporated this.
- Developments in supercritical CO₂ are proposed in project P5_D, which is directly applicable to a wider range of power generation technologies.
- Noise and vibration, including the fatigue that it drives, are large issues in oil and gas and aerospace, and the methods and capabilities can be readily transferred to project P7_C.
- Machine learning and model reduction methodologies are parts of projects P1_B and P6_C.
- Benchmarking of tools that are used in the aerospace and gas turbine industries could complement the engagement that is planned in project P2_A.

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There are also several technologies that could be considered as a high-priority and proactive efforts should be made to explore transfer and collaboration. Specifically:

- Oil and gas, chemical and process industries make extensive use of multiphase models and have large validation datasets. There is the potential to improve two-phase models relevant to nuclear thermal hydraulics by exploiting this; and
- The adoption of "digital twin" approaches to capture and predict the drivers for component damage mechanisms (many of which arise from thermal hydraulic effects), allowing a reduction in conservatism in life assessments.

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6 Research and Development Project Proposals

The primary output from this stage of the work has been the specification of proposals for research and development that will develop the UK (and the world) capability in nuclear thermal hydraulic modelling. They comprise 34 distinct projects, which is a testament to the knowledge and innovation of the UK nuclear thermal hydraulic community. All of the project proposals are included in Annex A. Each project has a reference of the format PN_A, PN_B... where N refers to the topic number (1 to 8) defined in Table 1 that denotes where it arose.

To complete all of the projects proposed is expected to be beyond the budget of short-term funding opportunities. However, the surplus of projects allows for extension of the programme beyond the original timeline and adaptation of the technical focus depending on the outcomes of other UK government initiatives. This is discussed further in Section 7.

- Section 6.1 analyses the proposals in the context of achieving the programme objectives.
- Section 6.2 discusses the overall contribution of the proposed research to UK capability.
- Section 6.3 summarises the potential for interaction with the new UK Test Facility.
- Section 6.4 discusses how these projects align with other parts of the broader Digital Reactor Design programme.

6.1 Analysis of Project Proposals

The purpose of the BEIS programme is not to perform research purely for the advancement of science, but to enhance UK capability and thereby enable the expansion of the UK civil nuclear industry. As discussed in Section 2, this needs to consider aspects of capability beyond the modelling tools themselves.

To appreciate if and how the proposed projects fit this objective it is important to understand how they deliver capability enhancements, and how they might be exploited. In order to achieve this, each of the proposed projects has been:

- Linked to the capability vision (Figure 1);
- Assessed in the context of achieving the BEIS programme objectives (Section 1.2); and
- Linked to the user requirements (Reference 5).

The links to the capability vision and the BEIS programme objectives are presented in Table 2 and Table 3. The links to the user requirements are included in Annex A, Section A.1.2. Table 2 highlights (in green) the types of capability development expected as an outcome from each proposal. It is noted that undertaking any of the proposed research in nuclear thermal hydraulics almost inevitably results in UK skills development, both for those undertaking the work and those attending the forums where it is presented - this is reflected in Table 2 by the lighter green highlighted regions.

Table 3 highlights (in green) where the project makes the strongest contribution to furthering the BEIS programme objectives. As discussed above it is noted that, if carried out in the UK, all of the projects will result in improvements to the skills of the UK workforce. Similarly all of the projects have the potential to result in an opportunity to get involved in an international programme (depending on future international activity in this area). This is indicated in the table by the lighter green highlighted regions.

The analysis concluded that all of the project proposals describe work which, if undertaken, would make a positive contribution to enhancing the UK capability and progressing the BEIS long term aims in addition to contributing to addressing the user requirements.

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Project Ref.	Project Title	Type of Capability Development							
		Personnel	Hardware/ infrastructure	Concepts and Doctrine	Modellii	ng Methodo	ogy and	Software	Solution
					Physical Understanding	Physical/ Empirical Mathematical Models	Modelling Tools	Inputs	Verification and Validation
P1_A	Development of innovative coarse grid models for reactor design								
P1_B	High fidelity modelling to improve the accuracy of low fidelity methods								
P1_C	Reducing the cost of CFD - Efficient and effective meshing								
P2_A	Increased participation in benchmarking								
P2_B	Maximising UK collaboration and collective learning								
P2_C	Sensitivity and Uncertainty Analysis of a Reduced-Order Model for Simulating BWR Dynamics								
P2_D	UK LWR predictive modelling validation centre								
P3_A	Improving the prediction of heat transfer by fundamental multi-scale modelling of bubble growth process								
P3_B	Improved two-phase flow regime transition modelling								
P3_C	Film dry-out modelling in CFD								
P3_D	Improved component scale boiling model								
P3_E	Prediction of DNB using CFD								

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Project Ref.	Project Title	Type of Capability Development							
		Personnel	Hardware/ infrastructure	Concepts and Doctrine	Modellii	ng Methodo	logy and	Software	Solution
					Physical Understanding	Physical/ Empirical Mathematical Models	Modelling Tools	Inputs	Verification and Validation
P4_A	Modelling of fuel clad ballooning following LOCA								
P4_B	CFD modelling of macroscopic convective boiling flows in NPP								
P5_A	Dissolved gas transport in molten metals and molten salts								
P5_B	Molecular dynamics capabilities for thermophysical, thermogravimetric phase equilibrium prediction over lifecycle								
P5_C	Heat transfer correlations for mixed convection and transitional flows in MSRs								
P5_D	Supercritical CO ₂ power cycles								
P5_E	Liquid metal heat transfer modelling								
P5_F	Modelling of cover gas dynamics								
P5_G	Predicting heat transfer to supercritical fluids								
P6_A	Coupled tool selection								
P6_B	Tritium generation and migration in advanced reactor coolants								
P6_C	Coupled 3D neutronics and CFD thermal hydraulics applied to BWR fuel channels								

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Project Ref.	Project Title	Type of Capability Development							
		Personnel	Hardware/ infrastructure	Concepts and Doctrine	Modellii	ng Methodo	logy and	Software	Solution
					Physical Understanding	Physical/ Empirical Mathematical Models	Modelling Tools	Inputs	Verification and Validation
P6_D	State of the art CRUD deposition models and the effects on heat transfer mechanisms								
P6_E	Modelling of air ingress accidents in HTGRs								
P7_A	Improved prediction of flow and thermal development in fuel pin cooling passages								
P7_B	Improved accuracy of RANS models for turbulent heat convection								
P7_C	Improving the ability to predict structural vibration in reactor design								
P7_D	Predicting and assessing thermal fatigue								
P7_E	Improved prediction of the stalling of natural circulation flows								
P7_F	improved prediction of passive cooling in NPP containment volumes								
P8_A	Investigate the impact of 'real' surfaces on NTH heat transfer modelling predictions								
P8_B	Improved wall models for accurate heat transfer								

Table 2: Project Links to Capability Development

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Project Ref.	Project Title			BEIS Program	nme Objectives		
		Enhanced designs and increased productivity	Increased uptake of modern digital engineering practices	Improved understanding of safety and through-life performance	Greater predictive modelling capacity and understanding of passive safety	Highly skilled workforce	Leverage to facilitate UK participation in international activities
P1_A	Development of innovative coarse grid models for reactor design						
P1_B	High fidelity modelling to improve the accuracy of low fidelity methods						
P1_C	Reducing the cost of CFD - Efficient and effective meshing						
P2_A	Increased participation in benchmarking						
P2_B	Maximising UK collaboration and collective learning						
P2_C	Sensitivity and Uncertainty Analysis of a Reduced- Order Model for Simulating BWR Dynamics						
P2_D	UK LWR predictive modelling validation centre						
P3_A	Improving the prediction of heat transfer by fundamental multi-scale modelling of bubble growth process						
P3_B	Improved two-phase flow regime transition modelling						
P3_C	Film dry-out modelling in CFD						
P3_D	Improved component scale boiling model						
P3_E	Prediction of DNB using CFD						
P4_A	Modelling of fuel clad ballooning following LOCA						
P4_B	CFD modelling of macroscopic convective boiling flows in NPP						

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Project Ref.	Project Title			BEIS Program	nme Objectives		
		Enhanced designs and increased productivity	Increased uptake of modern digital engineering practices	Improved understanding of safety and through-life performance	Greater predictive modelling capacity and understanding of passive safety	Highly skilled workforce	Leverage to facilitate UK participation in international activities
P5_A	Dissolved gas transport in molten metals and molten salts						
P5_B	Molecular dynamics capabilities for thermophysical, thermogravimetric phase equilibrium prediction over lifecycle						
P5_C	Heat transfer correlations for mixed convection and transitional flows in MSRs						
P5_D	Supercritical CO ₂ power cycles						
P5_E	Liquid metal heat transfer modelling						
P5_F	Modelling of cover gas dynamics						
P5_G	Predicting heat transfer to supercritical fluids						
P6_A	Coupled tool selection						
P6_B	Tritium generation and migration in advanced reactor coolants						
P6_C	Coupled 3D neutronics and CFD thermal hydraulics applied to BWR fuel channels						
P6_D	State of the art CRUD deposition models and the effects on heat transfer mechanisms						
P6_E	Modelling of air ingress accidents in HTGRs						
P7_A	Improved prediction of flow and thermal development in fuel pin cooling passages						
P7_B	Improved accuracy of RANS models for turbulent heat convection						

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Project Ref.	Project Title	BEIS Programme Objectives					
		Enhanced designs and increased productivity	Increased uptake of modern digital engineering practices	Improved understanding of safety and through-life performance	Greater predictive modelling capacity and understanding of passive safety	Highly skilled workforce	Leverage to facilitate UK participation in international activities
P7_C	Improving the ability to predict structural vibration in reactor design						
P7_D	Predicting and assessing thermal fatigue						
P7_E	Improved prediction of the stalling of natural circulation flows						
P7_F	Improved prediction of passive cooling in NPP containment volumes						
P8_A	Investigate the impact of 'real' surfaces on NTH heat transfer modelling predictions						
P8_B	Improved wall models for accurate heat transfer						

Table 3: Project Links to BEIS Objectives

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6.2 Contribution to UK Capability

Considering the content of the project proposals in the context of the type of capability development they describe (Table 2), a number of observations can be made about the proposals as follows:

- There is an emphasis on projects that develop modelling methods and tools. This is as expected, because it is the tools and the mathematical models which under-pin them that most people think of when they consider a modelling capability. This is consistent with the BEIS ITT for this task, which also refers to the capability in this way.
- Many of the projects provide an element of guidance and/or training, even if that is not main purpose of the work. This is an area that is in the forefront of the minds of many UK nuclear engineers who have experienced the decline in UK skills over several decades. It is a pertinent and timely concern, given that the UK will need to grow the magnitude of our capability, potentially quite quickly, to be able to be extensively involved in reactor design again.
- Many of the projects focus on the demonstration and validation of modelling techniques in a nuclear context. It is important to understand that a functionality to do something in a modelling tool does not in itself constitute an industry-ready capability. The demonstration and validation of methods in a nuclear context is key to their successful exploitation.
- There is an emphasis on further developing CFD modelling techniques over and above other modelling methods. This is illustrative of the UK's strengths and demonstrates where researchers believe they have most value to add. However, reactor designers also need lower fidelity methods (often as a higher priority), so this emphasis could be of concern, particularly if available international tools do not provide what is needed.
- Many of the projects focus on a particular technology or aspect of reactor design to demonstrate the intended innovation in an exploitable way. However, in many cases, this specific focus is not essential for a successful outcome. The detailed scope of these projects could be modified to be more generally applicable or to use an alternative demonstration vehicle depending on the overall content of the Phase 2 programme and reactor design activities in the UK.

By considering the type of capability development which would result from fulfilling the main objectives of the project proposals, the projects fall into three groups that are discussed in Section 6.2.1 to Section 6.2.3.

6.2.1 Enabling Projects

Two of the workshop discussion topic areas and a number of the developed projects consider the UK thermal hydraulic modelling capability at a high level. These projects are not primarily concerned with developing any specific aspects of the modelling of thermal hydraulics phenomena or any specific reactor technology, but are focused on developing, supporting and maximising the overarching aspects of what makes a capability successful.

Projects P2_A, P2_B and P2_D are examples of proposed projects that consider the development of the UK nuclear thermal hydraulics community and infrastructure with a high emphasis on collective learning, skills development and exploitation. It is recommended that Project P2_B should form an integral part of the management of Phase 2 of this programme, thereby reducing the cost and maximising the value of the Phase 2 programme.

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6.2.2 The Exploitation of Modelling Methods and Tools

A number of proposals (for example P1_A, P6_A or P7_C) look at either: reducing the cost to industry of using state-of-the-art tools; investigating techniques from other countries/industries in a UK nuclear thermal hydraulics context; combining existing methods in an innovative way; or applying advancements in modern computing to enable tools to be refined and used more effectively.

These projects do not therefore advance the science of nuclear thermal hydraulics; they enable the use of the most advanced methods in a UK industrial context. From a capability development perspective these projects are focused on producing exploitable outputs and short term benefits, and represent 'development' rather than 'research'.

6.2.3 The Advancement of Engineering Science

The majority of the project proposals are aimed at improving the state-of-the-art in thermal hydraulic modelling in a wide variety of NPP relevant areas. Many of these would form a valuable contribution and a step forward in world capability, as well as supporting UK based activity. Technical areas of interest include:

- Passive cooling;
- Boiling and two-phase heat transfer;
- Gen IV reactor fluids:
- Multiphysics modelling; and
- Single phase turbulent heat transfer.

6.2.4 Project Personnel

To achieve the aims of the programme, the project personnel should be chosen to maximise the development of industry capability. It is important to recognise that this does not mean that academic organisations do not have a role to play. Much of the most up to date knowledge in advanced reactor technologies, international nuclear contacts and significant expertise in the use of state-of-the-art methods and tools are within UK universities. To maximise the exploitation of these assets and knowledge transfer to UK industry it is recommended that industry and academic engineers work together on the majority of the Phase 2 tasks.

6.3 The UK Test Facility

The need to use experimental data to validate modelling advances is a key stage in providing confidence in the predictions of any model. In a highly regulated industry, such as civil nuclear, this confidence is of particular importance where the predictions relate to matters of nuclear safety. Referring back to the modelling capability depicted in Figure 1 and described in Section 2, testing directly contributes to:

- Improving physical understanding through observation;
- Providing data for the development of empirical mathematical models;
- Proving input data in the form of fluid material properties; and
- Validation of modelling results.

The provision of a UK test facility has always been seen as an integrated part of this programme of model development. Although, it is recognised that any new UK test rigs would not be available for use in the timeframe of Phase 2 of this project, much of the proposed research is one 'step' in a journey towards a complete solution and the ability to acquire additional data in

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the future is key to validation and ultimate exploitation. Each of the proposed research projects considers validation and assessment of applicability of the developed tools for NPP (taking into account test facility scalabilities and test and modelling uncertainties) and highlights where there is a significant risk that the required data is not currently available and further testing would be needed. The specific validation data needs associated with each of the proposed projects are documented in more detail Reference 7.

Project P2_C goes a step beyond identifying the need for additional validation data and actually proposes initiation of the concept design of a test rig to generate the required data as one of the tasks under the scope. It would be expected that a number of the other projects would also wish to do this as a 'next step' if appropriate validation data is not available in the public domain. For example, the availability of high quality experimental data for buoyancy driven flow has already been identified as an area of high risk.

6.4 Virtual Engineering Platform and Multiphysics Modelling (WP1)

The Virtual Engineering and Modelling and Simulation work streams form Work Package 1 of BEIS's Digital Reactor Design programme (with Thermal Hydraulics tasks comprising Work Package 2). As both work streams progress it is increasingly important that they collaborate to enable a cohesive outcome. To-date this has been progressed via input of the organisations involved into each other's projects, a number of dedicated meetings/ teleconferences and the NIP CG (Nuclear Innovation Programme Contractors Group).

The extent and specific scope of the collaboration at any point in time is heavily dependent on the capability of the 'virtual engineering platform' at that time. In principle, almost all of the research and development work proposed in Annex A could be carried out using a 'complete' virtual engineering platform. However, as both projects are progressing in parallel, it is likely that much of the thermal hydraulics projects will require functionality that is not yet available, especially at the Phase 2 stage.

The two projects are currently actively engaged in planning collaborative activities for Phase 2 and the number and range of these activities is likely to develop throughout the remainder of the Phase 1 stages. The following opportunities have been identified to date:

- The use of thermal hydraulic modelling tools as part of an integrated reactor design process is a key part of achieving the aims of the overall programme. Enabling the virtual engineering platform to interface with state-of-the-art commercial/international nuclear thermal hydraulic modelling tools would create collaboration opportunities with the thermal hydraulics project. Providing sufficient functionality is available near to the start of Phase 2 of this project, the opportunity for collaboration is specifically identified in projects P2_A and P2_B.
- The 'modelling and simulation' work package, under the Virtual Engineering project, is aimed at the integration of nuclear radiation modelling with CAD to improve the prediction of component through-life structural performance. This work is planned for Phase 2 of the Virtual Engineering, Modelling and Simulation project. A number of the projects proposed in Annex A consider multiphysics modelling, including the combination of thermal hydraulics and neutronics modelling (for example P6_A, P6_C). It is extremely likely that a collaborative approach to these projects would be of mutual benefit.

By the end of Phase 2 of both projects, the virtual engineering platform is anticipated to be considerably advanced. For Phase 3 of both projects it is recommended that the thermal hydraulics project make more extensive use of the platform. For example, projects P2_C, P2_D, P4_A, P7_C, P7_D, should be considered for extension under Phase 3 to include demonstration of coupling using the platform.

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7 R&D Prioritisation

As discussed previously, the entire portfolio of project proposals will likely exceed the short term funding opportunities. The projects vary in the size of their scope but, as an initial estimate, one could consider the budget for each would need to be between £300k and £1m. Choosing a mean value of £500k would result in all 34 projects requiring a total of around £17m to complete, which is considerably greater than the budget suggested for Phase 2 of this project. However, as discussed earlier in this document, the current UK strategy does not present any objective criteria on which to further down-select or prioritise the research. The process of prioritisation of UK nuclear thermal hydraulic research therefore becomes one that is both subjective and possibly contentious.

The contentious nature of any prioritisation stems from the current lack of clarity and range of possible futures for the UK civil nuclear industry. Many stakeholders have strongly held views and opinions on what they believe that future will or should be, and at the current time there is little empirical basis to narrow the field. The impact of this 'plurality of views' is discussed further, with examples, in Section 7.1. A number of risks and enablers to the current programme are discussed in Section 7.2

The subjectivity arises primarily because which projects are the most important, depends entirely on your point of view, goals and ambitions. For example, much of the two-phase flow model development work is of interest to light water reactor designers and operators, but of limited interest to those working in gas-cooled designs. Some of the projects have a wider technology remit, but may not be as easily exploited by any particular technology. In short, any assessment of the impact of the project is dependent on the stakeholder group you consider. Potential programmes of work depending on the future research focus are explored in Sections 7.3 and 7.4.

7.1 Plurality of Views

This project has sought throughout to engage with the UK and international community in addition to exploiting the expertise within the core team. Those consulted were requested to both prioritise and 'explain' at various stages, first their requirements, and secondly their proposed ideas. This engagement revealed a plurality of views, some of which could be considered as directly opposing 'schools-of-thought'. Because this project has been fortunate enough to enjoy contributions from many with long and illustrious careers in this area, it would be unwise to dismiss this lack of consensus. Strongly held differences in opinion on particular topics is often indicative of there being no single 'right' way forward and both points of view are likely to have merit.

To illustrate the challenge of the situation in the context of prioritising the proposed research in this project, two illustrative examples of opposing 'schools-of-thought' are given below:

Example 1: Should UK R&D prioritise LWR or Gen IV technologies?

- Viewpoint A: With the current Gen III new-build and UK based small PWR activity, the UK's most urgent requirement is for skills, methods and tools relating to the design and operation of LWR reactor technologies. The timescales for Gen IV reactor deployment are much longer and it is currently very uncertain that any will actually be designed or deployed in the UK. Therefore, R&D related to LWR technologies should clearly be the priority for the UK.
- Viewpoint B: LWR technologies and their associated methods and tools have been extensively developed internationally over several decades and are widely and

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successfully deployed. The UK has already 'missed the boat' in these areas; both BWR and PWR technologies are mature and further development in this area should not require government funding. In Gen IV technologies however, the door is still open for the UK to play a major role and investment in R&D at this stage could make a significant difference. It is clear that investment in R&D to support Gen IV technologies should be the priority for UK government.

Example 2: What is the future role of CFD in nuclear thermal hydraulics?

- Viewpoint A: We are on the verge of a revolution in nuclear thermal hydraulic modelling. Whilst previously a lack of computing power limited the extent to which detailed 3D modelling methods could be used, recent advances in HPC have removed those barriers and the next generation of nuclear reactors can be designed without the extensive (and expensive) empirical databases of the past. With these methods at our disposal the traditional tools will be superseded, so from an R&D perspective it is clear that CFD is where the UK should be investing our efforts.
- Viewpoint B: CFD is a flexible and powerful tool, but its ability to make a significant contribution to NPP thermal hydraulic modelling is far in the future. The complexity of NPP design and the importance of thermal hydraulics are such that it is not feasible to make predictions entirely from first principles. Furthermore, the regulatory framework requires, and will continue to require, experimental investigation and validation to underpin modelling predictions. The internationally used nuclear tools (system and sub-channel codes) provide a robust and accepted toolset that should be built on and expanded to encompass new designs.

These are only 2 examples, but it can be easily seen that which viewpoint is supported completely changes which projects should be undertaken as part of Phase 2. Indeed, such are the differences in opinion, it is likely that none of the contributing stakeholders or readers of this document will agree with all of what is proposed as R&D projects in Annex A.

7.2 Programme Risks and Enablers

Taking into account the fact that it will not be possible to satisfy everyone, and that there is more than one route to success, the key to the success of Phase 2 is that it aligns with UK policy and other UK R&D activities.

There is a significant risk that the breadth of the current programme will result in the Phase 2 budget being spread thinly over a variety of areas and therefore failing to make an impact in any. There is also a risk that the efforts of this project will not align well with the other areas of government funded research and the programme as a whole will fail to deliver a cohesive outcome. With no shortage of innovative ideas, what this project needs most urgently is a rationale for focusing its efforts. For the reasons discussed in Section 7.1, and that nuclear thermal hydraulics is only one aspect of the science and engineering of a nuclear reactor, it can be concluded that it is not sensible for the Project FORTE team (or indeed any of the UK nuclear thermal hydraulics community) to make this decision alone.

Since the start of this project other government civil nuclear initiatives have 'moved on'. For example, the 'Nuclear Sector Deal' (Reference 4) was published in June 2018 and there has been a clear demarcation between LWR technologies and 'advanced' reactor technologies with the SBRI Advanced Modular Reactor (AMR) Competition. It is hoped that the thinking behind such developments will enable some clearer guidance to be provided as to the short term (next 3 years) and longer term (next 15 years) goals for this programme.

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Areas where policy input would provide a key enabler for this project are:

- **Most importantly:** Direction regarding the relative emphasis to place on research that is predominantly targeted at LWRs and that which targets other, advanced reactor types.
- Direction regarding the relative importance of the benefits of this particular programme of research. For example, if the priority is developing a skilled workforce in the longer term, the use of university PhDs can be a good, if somewhat indirect, way of achieving this end. However, if the priority is on the achievement of exploitable outcomes, the use of more experienced researchers and organisations to complete the work will give a greater chance of success.
- Direction regarding which (if any) international programmes and partner countries are the highest priority. There are likely be political or technical reasons why some programmes should be targeted in preference to others. For example, a programme that offers good collaboration opportunities for a number of UK initiatives may be selected as a priority even if the nuclear thermal hydraulics aspects are no better than others. Additionally, it may be appropriate for the UK Government to seek or promote collaboration with some countries for political reasons.

7.3 Potential Programmes of Work

Given the expected budget available for Phase 2 and costs per-project, and the expectation that not all reactor technologies will ultimately be supported, it will be necessary to choose only a subset of the proposals that have been created. The resources required for the projects are primarily expressed in terms of engineer time. Although in some cases other costs are also anticipated, engineer time is considered to be the dominant factor in determining cost. A full time post-doctoral researcher, under full economic costing, costs approximately £100k to 125k per annum. An FTE (full-time equivalent) industrial consultant would cost £100k to £200k per annum depending on experience.

On this basis, the proposals have been grouped into programmes, centred on either a reactor technology or a modelling technology. These are described below with discussion on choosing a subset of projects to achieve a specific aim given in Section 7.3.4.

7.3.1 Reactor Technology Programmes

Based on the current new build projects in the UK, and the reactor developers selected in Phase 1 of the AMR competition (Reference 4), five project programmes (Table 4) have been identified that group the project proposals that are specific to supporting the following reactor technologies:

- RP_1. Gen III and SMR PWR New Build (PWR).
- RP_2. Gen III BWR New Build (BWR).
- RP_3. High Temperature Gas-cooled Reactors (HTGR).
- RP_4. Liquid Metal Fast Reactors (LMFR).
- RP_5. Molten Salt Reactors (MSR).

7.3.2 Modelling Technology Programmes

The majority of the projects are either generic or applicable to more than one reactor technology, therefore programmes of project proposals have been grouped by modelling application (

Table 5)

in the following areas:

MP_1. Improved value from UK modelling capabilities.

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- MP_2. Two-phase water modelling.
- MP_3. Support to structural integrity assessment.
- MP_4. Single phase heat transfer and passive cooling.
- MP 5. Support across all Gen IV technologies.
- MP_6. Support to supercritical CO₂ power cycles.

Supercritical CO₂ power cycles are a promising prospect for improving the efficiency of high temperature (Gen IV) reactors. The inclusion of a programme on its own (MP_6), as opposed to combining it with the broader Gen IV technologies (MP_5) reflects that it could be pursued as an international technology programme in its own right, not just as part of a Gen IV reactor development.

7.3.3 Phase 1 Projects

Research and development work currently underway under Phase 1 of this programme has already achieved significant progress. The work, led by the University of Manchester and the University of Sheffield (with direct contribution from the industry participants within the core team) comprises:

- 'Smart models for reactor components' develops innovative coarse-grid CFD, bridging the gap between high fidelity meshed methods and lower fidelity sub-channel methods. This project contributes to the development of tools by building on extant CFD and sub-channel modelling tools to provide an innovative, combined tool relevant across a range of reactor technologies.
- 'Single-phase active and passive flows and regimes' develops, refines and validates advanced models for a number of test cases covering both forced and naturally driven convection. This project considers both modelling tools and the underpinning mathematical models, addressing key thermal hydraulics phenomena affecting heat transfer and nuclear safety within a reactor.
- Innovative methods to model two-phase flow and heat transfer' develops and tests both conventional finite volume CFD and a novel Smoothed Particle Hydrodynamics (SPH) method. The projects demonstrate the use of these modelling tools relevant to both small and large PWR and BWR.
- Different cooling fluid media' recovers unpublished historical UK test data on sodium aerosols in a cover-gas and uses them to develop and validate a multiphysics model for an SFR cover gas region. It also develops a preliminary model for the upper plenum of the E-SCAPE test facility a 1/16th model of MYRRHA under commissioning at SCK·CEN. Further work continues to address the challenges of modelling fluids with a low Prandtl number. This project develops and demonstrates modelling tools and methods directly relevant to the development and licencing of LMFRs.
- Participation in an international benchmarking exercise comprising the modelling of a four-rod bundle under mixed convection. This work provided both useful validation evidence and enabled direct participation by the project in an international programme.

The output of these tasks is relevant to, or naturally leads to, a number of the proposed projects. Specifically, projects P1_A, P2_A, P4_B, P5_E, P5_F and P7_A summarise work that has already been progressed under the Phase 1 programme, and propose extensions to be carried forward in Phase 2. These are included on an equal footing with the new project proposals created but are highlighted in green in Table 4 and

Table 5.

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RP_1 - Su	pport to Gen III and SMR PWR New Build
P4_A	Clad ballooning following LOCA
P6_D	State of the art CRUD deposition models and the effects on heat transfer mechanisms
P7_F	Improved prediction of passive cooling in NPP containment volumes
RP_2 - Su	pport to Gen III BWR New Build
P2_C	Sensitivity and Uncertainty Analysis of a Reduced-Order Model for Simulating BWR Dynamics
P6_C	Coupled 3D neutronics and CFD thermal hydraulics applied to BWR fuel channels
RP_3 - Su	pport to High Temperature Gas Cooled Reactors
P6_E	Modelling of air ingress accidents in HTGRs
RP_4 - Su	pport to Liquid Metal Fast Reactors
P5_A	Dissolved gas transport in molten metals and molten salts
P5_E	Liquid metal heat transfer modelling
P5_F	Modelling of cover gas dynamics
RP_5 - Su	pport to Molten Salt Reactors
P5_A	Dissolved gas transport in molten metals and molten salts
P5_B	Molecular dynamics capabilities for thermophysical, thermogravimetric phase equilibrium prediction over lifecycle
P5_C	Heat transfer correlations for mixed convection and transitional flows in MSRs

Table 4: Programmes of project proposals to support specific reactor technologies

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MD 4 Jane	anne de cale a forma LIIV en a dell'e e camp dell'idea
	proved value from UK modelling capabilities
P1_A	Development of innovative coarse grid models for reactor design
P1_B	High fidelity modelling to improve the accuracy of low fidelity methods
P1_C	Reducing the cost of CFD - Efficient and effective meshing
P2_A	Increased participation in benchmarking ²³
P2_B	Maximising UK collaboration and collective learning
	o-phase water modelling
P2_D	UK LWR predictive modelling validation centre
P3_A	Improving the prediction of heat transfer by fundamental multi-scale modelling of bubble growth process
P3_B	Improved two-phase flow regime transition modelling
P3_C	Film dry-out modelling in CFD
P3_D	Improved component scale boiling model
P3_E	Prediction of DNB using CFD
P4_B	CFD modelling of macroscopic convective boiling flows in NPP
MP_3 - Sup	pport to structural integrity assessment
P7_C	Improving the ability to predict structural vibration in reactor design
P7_D	Predicting and assessing thermal fatigue
MP_4 - Hea	at transfer and passive cooling modelling
P7_A	Improved prediction of flow and thermal development in fuel pin cooling passages
P7_B	Improved accuracy of RANS models for turbulent heat convection
P7_E	Improved prediction of the stalling of natural circulation flows
P8_A	Investigate the impact of 'real' surfaces on NTH heat transfer modelling predictions
P8_B	Improved wall models for accurate heat transfer
MP_5 - Sup	oport across all Gen IV technologies
P6_A	Coupled tool selection
P6_B	Tritium generation and migration in advanced reactor coolants
MP_6 - Sup	oport to supercritical CO ₂ power cycles
P5_D	Supercritical CO ₂ power cycles
P5_G	Predicting heat transfer to supercritical fluids

Table 5: Programmes of project proposals of related modelling technologies

²³ Depending on the chosen benchmark problems, this project could support any of the MP programmes.

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7.3.4 Applicability and Choosing a Project Set

The applicability of the modelling technology programmes to underpin the reactor technology programmes is shown in Table 6.

The intention is that, for a given reactor technology decision, projects from the relevant reactor programme, along with a selection from applicable supporting modelling programme areas can be pursued as a coherent set (see Section 7.4 for a number of examples).

In the absence of a chosen or prioritised reactor technology, it can be seen from Table 6 that undertaking work in many of the modelling programmes can be widely applicable, or could be directed towards collaboration with international partners. However, even within the modelling programme areas, the projects themselves cannot be fully generic and require to be targeted at a specific problem of some kind, especially to derive the most exploitable result.

In most cases, the projects in each programme category need not be funded on an 'all-or-nothing' basis, i.e. the projects that best fulfil the needs and capabilities of the beneficiary of the investment should be selected. For example, to support liquid metal fast reactors with a core heat transfer emphasis, P5_E would be key, and the other projects from RP_4 could be given a lower priority and balanced against the benefits obtained from selecting from MP_1 and MP_4.

However, when selecting a project proposal set, it should be noted that there are sequential dependencies and parallel links recommended in some projects. Specifically:

- It is recommended that Projects P3_A and P3_B are carried out before P3_D and, to a lesser extent, P3_E;
- P3_C and P3_B have potential to be of mutual benefit to each other;
- ▶ P4_B would benefit from the work carried out in P3_A and by collaboration with P3_B.
- P5_A has the potential to benefit from P3_A, and can make use of knowledge or data gained from P5_F;
- Methods developed and used in P5_G are also applicable to P5_D;
- P5_B is potentially able to supply data to P5_A and P5_C;
- Progress can be made more effectively in P5_D by using data/results from P5_G;
- P7 A is a key enabler for P7 B;
- P7_E and P7_F can benefit from working closely with P7_A, P7_B and P7_D; and
- P7 D, P8 A and P8 B could be of mutual benefit to each other.

	Reactor Technologies				
Supporting Modelling Technology Programmes	PWR	BWR	HTGR	LMFR	MSR
Improved value from UK modelling capabilities					
Two-phase water modelling					
Support to structural integrity assessment					
Heat transfer and passive cooling modelling					
Support across all Gen IV technologies					
Support to supercritical CO ₂ power cycles					

Table 6: Applicability of modelling technology programmes to supporting reactor technologies

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7.4 Programme Scenarios

Three examples have been created to help illustrate and explore how the project proposals can be assembled into programmes to address a particular aim or focus:

- A programme to enhance UK capability and involvement in current and future Gen IV reactor programmes.
- A programme to enhance UK modelling capability in heat transfer and passive cooling across all reactor technologies, to reduce costs and improve safety.
- A programme to support rapid developments of UK LWR modelling capability to maximise benefits to UK industry from current new build and to support a UK SMR programme.

It should be stressed that none of these is considered a definitive recommendation and there will be the need to align any future programme to other UK Government initiatives, to the specific objectives and desired outcomes at that time and, critically, to the budget available.

The three example programmes are shown in Figure 5 to Figure 7 (page 59 to 61) and are discussed in Sections 7.4.1 to 7.4.3 below.

7.4.1 Gen IV Technologies

Gen IV reactors are currently being developed across the world funded by private enterprise and government supported international programmes. These reactors are designed to offer a variety of benefits over current LWR technologies in sustainability, economics, safety and reliability, proliferation resistance and physical protection²⁴. Interest in these designs forming part of the portfolio of UK electricity generation has increased over the last 5 years and the UK has recently re-joined the Gen IV International Forum as an active member.

In terms of thermal hydraulic modelling, many of the Gen IV technologies have significant R&D needs, due to the more unusual fluids used. In addition, they have a strong case for requiring government support, as many designs are at a lower level of maturity and have no operational commercial plants to generate a source of income.

Figure 5 presents a programme of work designed to develop the UK capability in nuclear thermal hydraulics relating to Gen IV reactor technologies. This example programme does not attempt to down-select or prioritise one technology. Instead it recommends work of interest to a range of technologies with a view to growing international connections and UK reputation, whilst producing outputs of value to provide leverage for future participation in international reactor programmes.

Advantages of this programme:

- The focus on Gen IV technologies co-ordinates well with the AMR development workstream under the BEIS NIP.
- The focus on Gen IV technologies presents a strong case for requiring government funding, due the high level of investment needed and the long timescales and high risk associated with a return on this investment.
- The lower TRL of Gen IV reactor designs compared with LWRs and lower level of maturity of much of the associated thermal hydraulics modelling, makes it easier for the UK to make an impact, with a relatively small amount of work.

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²⁴ https://www.gen-4.org/gif/jcms/c 9502/generation-iv-goals



The work packages have been chosen to address specific areas of need for current international reactor development programmes, thereby maximising the potential for international engagement across a wide range of countries and organisations.

Disadvantages of this programme:

- The low maturity of the majority of the Gen IV reactor designs and the timescales associated with their deployment, mean that the timescales for UK industry to gain an economic benefit from the research are uncertain and potentially quite long.
- The UK does not require all of the different Gen IV reactor technologies and it is currently unclear which, if any, will be most successful. This implies that some of the research will be of lower long-term value to UK industry, if that technology is not successful here.
- As the work is sub-divided into work packages that are tailored to the needs of different technologies and designs, the progress that can be made within in each technology is lower than if the whole programme was focused on a single technology.
- Excluding LWRs from this programme fails to address the majority of the LWR requirements for thermal hydraulic model development highlighted in Reference 5. Since LWR SMR designs are likely to be the first that are commercially deployed, this may limit the utility of the outputs in the short term.

7.4.2 Heat Transfer and Passive Cooling

The normal operation of traditional reactor designs involves the primary working fluids being pumped around the circuit. Increasingly, however, new designs are making more extensive use of buoyancy driven flow to achieve 'passive cooling' via natural circulation. This offers significant benefits in terms of enhanced safety and reduced plant complexity and cost. Some recent designs use natural circulation under normal operations, but even those that do not (pumping the coolant in the primary circuit) are now designed such that natural circulation can be used to dissipate decay heat in the event of a fault.

Figure 6 presents a programme of work to improve UK capability in the thermal hydraulic modelling of heat transfer and passive cooling. The programme considers the challenges across all technologies and looks to progress strong capabilities into world-leading ones as well as expanding the capability into 'Gen IV' fluids.

Advantages of this programme:

- The focus on passive cooling co-ordinates well with the envisaged future direction of international nuclear reactor design.
- The theme of passive cooling and heat transfer is of relevance to all reactor technologies, (many high temperature AMR designs have converged on similar passive cooling arrangements) thereby mitigating the risk of a proportion of the work being of lower value depending on the future technology choices made.
- The work programme aligns well with the initial theme recommended for the UK test facility in Reference 7.
- Much of this work is of immediate industrial value to both new and existing plants, thereby maximising the potential for rapid industry exploitation.
- This work offers the potential for the UK to develop a world-leading capability, rather than simply 'making up ground' between the UK and international centres of excellence.

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Disadvantages of this programme:

- Although the theme of passive cooling and heat transfer is of relevance to all reactor technologies, the details of the thermal hydraulics modelling required to address the challenges of each reactor design are different. It may therefore be difficult for all aspects of the work to be universally appealing and exploitable.
- By focusing around a single theme that is of importance across all technologies, the programme may exclude areas that are of the highest importance to a particular technology.
- Similarly, while important for safety justification, passive cooling and heat transfer in themselves do not comprise all aspects of the 'broad-spectrum' capability necessary to design a new reactor.

7.4.3 Light Water Reactors

The current new build programmes underway in the UK are delivering new 'large' light water reactors. The most mature SMR designs are primarily based around LWR technologies. It can therefore be argued that the most urgent requirement for UK industry is to improve capability in LWRs such that UK industry can gain the maximum benefit from these projects.

As mentioned in Section 2.3, despite the maturity of large LWR plants there are still significant gains to be made by improving the ability to more accurately predict the thermal hydraulic performance. The economic and safety justification benefit of being able to predict the heat transfer under particular two-phase flow conditions is such that there has been decades of significant international R&D activity in this area (funded by governments and industry) which still continues. Figure 7 depicts a programme of work focussed around LWR technologies, which focusses on the highest priority challenges raised for both large and small LWRs.

Advantages of this programme:

- LWR thermal hydraulic modelling challenges are mature and well understood enabling focused R&D to be performed with clear objectives.
- There is significant international activity and expertise in LWR thermal hydraulics, providing a range of attractive options for collaborative projects.
- Much of this work is of immediate industrial value to both new SMRs and existing plant designs, thereby maximising the potential for rapid industry exploitation.
- The work addresses a (potentially urgent) need for the UK to upskill in this area, so that the UK has the understanding and tools needed to operate the new LWRs in the UK nuclear fleet.

Disadvantages of this programme:

- Due to the maturity and commercial success of many LWR designs, the case for government funding for R&D is less clear (although the development of UK SMR designs strengthen this case).
- The exclusion of R&D to specifically support AMR technologies makes it hard for this project to integrate successfully with the current NIP AMR development work-stream.
- The level of international knowledge and expertise in LWR technologies, and the fact that the remaining challenges in LWRs are difficult to solve, may make it hard for the UK to make a significant impact within the likely budget and timeframes of this programme.

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7.5 Recommendations

As discussed in Section 7.2 and also in Section 2.4, it is highly recommended that the content of future phases of this programme are both co-ordinated with other UK civil nuclear initiatives and remains flexible to respond to the changes in the landscape that are likely over the next 5 years.

To align the precise content of Phase 2 with the most up-to-date government policy and budgetary constraints (and to avoid falling into the trap of being unduly influenced by one particular 'school of thought') it is strongly recommended that the contents of this report are reviewed and discussed with BEIS before a Phase 2 scope is defined.

However, there are a number of areas where clear recommendations can be made, applicable to many possible future directions of the project:

- The vision for P2_B is that it forms an integral part of the future management of this programme, including linking with other current UK initiatives (e.g. the UK-FN Nuclear Thermal Hydraulics Special Interest Group) and the other nuclear innovation programmes (e.g. Virtual Engineering). This project is recommended for inclusion in Phase 2 regardless of any other decisions.
- Project P2_A describes initial work to both increase and co-ordinate UK involvement in international nuclear thermal hydraulic benchmarking. This was (uniquely) considered to be of high importance by all of our stakeholder groups and, by its nature, can develop and adapt to changing priorities. Additionally, it represents a relatively 'easy win' in terms of increasing the visibility of the UK in international programmes. This project is recommended for inclusion in Phase 2 with its precise scope to be defined in the context of the rest of the programme.
- It is recommended that the technical content of the Phase 2 scope is built around a theme or a subset of technologies as illustrated by the examples in Figure 5 to Figure 7. This theme could be mandated by BEIS or suggested by the supplier and agreed with BEIS. This acknowledges that it will not be practical or sensible to attempt to address all the requirements raised in Reference 5 or all of the projects proposed in this specification within a single programme.
- It is suggested that the reach of the budget could be extended by co-funding arrangements with industry, such as in-kind contributions. Additionally, the possibility to link some of the more academically slanted research to Engineering and Physical Sciences Research Council (EPSRC) funding (Reference 4) may also allow greater exploitation of the proposals. It is recommended that both of these avenues are explored in the early stages of Phase 2 and again 12 months into the two year Phase 2 timescales (it will likely be appropriate or indeed necessary for BEIS to be involved in/party to a subset of these discussions).
- It is recommended that this project continues to collaborate with the Virtual Engineering, Modelling and Simulation work stream to ensure a cohesive programme.
- The use of High Performance Computing (HPC) is key to many modelling advances. Although not within the scope of a thermal hydraulics project, it is strongly recommended that the availability of HPC to UK industry is explored and, if necessary, expanded.
- It is strongly recommended that the UK take a collaborative approach to nuclear thermal hydraulic modelling, adopting such international tools as are available and building on them rather than re-inventing our own. The cost of developing and maintaining UK specific tools, which duplicate much of the capability already available internationally, would be extensive and is not justified in the medium term.

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The programme of R&D projects presented here is an example of how Government investment in nuclear thermal hydraulics research and development under Phase 2 of 'Digital Reactor Design - Thermal Hydraulics' can be used to expand the UK's international position and capability in Generation IV advanced reactors, whilst not committing, in the short term, to one technology.

The programme has been designed on the premise that funds available under Phase 2 are to be targeted towards the developments most relevant for enhancing UK involvement in current and future Gen IV reactor programmes, as opposed to other possible objectives. This is not the only programme that could have been designed from the outputs of Phase 1 and should not be considered as a definitive recommendation from

The programme is intended to enhance the current UK capability as follows:

	Current UK Position	Outcome
Thermal hydraulic modelling	Strong capability and active research in advancing the state of the art in general purpose CFD modelling in water and gases. Capability in TH nuclear codes primarily limited to current UK reactor fleet.	Expanding capability in CFD for Gen IV reactor fluids, keeping the UK in a leading position. Increased knowledge of Gen IV potential for further UK based code development.
Gas cooled reactors	Strong general capability in nuclear thermal hydraulics (NTH) gas modelling.	Further demonstration and consolidation of UK skills in NTH gas modelling.
	Limited knowledge and experience of HTGR specific needs. UK involvement in HTGR design limited to small number of organisations and primarily one new design.	Increased and growing pool of HTGR skilled resource. Demonstrated UK contribution in an area of importance to all HTGR designs, leveraging an expanded UK presence in international programmes.
Liquid metal fast reactors	Dwindling historic capability with up-to-date skills present only in a limited number of institutions. CFD modelling solutions more	Increased and growing pool of resource skilled in modern LMFR thermal hydraulic design and analysis best practice.
	difficult due to high liquid metal thermal conductivity.	Enhanced UK CFD modelling capability in liquid metals.
	No current significant involvement in reactor design.	UK presence in at least one reactor programme and leverage for UK participation in current and future LMFR programmes.
Molten salt reactors	Low level of NTH capability limited to only a few organisations.	A'kick-started' and growing capability in NTH analysis for molten salt with presence in at least one design programme.
	Low level of reactor design and analysis knowledge vested in only a few organisations. One UK organisation pursuing reactor design, but increasingly having to look outside of UK for support as design progresses.	Initiation of a growing pool of skilled resource with an understanding of molten salt reactors and specific NTH expertise.
2030 horizon nuclear innovation	UK academia sporadically engaged in highly innovative projects at a low TRL. Industry focus in life-extension and realising marginal gains related to	UK industry and academia working together with international collaborators to realise 'game changing' development in NTH and reactor design.
	currently deployed technologies.	

Supercritical CO2 power cycles Funding the activies proposed would place the UK at the forefront of a step-change in power conversion technology, of particular relevance to mitigiating cost and safety concerns for sodium cooled reactors.

Advanced Reactor R&D with a Focus on Internationally Exploitable Outcomes, Keeping a Wide Range of Technology Options Open

Estimated Budget: £8 million to £10 million over 3 years

Overarching Projects Reinvigorating and Sustaining the UK Nuclear Thermal Hydraulics Community

Maximising UK collaboration and collective learning

To create a co-ordinated and exploitation focused nuclear thermal hydraulic research and development initiative and to develop the ways of working needed to ensure an enduring capability

Increased participation in benchmarking

To promote UK-wide and international collaboration. To initiate a UK model validation programme, setting us up to maximise the value from a UK test facility.

Technology Projects Addressing Key Gen IV Reactor Technology Challenges

Liquid metal heat transfer modelling

Tritium generation and migration in advanced reactor coolants

Modelling of air ingress accidents in HTGRs

Heat transfer correlations for mixed convection and transitional flows in MSRs

Iolecular dynamics capabilities for thermophysical, thermogravimetric phase equilibrium prediction over lifecycle

Dissolved gas transport in molten metals and molten salts

Modelling of cover gas dynamics

- Directly addressing high priority challenges in current reactor programmes to enable reactor design and deployment,
- Capability development with UK industry by knowledge transfer from academia and/or international sources.
- \bullet Developing UK reputation for Gen IV and enables the UK to play a role in international reactor programmes.
- Could be used as 'ice-breaker' projects to engage with Gen IV international forum.

Innovation Projects Enabling a Step-Change in UK Modelling Capbability or International Presence

Coupled tool selection (adopting the best available cutting-edge international technology)

Supercritical CO₂

power cycles

High fidelity modelling to improve the accuracy of low fidelity methods delivered via machine learning

Development of innovative coarse grid models for reactor design

· Additional capabilities that would allow more advanced and higher fidelity modelling methods to be deployed that are not currently practical for reactor design.

· Step-changes in technology that are not essential for reactor development and deployment, but may substantially reduce costs or timescales.

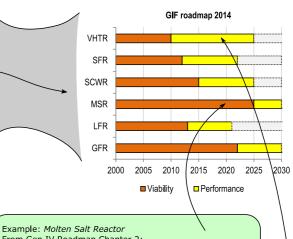
This research forms the necessary immediate steps and lays the foundations to play an enduring role in exploiting the advantages of advanced reactors in the 2030 to 2050 timeframe.

They develop and sustain the skills and knowledge as well as build the international links that will be essential on an ongoing basis, in-line with the government, academic and industry actions on the OECD/IEA/NEA Nuclear Energy Technology Roadmap, 2015: https://www.oecd-nea.org/pub/techroadmap

The work supports achieving the 'Reactor Technology', 'Licensing and Regulation, Nuclear Safety', 'Training and Capability Development' and 'Codes and Standards' milestones.

Research and development Technical Projects are all targeted at the near-term issues in the development of Gen IV reactors thereby enabling rapid UK involvement and a clear demonstration of exploitable value.

> Source: Technology Roadmap Update for Generation IV Nuclear Energy Systems https://www.gen-4.org/gif/jcms/c_9352/technology-road



From Gen IV Roadmap Chapter 2:

- mastering the technically challenging technology will require concerted long-term international R&D efforts, namely:
- · studying the salt chemical and thermodynamic properties, including with
- · development of efficient techniques for gas extraction from the coolant; • system design: development of advanced neutronic and thermal-hydraulic
- The projects defined address all three of these directly, delivering immediate benefits.

Example: Very High Temperature Gas Reactor The projects defined create a modelling cabaility to address the main safety concerns for VHTRs, including those connected to hydrogen production facilities

Building on the 'Digital Reactor Design – Virtual Engineering' framework to realise exploitable benefits in the coupling of thermal hydraulics models with neutronics.

Figure 5: Programme Focussing on Gen IV Technology

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The programme of R&D projects presented here is an example of how Government investment in nuclear thermal hydraulics research and development under Phase 2 of 'Digital Reactor Design – Thermal Hydraulics' can be used

This programme has been designed on the premise that the funds available under Phase 2 are to be targeted at enhancing nuclear safety and reducing costs by enabling a better level of understanding in both heat transfer and passive cooling for AMR and SMR technologies. This is not the only programme that could have been designed from the outputs of Phase 1 and should not be considered as a definitive recommendation from the project.

The programme is intended to enhance the current UK capability as follows:

	Current UK Position	Outcome
Thermal hydraulic modelling	Strong capability and active research in advancing the state of the art in general purpose CFD modelling in water and gases.	Expanding capability in the use of CFD for the prediction of passive cooling in both reactor 'loops' and plena/containment volumes.
	Capability in TH nuclear codes primarily limited to current UK reactor fleet and codes relevant to defence applications.	Extended capability and better understanding of best practice in the use of CFD to model heat transfer in water, gases and advanced reactor fluids. Improving the capabilities of lower fidelity
	аррисанолог ———————————————————————————————————	TH methods and the coordinated use of low and high fidelity methods to construct reactor models.
LWRs and SMRs	Capability in design and operation of PWRs vested in a small number of organisations.	Increased and growing pool of resource with knowledge and experience of PWR, SMR and BWR thermal hydraulics. Focused R&D outputs exploited within a reactor development programme.
	Single UK organisation pursuing a PWR SMR design. Minimal specifically relevant	Demonstration of understanding of the most pertinent LWR heat transfer and passive cooling issues leveraging involvement of the UK supply chain in
	capability in BWRs in UK	international LWR development.
Gas cooled reactors	Strong capability in nuclear thermal hydraulics gas flow and heat transfer modelling.	Development of strong core skills into a world leading capability in the modelling of heat transfer and natural and mixed convective flow in single phase gases.
	Limited knowledge and experience of specific needs for HTGR passive cooling.	Demonstrated UK contribution in key areas of importance to all HTGR designs, leveraging an expanded UK presence in
	UK involvement in HTGR design limited to small number of organisations.	international programmes.
Liquid metal fast reactors	Dwindling historic capability with up-to-date skills present only in a limited number of institutions.	Increased and growing pool of resource skilled in modern LMFR thermal hydraulic design and heat transfer analysis best practice.
	TH modelling solutions more difficult due to high liquid metal thermal conductivity.	UK development of a potentially world leading capability in state-of-the-art liquid metal modelling.
	No current significant involvement in reactor design.	UK presence in at least one reactor programme and leverage for UK participation in current and future LMFR programmes.
Molten salt reactors	Low level of molten salt specific capability, limited to only a few organisations. Difficulties in the modelling	A 'kick-started' and growing capability in NTH analysis for molten salt with presence in at least one design programme.
	of molten salts due to uncertainty and variability in the material properties of the fluid.	Initiation of a growing pool of skilled resource with an understanding of molten salt reactors and the development of a specific capability in the molten salt heat transfer most relevant for reactor design
	Low level of reactor design and analysis knowledge	and safety substantiation.
2030 horizon nuclear innovation	UK academia sporadically engaged in highly innovative projects at a low TRL.	UK industry and academia working together with international collaborators to realise 'game changing' development in NTH and reactor design.
	Industry focus in life- extension and realising marginal gains related to currently deployed technologies.	

Heat Transfer R&D with a Focus on Natural Circulation and Passive Cooling Estimated Budget: £8 million to £10 million over 3 years

Overarching Projects Reinvigorating and Sustaining the UK Nuclear Thermal Hydraulics Community

Maximising UK collaboration and collective learning

To create a co-ordinated and exploitation focused nuclear thermal hydraulic research and development initiative and to develop the ways of working needed to ensure an enduring capability

Increased participation in benchmarking

To promote UK-wide and international collaboration. To initiate a UK model validation programme, setting us up to maximise the value from a UK test facility.

Technology Projects Addressing Key Heat Transfer and Passive Cooling Challenges

Improved accuracy of RANS models for turbulent heat convection

Improved wall models for accurate heat transfer

Predicting and assessing thermal fatigue

Improved prediction of the stalling of natural circulation flows

Investigate the impact

of 'real' surfaces

on NTH heat transfer

modelling predictions

Liquid metal heat transfer modelling

Improved prediction of passive cooling in NPP containment volumes

to enable reactor design ar
 Capability development wacademia and/or internation

- Directly addressing high priority challenges in current reactor programmes to enable reactor design and deployment.
- \bullet Capability development with UK industry by knowledge transfer from a cademia and/or international sources.

Innovation Projects Enabling a Step-Change in UK Modelling Capbability or International Presence

Heat Transfer Correlations for Mixed Convection and Transitional Flows in MSRs High fidelity modelling to improve the accuracy of low fidelity methods delivered via machine learning)

Development of innovative coarse grid models for reactor design

Predicting heat transfer to supercritical fluids

- Additional capabilities that would allow more advanced and higher fidelity modelling methods to be deployed that are not currently practical for reactor design.
- Step-changes in technology that are not essential for reactor development and deployment, but may substantially reduce costs or timescales.

Passive cooling for fault recovery has been a desirable part of the assurance of nuclear safety for a long time. The potential benefits are clear: passive systems require no operator actions or power supply to work and have the potential to both enhance safety and reduce plant complexity and cost. However, it is has previously been difficult to claim passive thermal hydraulic phenomena as anything other than a last line of defence, primarily due to challenges in showing with confidence that it is possible to predict that the heat transfer performance will be sufficient under all conditions.

With the development of both SMR and AMR designs that make claims of passive safety, or in some cases use natural circulation under normal operating conditions, a step change in the level of confidence with which they can be predicted is needed. This research looks to specifically address this challenge with both short term and long term benefits across all reactor technologies.

Validation is key to increasing prediction confidence and the main development aspects of this programme can be strongly linked with the planned UK Test Facility. The work provides the analysis necessary to focus the design and operation of rigs to the areas where there are the greatest knowledge gaps, and to areas that provide immediate benefits to UK industry.

The work supports the government, academic and industry actions on the OECD/IEA/NEA Nuclear Energy Technology Roadmap, 2015:

https://www.oecd-nea.org/pub/techroadmap

- Reactor technology accelerating the development of SMR and AMR designs and promoting partnerships within UK industry and academia.
- Nuclear Safety and licensing Unlocking the use of passive safety as an integral part of future NPP design.
- Training and Capability Enhancing UK capability by innovation, co-ordination and knowledge dissemination in the state-of-the-art modelling in convection and heat transfer.

Development of innovative coarse grid models for reactor design

The development of a disruptive tool with the potential to achieve a significant step forward in practical nuclear thermal hydraulic analysis and be applied across all reactor technologies.

Predicting heat transfer to supercritical fluids Funding the activities proposed would place the UK at the forefront of a step-change in power conversion technology, of particular relevance to mitigating cost and safety concerns for sodium-cooled reactors.

Figure 6: Programme Focussing on Heat Transfer and Passive Cooling

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The programme of R&D projects presented here is an example of how Government investment in nuclear thermal hydraulics research and development under Phase 2 of 'Digital Reactor Design – Thermal Hydraulics' can be used

This programme has been designed on the premise that the funds available under Phase 2 are to be targeted at enhancing nuclear safety and reducing costs by enabling a better level of understanding in thermal hydraulics related to both small and large light water reactors (LWRs). This is not the only programme that could have been designed from the outputs of Phase 1 and should not be considered a definitive recommendation from the project.

The programme is intended to enhance the current UK capability as follows:

-	Current UK Position	Outcome
Thermal hydraulic modelling	Strong capability and active research in advancing the state of the art in general purpose CFD modelling in water and gases.	Expanding capability in the use of CFD for the prediction of all areas of thermal hydraulics relevant to LWR design and operation.
	Capability in TH nuclear codes primarily limited to current UK reactor fleet and codes relevant to defence applications.	Improving the capabilities of lower fidelity TH methods and the coordinated use of low and high fidelity methods to construct reactor models.
		Initiation of a centre of excellence for LWR predictive modelling in North Wales.
PWRs	Good capability in PWRs vested in a small number of organisations for both defence and civil nuclear plant operation and design in a defence context.	Increased and growing pool of resource with knowledge and experience of PWR thermal hydraulics relevant to both SMRs and large reactor operation.
	Single UK organisation pursuing a PWR SMR design.	Focused R&D outputs exploited within a new reactor development programme.
		Demonstration of UK development and understanding in single and two-phase PWR heat transfer, leveraging involvement of the UK in international PWR research and development.
BWRs	Low level of experience in BWR thermal hydraulics in UK industry.	Considerable step forward in UK understanding of BWR thermal hydraulics.
	Capability in BWR thermal hydraulics present in a small number of UK academic institutions.	Development of skills to support UK BWR licensing and operation.
		Initial development and demonstration of UK capability to contribute to future BWR design.
2030 horizon nuclear innovation	UK academia sporadically engaged in highly innovative projects at a low TRL.	UK industry and academia working together with international collaborators to realise 'game changing' development in NTH and
	Industry focus in life- extension and realising marginal gains related to currently deployed technologies.	reactor design.

Developing sensitivity and uncertainty methods for BWR dynamics

Using BWR as an example, this work will deliver specific enhancement and improved UK skills in an area key for the licencing of all reactors, unlocking the potential for more expansive use of digital methods in a nuclear context.

Light Water Reactor R&D with a Focus on Internationally Exploitable Outcomes, Relating to PWRs, BWRs and SMRs

Estimated Budget: £8 million to £10 million over 3 years

Overarching Projects Reinvigorating and Sustaining the UK Nuclear Thermal Hydraulics Community

Maximising UK collaboration and collective learning

To create a co-ordinated and exploitation focused nuclear thermal hydraulic research and development initiative and to develop the ways of working needed to ensure an enduring capability

Increased participation in benchmarking

To promote UK-wide and international collaboration. To initiate a UK model validation programme, setting us up to maximise the value from a UK test facility.

Technology Projects Addressing Key LWR Reactor Technology Challenges

Improved prediction of the stalling of natural circulation flows CFD modelling of macroscopic convective boiling flows in NPP Improved two-phase flow regime transition modelling

UK LWR Predictive Modelling Validation Centre Predicting and assessing thermal fatigue

Improved prediction of passive cooling in NPP containment volumes

Improving the ability to predict structural vibration in reactor design

- Directly addressing high priority challenges in current reactor programmes to enable reactor design and deployment.
- Capability development with UK industry by knowledge transfer from academia and/or international sources.

Innovation Projects Enabling a Step-Change in UK Modelling Capbability or International Presence

Coupled tool selection (adopting the best available cutting-edge international technology) High fidelity modelling to improve the accuracy of low fidelity methods (delivered via machine learning) Development of innovative coarse grid models for reactor design

Developing sensitivity and uncertainty methods for BWR dynamics

- Additional capabilities that would allow more advanced and higher fidelity modelling methods to be deployed that are not currently practical for reactor design.
- Step-changes in technology that are not essential for reactor development and deployment, but may substantially reduce costs or timescales.

With LWR new-build projects underway in the UK and the likelihood that the first SMRs to market will be based around LWR technology, it could be argued that the most urgent requirement for the UK is to upskill in all areas relating to LWR operation.

Nuclear thermal hydraulics is no exception and, despite the continued operation of Sizewell B, UK capability in thermal hydraulic modelling related to civil PWRs is neither extensive nor representative of the current state-of-the-art. For BWRs, UK capability is low and well developed thermal hydraulics understanding and experience is vested in only a small number of individuals.

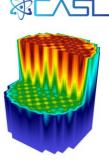
This research is focussed at achieving rapid and significant growth in UK capability in the thermal hydraulic modelling of light water reactors. This is undertaken with a view to:

- Developing a skilled UK workforce for the current wave of new-build reactors;
- Developing industry skills to support the development of a UK based SMR design;
- Leveraging opportunities for international collaboration in the huge, global LWR market.

Validation is key to increasing confidence and a number of projects within this programme can be strongly linked with the planned UK Test Facility. The work provides the analysis necessary to focus the design and operation of rigs to the areas where there are the greatest knowledge gaps and how the uncertainty in modelling predictions could be reduced by testing.

Opportunities exist to enhance UK LWR new build programmes by collaboration with international research.

For example, the US Consortium for Advanced Simulation of Light Water Reactors (CASL) DoE Energy Innovation Hub, which is creating the Virtual Environment for Reactor Applications (VERA). This comprises software tools and infrastructure able to solve coupled physics problems including neutronics, thermal-hydraulics and fuel performance, including uncertainty quantification. https://www.casl.gov/vera



PWR coolant temperature distribution prediction from CASL report: Watts Bar Unit 2 Startup Results with VERA https://www.casl.gov/sites/default/files/docs/CASL-U-2017-1306-000.pdf

Courtesy of Oak Ridge National Laboratory, U.S. Dept. of Energy

The work supports the government, academic and industry actions on the OECD/IEA/NEA Nuclear Energy Technology Roadmap, 2015:

- https://www.oecd-nea.org/pub/techroadmap
- Reactor technology accelerating the development of SMR designs and reducing their cost.
- Nuclear Safety and licencing Development of the skills necessary to enable the licencing of new LWR designs in the UK.
 Training and Capability – Enhancing UK capability by
- innovation, co-ordination and knowledge, dissemination in the state-of-the-art modelling relating to LWR thermal hydraulics. Promoting partnerships within UK industry and academia.

Figure 7: Programme Focussing on Light Water Reactors

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8 Abbreviations

ABWR Advanced Boiling Water Reactor
AGR Advanced Gas-cooled Reactor
AMR Advanced Modular Reactor

BARC Bhabha Atomic Research Centre (India)

BEIS Department for Business, Energy and Industrial Strategy

BWR Boiling Water Reactor
CAD Computer Aided Design

CASL Consortium for Advanced Simulation of Light Water Reactors (USA)

CCS Carbon Capture and Storage

CEA Commissariat à l'énergie atomique et aux énergies alternatives (France)

CESAR Centre for Exascale Simulation of Advanced Reactors (USA)

CFD Computational Fluid Dynamics

CHF Critical Heat Flux

CRP Coordinated Research Projects (IAEA)

CRUD Chalk River Unidentified Deposits (apocryphal backronym)
CSNI OECD NEA Committee on the Safety of Nuclear Installations

DECC Department of Energy and Climate Change

DNB Departure from Nucleate Boiling
DNS Direct Numerical Simulation

DOE-NEUP Department of Energy Nuclear Energy University Program (USA)

EDF Électricité de France

EPRI Electric Power Research Institute (USA)

FSI Fluid-Structure Interaction
FTE Full Time Equivalent

HPC High Performance Computing

HTGR High Temperature Gas-cooled Reactor
HVAC Heating, Ventilation, and Air Conditioning
IAEA International Atomic Energy Agency
INL Idaho National Laboratory (USA)

IRSN Institut de radioprotection et de sûreté nucléaire (France)

JAEA Japan Atomic Energy Agency

JRC European Commission Joint Research Centre

LES Large Eddy Simulation
LFR Lead-cooled Fast Reactor

LMFR Liquid Metal-cooled Fast Reactor

LOCA Loss of Coolant Accident
LWR Light Water Reactor
MD Molecular Dynamics
MSFR Molten Salt Fast Reactor
MSR Molten Salt Reactor

MYRTE MYRRHA Research and Transmutation Endeavour

NEAMS Nuclear Energy Advanced Modelling and Simulation Program

NIP Nuclear Innovation Programme

NIP CG Nuclear Innovation Programme Contractors Group NIRAB Nuclear Innovation and Research Advisory Board

NNL National Nuclear Laboratory (UK)

NPP Nuclear Power Plant

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NRC Nuclear Regulatory Commission (USA)

NTH Nuclear Thermal Hydraulics
ONR Office for Nuclear Regulation (UK)
ORNL Oak Ridge National Laboratory (USA)

PIV Particle Image Velocimetry

POD Proper Orthogonal Decomposition

PTS Pressurised Thermal Shock PWR Pressurised Water Reactor

RANS Reynolds-Averaged Navier-Stokes

SAMOFAR Safety Assessment of the Molten Salt Fast Reactor

SCK•CEN Studiecentrum voor Kernenergie • Centre d'Étude de l'énergie Nucléaire (Belgium)

SCWR SuperCritical Water Reactor

SESAME Simulations and Experiments for the Safety Assessment of Metal cooled reactors

SFR Sodium-cooled Fast Reactor SIG Special Interest Group SMR Small Modular Reactor

SPH Smoothed Particle Hydrodynamics

STFC Science and Technology Facilities Council

THINS Thermal Hydraulics of Innovative Nuclear Systems
URANS Unsteady Reynolds-Averaged Navier-Stokes
VERA Virtual Environment for Reactor Applications (USA)

VHTR Very High Temperature Reactor

WGAMA CSNI Working Group on Analysis and Management of Accidents

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ANNEX A - RESEARCH PROPOSALS

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A1 Introduction

This annex contains outline proposals for 34 potential research and development projects intended to enhance the UK capability in nuclear thermal hydraulics. Table A2 in Section A.1.2 shows the page number where each project is defined.

It is important for the programme to recognise that the technical thermal hydraulic modelling challenges addressed by these projects are 'world challenges'. Fluids do not behave differently in the UK! These challenges are known and recognised by the organisations to which they are relevant and international industry and academic researchers alike are currently working on solving them. It is possible that work may be published which removes the need for or changes the emphasis of any of the projects before Phase 2 of this programme begins. Additionally, all of the project proposals are presented at quite a high level to enable inclusion in this document without it becoming unwieldy (i.e. all proposals were limited to 3-4 pages in length).

Therefore, it is important that all projects start with a brief review of the latest research in that specific area and that the scope is refined and potentially updated based on the findings of that review. Where a slightly more extensive review is needed as an enabler to the project itself, this is included in the scope of work.

As discussed in Section 6.3, the availability of suitable test data to enable validation is a challenge for many of the projects. In all cases, it is recommended that consideration be given to whether the UK test facility could offer the opportunity to acquire additional data in specific areas.

A.1.1 Format of Proposals

The proposals have all been developed and presented in a consistent format. Table A1 below defines the content of the template.

Project Title					
Topic	Workshop topic most closely related to project content				
Reference	Unique project reference number, of the format PN_A, PN_B where N refers to the topic number (1 to 8) defined in Table 1.				
Source	Where the project idea came from (e.g. the workshop, the core team or another other stakeholder)				
Location on Capability Map	What type of capability development does this project represent? Link to capability structure (Figure 1).				
R&D Spectrum	The level of maturity of the project in terms of the R&D lifecycle. Basic Research - The enhancement or acquisition of fundamental knowledge and understanding without a well-defined application. Applied Research - The enhancement of knowledge to fill a recognised gap or need.				
	Early Development - The initial development of tangible tool, system, method or process e.g. development of approach. Late Development - The demonstration that a tangible tool, system, method or process is ready/appropriate for implementation.				

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Technical Objectives	What the project is hoping to achieve?
	To include relevant background information, a description of where the project is going long term and the objectives for this specific task, as relevant.
Benefits	What are the specific technical benefits of doing this work?
	What are the benefits to the UK nuclear industry?
Scope & Approach	Defines the key tasks and activities to be performed to achieve the project objectives i.e. what is actually going to be done?
Validation Requirements	Need to consider what would be needed to enable validation.
	Does suitable data already exist? If not where and how it could be obtained? How could the UK facility contribute?
Output	The specific outputs/deliverables of the task.
Existing Research & Body of Knowledge	This should include an initial overview of existing or ongoing research and opportunities for international collaboration.
International Programmes	(This information will almost certainly be preliminary and incomplete at this stage)
Risks	Highlight any significant project or technical risks (e.g. very small pool of people with the right skills or very challenging research with only a moderate chance of success).
Timeline and Prerequisites	An estimate of how long the work might take and if there are any prerequisites to completing it.
	Does this project have links with others in the programme?
Resource/Costs	Need to consider both type and quantity of resource needed.
	e.g. 1 FTE researcher + 0.25 FTE industrial specialist for 1 year.
	Are there any other costs?
Exploitation	It is important that the project is capable of producing or at least
Recommendations	progressing exploitable outputs.
	Recommendation of the route to maximise the benefits of the work.

Table A1: Project Proposal Structure

A.1.2 Linking of Proposals to User Requirements

The analysis of the proposed projects in the context of the user requirements (Reference 5) identified that, in many cases, the solution to multiple requirements would be progressed by completing the proposed work. Table A2 presents the linking of the projects to the user requirements in two ways. Where the proposed work specifically addresses or progresses a solution to a requirement, it is defined as a 'strong' link. Where the proposed work is considered to provide output that adds to the relevant body knowledge in a way that is helpful to addressing a specific requirement, this has been defined as an 'indirect' link. A brief discussion of the applicability of the potential work beyond nuclear thermal hydraulics is also included.

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Project Ref.	Page No.	Project Title	Linked Requirements Strong	Linked Requirements Indirect	Wider Applicability
P1_A	74	Development of innovative coarse grid models for reactor design	AGR_M_02, AGR_M_03, AGR_M_09, LMFR_M_03, PWR_M_06	AGR_M_01, LMFR_M_15, PWR_M_18	Developments could assist in the TH modelling of a range of complicated engineering systems, especially those encompassing a wide range of scales.
P1_B	78	High fidelity modelling to improve the accuracy of low fidelity methods	AGR_M_03, AGR_M_08, LMFR_M_03, LMFR_M_06	HTGR_M_04, PWR_M_06	Potentially wide applicability across all industries employing complex TH analysis across a range of scales.
P1_C	81	Reducing the cost of CFD - Efficient and effective meshing	AGR_M_03	LMFR_M_07, LMFR_M_08	Developments could assist in all industries where CFD is used to model complex internal flow passages.
P2_A	85	Increased participation in benchmarking	PWR_M_20, PWR_M_21, AGR_M_05, LMFR_M_06, SCWR_M_01	Many possible - depending on precise benchmarks chosen	Findings likely to be of interest to all industries where thermal hydraulic modelling is used to model complex internal flow passages.
P2_B	88	Maximising UK collaboration and collective learning	PWR_M_20, PWR_M_21, AGR_M_05	All UK NTH R&D	Potential for valuable links with other industry R&D collaborations.
P2_C	92	Sensitivity and Uncertainty Analysis of a Reduced- Order Model for Simulating BWR Dynamics	PWR_M_21, BWR_M_04, BWR_M_08, BWR_M_09	PWR_M_14	The demonstration of methods for quantifying uncertainty in an NTH context could be used in the future for modelling tools associated with other reactor technologies and indeed other industries.
P2_D	98	UK LWR predictive modelling validation centre	BWR_M_04, BWR_M_05, BWR_M_08,	All light water system and sub-channel codes.	This project is focused on providing a means of model validation and model improvement in association with the new UK test facility. In time this could be expanded to encompass other reactor technologies.
P3_A	101	Improving the prediction of heat transfer by fundamental multi-scale	BWR_M_02, PWR_M_01,	LMFR_M_05, PWR_M_03	Relevant to any industry where convective boiling is important.

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Project Ref.	Page No.	Project Title	Linked Requirements Strong	Linked Requirements Indirect	Wider Applicability
		modelling of bubble growth process			
P3_B	105	Improved two-phase flow regime transition modelling	BWR_M_02, PWR_M_01, PWR_M_18	BWR_M_01, BWR_M_06, BWR_M_07, PWR_M_09, PWR_M_17	The implementation of boiling phase transition models into a CFD framework, could be of value to any industry where boiling is important.
P3_C	108	Film dry-out modelling in CFD	BWR_M_01, BWR_M_02, PWR_M_01	BWR_M_03, PWR_M_10, PWR_M_17	This work would further add to the capability to model boiling and film flows with CFD and has potential applicability to any industry where these are important.
P3_D	112	Improved component scale boiling model	BWR_M_07, PWR_M_09	BWR_M_04, BWR_M_08, PWR_M_01	This work would further add to the capability to model boiling and film flows with CFD and has potential applicability to any industry where these are important.
P3_E	117	Prediction of DNB using CFD	BWR_M_06, BWR_M_07, PWR_M_09	BWR_M_03, PWR_M_03, PWR_M_17	The prediction of this most important boiling phase transition would be of value to any industry where boiling heat transfer is important.
P4_A	120	Modelling of fuel clad ballooning following LOCA	PWR_M_22	MSR_M_02	Although this particular problem is very industry specific, the methods for coupling of the flow, thermal and structural response could be of value to other industries.
P4_B	123	CFD modelling of macroscopic convective boiling flows in NPP	PWR_M_01	BWR_M_07, PWR_M_09	This work is necessarily quite application specific. The outcome will however add to the body of knowledge relating to the use of CFD for two-phase flow modelling.
P5_A	127	Dissolved gas transport in molten metals and molten salts	LMFR_M_16		This work would be applicable to any industry where entrainment into liquid or molten material is important, for example casting.
P5_B	130	Molecular dynamics capabilities for	MSR_M_01		Any industry or scientific process where complex chemical species and their evolution

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Project Ref.	Page No.	Project Title	Linked Requirements Strong	Linked Requirements Indirect	Wider Applicability
		thermophysical, thermogravimetric phase equilibrium prediction over lifecycle			produces changes in material properties that are unknown in advance could benefit from the methods developed.
P5_C	132	Heat transfer correlations for mixed convection and transitional flows in MSRs	MSR_M_05	MSR_M_03, MSR_M_06, MSR_M_07	Mixed convection is a difficult heat transfer regime to make accurate predictions for. Maintaining and extending expertise for creating such correlations will create skills and methods that can be applied in many other industrial contexts.
P5_D	134	Supercritical CO ₂ power cycles	LMFR_M_17		Supercritical CO ₂ technology has wide applicability in many forms of high temperature power generation: e.g. nuclear, solar, conventional, energy storage, carbon capture and storage.
P5_E	136	Liquid metal heat transfer modelling	LMFR_M_01, LMFR_M_04, LMFR_M_13		This work would be applicable to any industry where molten metals are used, casting for example.
P5_F	139	Modelling of cover gas dynamics	LMFR_M_16		Any industry where heat transfer through aerosol particle laden gas is present would benefit from this work.
P5_G	142	Predicting heat transfer to supercritical fluids	SCWR_M_03, SCWR_M_05	SCWR_M_06	Supercritical fluids are used in many industries, and are applied in conventional power cycles, and so this work would be of widespread value.
P6_A	145	Coupled tool selection	BWR_M_04, MSR_M_01, PWR_M_14		This project focusses on building international links through the use of common tools; this should provide wider benefits naturally through increased collaboration and cooperation.

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Project Ref.	Page No.	Project Title	Linked Requirements Strong	Linked Requirements Indirect	Wider Applicability
P6_B	148	Tritium generation and migration in advanced reactor coolants	HTGR_M_06		While this project was raised in the context of an HTGR UR, MSRs and LMFRs will encounter this issue to some extent, and can benefit from this work. Control of tritium transport is a relevant problem in nuclear fusion and other activities where it is generated or stored, and they could also benefit.
P6_C	150	Coupled 3D neutronics and CFD thermal hydraulics applied to BWR fuel channels	BWR_M_03, BWR_M_04, BWR_M_05, BWR_M_06, BWR_M_07, PWR_M_14	BWR_M_09	Coupled general purpose 3D CFD and 3D neutronics can be readily applied to all nuclear reactor types.
P6_D	152	State of the art CRUD deposition models and the effects on heat transfer mechanisms	PWR_M_11		This is a potential route into a more widespread application of the most modern US high fidelity modelling tools (e.g. MOOSE, VERA).
P6_E	154	Modelling of air ingress accidents in HTGRs	HTGR_M_08, HTGR_M_09	HTGR_M_07	This project has been proposed in the context of one HTGR reactor design, but would be able to be applied to any design in the same category.
P7_A	156	Improved prediction of flow and thermal development in fuel pin cooling passages	AGR_M_01, AGR_M_04, PWR_M_05	LMFR_M_04, PWR_M_15	This work could be of benefit to any application requiring the modelling of unsteady flow phenomena in narrow internal passages.
P7_B	160	Improved accuracy of RANS models for turbulent heat convection	AGR_M_04, PWR_M_05, PWR_M_15	AGR_M_06, HTGR_M_01, LMFR_M_07, LMFR_M_08, LMFR_M_09, LMFR_M_12, PWR_M_07, SCWR_M_02, PWR_M_20	The modelling of turbulent flow using CFD represents the state-of-the-art in fluid dynamics modelling in many industries. The specific work proposed here would enhance capability in the modelling of buoyancy driven flow in all industry applications.

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Project Ref.	Page No.	Project Title	Linked Requirements Strong	Linked Requirements Indirect	Wider Applicability
P7_C	164	Improving the ability to predict structural vibration in reactor design	HTGR_M_02, PWR_M_12	SCWR_M_04, LMFR_M_12, PWR_M_20	Structural vibration induced by fluid flow is seen across a range of industries, most notably aerospace and automotive. Although this project initially examines adopting methods from other sectors for civil nuclear application, any learning gained in the strengths and limitations of the methods will likely benefit all who use them.
P7_D	168	Predicting and assessing thermal fatigue	LMFR_M_10, LMFR_M_11, PWR_M_08	LMFR_M_12, PWR_M_13, PWR_M_15	The development of improved transient thermal modelling capability and improved conjugate heat transfer modelling would likely be of benefit to industries such as oil and gas.
P7_E	172	Improved prediction of the stalling of natural circulation flows	LMFR_M_11, PWR_M_05, AGR_M_04	HTGR_M_01, LMFR_M_09, PWR_M_15,	This work adds to the general body of knowledge regarding the reliable modelling of single phase flow and heat transfer with CFD.
P7_F	177	Improved prediction of passive cooling in NPP containment volumes	HTGR_M_01, PWR_M_05, PWR_M_15	MSR_M_07, PWR_M_16	The modelling of single phase buoyancy driven flow in a volume with CFD has wider industrial application: for example in the design of passive cooling for buildings.
P8_A	181	Investigate the impact of 'real' surfaces on NTH heat transfer modelling predictions	AGR_M_06, HTGR_M_03	PWR_M_11	Although this work focusses specifically on typical NPP surfaces, it will add to the body of knowledge regarding the effect of surface details on heat transfer.
P8_B	185	Improved wall models for accurate heat transfer	AGR_M_06, HTGR_M_03, PWR_M_05	AGR_M_01, PWR_M_05, LMFR_M_15, PWR_M_20	This work would be of benefit to all industries where CFD is used to predict surface heat transfer.

The following User Requirements are not satisfied by any of the project proposals: AGR_M_07, HTGR_M_05, HTGR_M_10, LMFR_M_02, LMFR_M_14, MSR_M_04, PWR_M_02, PWR_M_04, PWR_M_19.

Table A2: Project Links to User Requirements

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A2 Proposed R&D Projects

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Project Title	Development of Innovative Coarse-Grid Models for Reactor Design			
Topic	Multi-fidelity			
Reference	P1_A			
Source	Workshop Group	o 1 and current Ph	nase 1 developme	ent work.
Location on Capability Map	Modelling Tools Physical/Empirical Mathematical Models			
R&D Spectrum	Basic Applied Early Late Research Research Development Developm			
		\boxtimes	\boxtimes	
Technical Objectives	detailed geomet new improved m capture the flow is currently prohi entire plant, or e the medium term codes) are availal larger scale, but specific empirical A key objective of the benefits of dimethods in a fratimescales. Muc methods/codes of multiphysics charapproach directly coarse-grid CFD within a single from the properties of fuel-chance design/enging to develop of the properties o	ry and multiscale/ nodels are being divided within these complications are not received and entire fueld and these are necessed data which limits of current NTH more tailed modern the mework which can hinternational effort different fidelities of combining some model so the multiple and whole-concering calculation methods to enable thous/models; validated-smart-fuels and validate multiple with the constant of t	e better combination rel-channel models lti-channel/whole-cor both light-water	nods exist (and noreasonably hall scale, but it he scale of an remain so for b-channel predictions on a dent on plant or applicability. It is to capture odelling strially useful ted to coupling multi-scale and novative dels into a new exist addressed is project are: ology for models one for routine on of coarse and other or and other
Benefits	engineering calc	ulation methodolo by making use of	odernise the react ogies (e.g. system the recent develop s (e.g. CFD). More	and sub- oments in

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	 Enabling CFD models to be used to simulate more complex systems within realistic computing resources such that they can be applied within industry as design tools; Developing tools that can be calibrated and validated for specific systems and produce results in short turnover times, serving a similar purpose to the system/sub-channel codes but with enhanced capability (i.e. including 3D effects, plant aging etc.); Enabling a natural coupling with conventional CFD, and hence enabling models to resolve local flow physics to be included in the solution as required, resulting in reduced uncertainty in methods; Enabling an overall modelling strategy to be developed that uses both empirical and resolved methods with a reduced number of software tools, thereby reducing both training requirements and the risk of user error.
Scope & Approach	The approach chosen for this work is to develop innovative methodologies for coarse-grid methods aimed at significantly improving the performance of the widely used porous medium approach, which suffers from various deficiencies when applied to reactors. Various innovative ideas are worth developing/testing, including, as proposed here, making use of the sub-channel strategies and correlations. The scope of this project will include: • Develop, evaluate and integrate empirical models for coarse-grid CFD (replacing wall functions) by comparison with experimental data or with the aid of high-fidelity CFD for reactor relevant flow and heat transfer physics, including for example, cross flows, rough surfaces and buoyancy (for single phase flow in the first instance). • Develop interfacing methods to enable smooth transition between coarse/fine mesh models, improving representations of flow physics/turbulence and numerical stability. • Develop a number of 'smart' models for fuel channels to demonstrate the techniques; validate against sub-channel
	 codes for simple cases and against detailed CFD or experiments for 'complex' cases. Build, test and validate models for multiple channels/the whole core for very large systems to demonstrate the full capability and advantages of the new methodology and to gain acceptance from the community.
Validation Requirements	 Verification: the developed methodology should be carefully tested under various scenarios for physical consistency and numerical stability. Validation of full representation (smart fuel channel model, for example): validate the model against sub-channel codes for simple cases (e.g. normal operation conditions where sub-

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	channel models are well validated) and against detailed CFD or experiments for 'complex' cases.
Output	 Innovative coarse-grid CFD methodology with potential for simulating large reactor systems (fuel channels, core) in short turnover time.
	 Validated smart fuel channel model in open source CFD code to demonstrate the full capability.
	 Initial model(s) for larger system (e.g. multiple-channels, whole- core).
	 Documentation of the developments in 2-3 academic papers.
Existing Research & Body of	Existing porous representations in current CFD codes.
Knowledge International Programmes	▶ Few examples of research into coarse-grid CFD models. These adopt different approaches from those proposed in this project, but some aspects are likely to be of relevance.
	Existing sub-channel models.
	 Various current/previous US/EU consortia in reactor systems modelling (NEAMS, SESAME, THINS), all include some elements of CFD/system coupling and component modelling.
	 Feasibility study of innovative ideas of coarse-grid CFD carried out in the current Phase 1 project has shown excellent potential.
Risks	It may take time to gain acceptance from industry/regulators even though the methodology/models may be technically sound.
	Existing sub-channel and system code methods are already considered 'adequate' for current reactor designs, this may delay take-up of new innovations in light water technologies. However, the benefits to new reactor design could be realised without this barrier.
Timeline and Prerequisites	First phase – 2 years to create initial models and test feasibility of approach (as part of the current BEIS program).
	Second phase – 3 years to develop the models to an exploitable state.
Resource/Costs	2 researchers (CFD code development experience and a good understanding of existing methodology of 'coarse-grid' and porous models.)
	Access to open source code (with source and version control)
	Industrial partner for support with demonstration cases and data. Access to HPC resources and expertise (e.g. STFC).
Exploitation Recommendations	 Publish methodology in reports and papers to seek dissemination, acceptance and further development; make recommendations for future developments.
	 Demonstration models implemented in open source code to remove financial barriers to exploiting the advancements.

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▶ Likely future exploitation will be development of validated, reactor-specific, smart models for reactor components/whole-core for relevant designs of both advanced light water and other, Gen IV technologies (this is likely to be carried out by industry and will result in proprietary models based on the method developed by this project).

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Project Title	High Fidelity Modelling to Improve the Accuracy of Low Fidelity Methods			
Topic	Multi-fidelity			
Reference	P1_B			
Source	Workshop Group	o 1		
Location on Capability Map	Modelling Tools and Concepts and Doctrine			
R&D Spectrum	Basic Applied Early Late Research Research Development Development			
		\boxtimes	\boxtimes	
Technical Objectives	Low fidelity tools (e.g. system codes) are an important part of the suite of methods available to the nuclear thermal hydraulic engineer. They are essential in early design and safety substantiation and, once developed, they represent a fast, inexpensive way of analysing a complex reactor system. However their low fidelity nature leads to regions of a reactor where their accuracy is low, and confidence in their results cannot be high in the absence of empirical closure relations (correlations) derived from test data characterisations of components and flows. Higher fidelity modelling techniques exist that can accurately capture the flows in complex regions of a reactor, but it is not currently practical to use them to model an entire system and the use of simpler models where possible will always offer cost and timescale benefits. The technical objective of this work is to improve the accuracy of low fidelity tools by incorporating more detailed descriptions/submodels in areas where the former are known to be of low accuracy.			
Benefits	 The benefits of this work package are: To improve the accuracy and range of applicability of system codes; To realise the benefits of high fidelity modelling techniques in whole reactor analyses; To potentially reduce the reliance on test data thereby reducing the costs and timescales to produce suitable predictions; To reduce the timescales and costs in developing the inputs needed for reactor specific modelling by making use of modern computational techniques. To involve the UK in research at the forefront of an emerging technology with wide applicability (i.e. beyond NPP analysis). 			
Scope & Approach	There are a number of different approaches that could be taken for this work. The explicit embedding of high fidelity modelling (e.g. CFD) in a lower fidelity model is a method that has been and is being actively explored. Challenges include issues of			

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	 interoperability of tools, their relative computational demands and differences in the timescales associated with the physics captured by different modelling approaches, which makes handling the interface between models hard. This project is intended to develop an alternative approach; building on state-of-the-art machine learning techniques to capture the benefits of high fidelity modelling within a lower fidelity framework. This project will be a proof-of-concept for the generation of higher fidelity 'sub-models' for use in lower fidelity NPP analysis codes using this approach. The expected activities are: Investigate the suitability of driving reduced order models using Proper Orthogonal Decomposition (POD) based on high fidelity training data and simulations. Investigate the feasibility of and, if possible, identify a suitable machine learning approach to provide, for example, flow regime classified lower order models or emulated response predictions based on high fidelity training data (could be a mix of simulation and test). Based on the findings of the feasibility of the approach, agree a realistic set of required submodels, focussed on priority areas. Create a hierarchy of reduced models for specific flows to be embedded in higher level models (e.g. system codes) models. Demonstrate the approach by incorporating specific, improved low order models in a system code.
Validation Requirements	An improved system code could be validated against the available large scale data against which the empirical closures have already been validated. A more complex embodiment could be based on suitable benchmark problem, with validation data available.
Output	The developed demonstrator and associated documentation made available for industry exploitation and further research.
Existing Research & Body of Knowledge International Programmes	Research is starting to gain traction using POD and machine learning to exploit LES and DNS. The methods are transferrable to thermal hydraulics. For example, a very recent, highly relevant example from rocket propulsion provides a template to follow: Common Proper Orthogonal Decomposition-Based Spatiotemporal Emulator for Design Exploration, Shiang-Ting Yeh, Xingjian Wang, Chih-Li Sung, Simon Mak, Yu-Hung Chang, Liwei Zhang, C. F. Jeff Wu, and Vigor Yang, AIAA Journal (to appear) https://doi.org/10.2514/1.J056640 Preprint available: https://arxiv.org/abs/1709.07841
Risks	Ideally a demonstrator would be similar to a real operational reactor, but this may create problems with proprietary inputs.

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	The novelty, and difficulty of the technical challenge may mean that it is hard to demonstrate a significant improvement over current industry working practices in the first instance. Machine learning is an emerging technology; people with skills in this area are scarce and in-demand in other industries.
Timeline and Prerequisites	A demonstrator could likely be achieved in 3 years.
Resource/Costs	2 FTE researchers plus 0.5 FTE industrial contributors for three years. Resources with an understanding of reactor thermal hydraulics and relevant experience with POD and machine learning are needed. Industry and academic collaboration would be beneficial to ensure that the demonstration is as credible as possible.
Exploitation Recommendations	The demonstration system code and submodels could be used as a starting point to develop improved system codes for industrial use.

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Project Title	Reducing the Cost of CFD – Efficient and Effective Meshing			
Topic	Multi-fidelity			
Reference	P1_C			
Source	Workshop Groups 1 and 4 and subsequent core team development			
Location on Capability Map	Personnel Concepts and Doctrine Modelling Tools			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		\boxtimes
Technical Objectives	To investigate methods for reducing the time taken to develop high quality, optimally sized CFD meshes for thermal hydraulic modelling. To document guidance relevant to NTH engineers wishing to use			
Benefits	 The engineering time taken to develop a mesh can represent a significant proportion of the cost to industry of using CFD. Furthermore, the size and quality of the mesh can have a significant impact on computational expense and final accuracy of the analysis. Reducing the engineer time taken to develop meshes for nuclear thermal hydraulic CFD will directly reduce the cost to industry of using advanced methods. Improving the quality of CFD meshes used in the UK will maximise the benefits of using these methods and help prevent rework and thereby reduce the time taken (and the cost) overall to achieve the required solution. 			
Scope & Approach	 There are a variety of methods and tools available for creating meshes suitable for NTH CFD application. These can vary from: The highly automated e.g. a mesh generated by automatic surface wrapping and automatic tetrahedral, hierarchical hexahedra or unstructured polyhedral volume mesh generation, to, The highly manual e.g. laboriously hand-crafted mesh using block structured, hexahedral volumes. Both methods have a range of applications where they are the best solution, and choosing when to employ each technique (or the large range of options between and aside from them) is not always clear. When a technique is chosen, there are significant elements of skill and judgement that are needed to produce a high-quality mesh with appropriate refinement in the regions of most importance. 			

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Furthermore, learning a new technique or tool is a substantial training investment.

Comprehensive knowledge of meshing strategies and how to implement the optimally sized, high quality mesh is not widespread in the academic or industrial CFD user-base. Knowledge of the effect that the mesh quality metrics reported by meshing tools on the accuracy and stability of solutions is also not widespread, or well documented, and is to some extent CFD solver specific.

The detailed development of automatic meshing algorithms is a challenging and specialist area, which is owned by the vendors of such tools, and the details of any guidance that can be offered by them is inevitably tool and algorithm dependent. It is often the case, however, that the tool developers are not best placed to make flow and component specific judgements on the best meshing approach to use because they cannot be expected to have comprehensive knowledge of all of the real-world applications to which their tool may be applied. This knowledge is typically held by experienced users, depends strongly on the toolchain involved and is rarely rigorously subject to uncertainty analysis, formally recorded or communicated. There is a shortage of such users within the UK, so it is the case that this knowledge is not disseminated where it is needed the most.

This project will consider and define the requirements of a mesh for nuclear thermal hydraulic modelling using CFD using a number of prototypical examples. The emphasis of the project is create a suitable quality mesh in the minimum time. The scope of the project will be:

- Identify non-proprietary but prototypical test cases. These need to be sufficiently geometrically complex to be useful, i.e. not basic 'benchmark' style geometries.
- ▶ Identify the flow conditions to be used for the comparison and the high-level CFD solution being targeted: heat transfer or pressure drop, using modelled (RANS) or resolved (e.g. LES) turbulence.
- Create a high quality reference solution for each test case.
- Apply a variety of meshing strategies and tools to each case, recording: the time taken, any areas of difficulty, and any shortcuts. To include meshes with a relatively low cell count as well as highly resolved cases (the emphasis of this project is to produce meshes that are of a size for practical industry use).
- Use the meshes to calculate a CFD solution in each case and compare the convergence behaviour and results.
- Comprehensively report the method, tools and steps used to construct the mesh including: description of mesh in terms of relevant parameters (e.g. cell types, skewness, y+ etc.); guidance on any difficult areas; an estimate of the time taken to reconstruct a similar mesh using the guidance; the resulting

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	 CFD solution; a comparison with the high fidelity solution; and the result of any mesh sensitivity studies. Consider and plan, if required, an extension to this project to include less well used meshing techniques such as overlapping or sliding meshes.
Validation Requirements	Explicit validation is not required, because the emphasis is not the accuracy of the CFD solution per-se. The reference solution fulfils this role.
Output	A guidance document for each prototypical example for how to implement a mesh for a given component in a given meshing tool (or following a high level approach), for a defined flow condition. An over-arching summary document describing the results of the project as a whole.
Existing Research & Body of Knowledge International Programmes	Knowledge resides with users experienced in applying CFD to complex industrial geometries, and is distributed worldwide. CSNI 'Best Practice Guidelines for the Use of CFD in NRS Applications' [NEA/CSNI/R(2014)11] contains some relevant information and guidance, although the focus is not industrial efficiency.
Risks	The correct decisions on meshing are not mathematically derivable in the general, 3D case, and are often a matter of opinion, custom-and-practice, or acceptance of defaults. They are also often not directly transferrable between tools. The project may become a comparison or competition between strongly held existing positions, without a clear metric on which to compare relative merit. The mitigation in this case is to report the differently held opinions and highlight that there is subjectivity in approaches in this case. The tools available for CFD meshing are constantly being improved. Some aspects of the outputs of this project could become out-of-date relatively quickly. This is unavoidable in the fast developing CFD industry and the more generic and strategic findings of the work will have a much longer life span.
Timeline and Prerequisites	Provided that a high-quality reference solution can be produced, each prototypical example, with associated documentation, could be produced in approximately six months. Interaction with CFD code developers to establish better guidelines for the effect of cell quality may be needed to unambiguously identify how to make the most appropriate choices, and what thresholds for mesh quality can be accepted. Licences to commercial CFD and meshing tools and access to skilled users is required. The timescales could be as little as one year if multiple organisations are working parallel.
Resource/Costs	The best value could be gained by involving a variety of organisations, thereby capturing the knowledge and experience

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	within each. Additionally, it is unlikely that a single organisation will have access to or skills in all of the available tools.
	Resources used should be engineers with a significant level of experience in building complex 3D meshes for NTH CFD. The project could consider including contributors from other relevant industries.
	Approximately 6 - 9 months FTE effort per example depending on the complexity of the case and number of meshes generated.
Exploitation Recommendations	The documented results of the study should be publically available and could be immediately exploited by all UK organisations who perform CFD for the purpose of NTH analysis.
	This knowledge is not fundamentally nuclear specific, and could be readily applied to other industries that use CFD simulations. It is also neither a UK specific issue, nor a problem that is particularly well solved and publically disseminated elsewhere, so it would represent a strong contribution to international programmes.

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Project Title	Increased Participation in Benchmarking			
Topic	Best practice and uncertainty evaluation			
Reference	P2_A			
Source	Workshop Group 1			
Location on Capability Map	Verification and Validation Concepts and Doctrine Personnel			
R&D Spectrum	Basic Applied Early Late Research Research Development Development			
		\boxtimes	\boxtimes	
Technical Objectives	The process of benchmarking is fundamental to the assurance of quality and understanding of uncertainty in all modelling tools. International benchmarking programmes exist to enable the investigation of new modelling techniques, but UK involvement in NTH benchmarking is sporadic and often 'tagged onto' other work thereby limiting its value. The objectives of this project are to re-engage with NTH international benchmarking programmes in order to: Provide information to improve the quality assurance of NTH modelling in the UK thereby expanding its use in support of both design and nuclear safety substantiation. Quantify the uncertainties of different modelling techniques applied to nuclear thermal hydraulic cases. Enable the evaluation and quantification of 'software user effects' i.e. the effect that the detailed user inputs, chosen software and hardware have on the results within a set of nominally identical analyses.			
Benefits	 The overall purpose of this work is to increase the benefits of NTH modelling tools by improving UK user knowledge and evidence for validation. This will lead to a reduction in wasted effort and therefore reduced costs in both reactor design and substantiation. Improved best practice by better understanding model strengths and limitations. Improved confidence that applied software can be used to support reactor design and demonstrate safety to regulators. Creation of valuable training opportunities (involvement in benchmarking is excellent training) Promoting collaborative working within the UK NTH community. Promoting international collaboration and enhancing the UK's reputation through involvement in relevant programmes. 			

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Scope & Approach	The approach for the work is the organisation of a co-ordinated UK initiative to increase participation in benchmarking and maximise the exploitation of value gained from such participation. This could include participation in OECD/CSNI WGAMA benchmarks and/or IAEA Coordinated Research Project (CRP) benchmarks (or proposal of a new benchmark case). This project should review the functionality of the platform under development by the WP1 – Virtual Engineering programme and
	consider if it can be used to perform this project.
	Define scope (activities) of a UK thermal hydraulics working group. Consider US National Lab models for industry/academic collaboration (link with project P2_B).
	2. Select suitable existing benchmarks in the framework of training and an initial UK exercise. It is recommended to undertake 'blind' benchmarking in the first instance followed by comparison with data and other published modelling results. Selection of benchmark could be made to maximise benefits to other research projects.
	 Unlike some benchmarking exercises, emphasis should be on exploring the valid ranges of models, so identification of methods/approaches that compare badly are just as valuable as those that compare well.
	Consider the use of DNS to supplement data available for an existing benchmark.
	5. Depending on the project progress and opportunities available, the UK could propose a new benchmark. The specific case should be determined by the UK priorities at the time, but possible ideas include:
	a. Void distribution (drift) in BWRs or droplet size and entrainment rate models as two-phase flow examples.
	 b. Fluid-structure interaction or thermal fatigue as single phase flow examples.
	 c. Natural circulation/passive cooling in a single and/or two- phase environment.
	All findings should be presented at UK working group and disseminated to UK Nuclear Thermal Hydraulic Community.
Validation Requirements	This project is a validation and uncertainty quantification exercise. Benchmark cases need to be chosen based on both their relevance and the quality of the validation data available. The new UK test facility could be used to create suitable new experimental data to support the proposal of a new benchmark case.
Output	Reported comparison of results, report should be complete and detailed regarding all modelling assumptions, inputs and the most important sources of result discrepancies (sources of uncertainties and errors).

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	Presentation of findings at relevant UK working group.
Existing Research & Body of Knowledge International Programmes	Existing research and knowledge in UK i.e. involvement in previous benchmarking exercises (both in nuclear and in other industries e.g. combustion). International benchmarking programmes: OECD/CSNI WGAMA, ASME V&V 20 and 30 standard committees, IAEA CRP
	benchmarking exercises.
Risks	Availability of existing test data, or experimental facility (if new data are needed) for any new benchmark proposed.
Timeline and Prerequisites	Initial time needed to choose cases potentially linking with other nuclear thermal hydraulic Phase 2 projects.
	Each benchmark should be expected to take between one and two calendar years (depending on the complexity of the problem).
	It would reduce the costs of this project if it were run in parallel with P2_B, as the 'working group' included in the scope could be coordinated with that for other collaborative projects.
Resource/Costs	Actual benchmarking exercises should be carried out by a combination of academic and industry contributors in order to maximise the training benefits.
	Support from industry would certainly be needed in the selection of the most valuable benchmarks and tools to be tested.
	The precise resource and costs would depend on the benchmark chosen and tools used and could, to some extent, be modified to fit the available budget. Typical costs estimated as 1FTE researcher for 1 year to carry out a variety of analyses associated with a single benchmark.
	Likely to need approximately 3 FTEs for 1-2 years to complete a more comprehensive set of studies on a number of different benchmarks.
	Working group would comprise a number (minimum of 4-5) of different organisations and meetings etc. would also require funding.
Exploitation Recommendations	Results to be as widely disseminated as possible throughout UK community. Findings should be clearly and completely reported to maximise value.

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Project Title	Maximising UK Nuclear Thermal Hydraulics Collaboration and Collective Learning			
Topic	Best practice and uncertainty evaluation			
Reference	P2_B			
Source	Workshop Group	1		
Location on Capability Map	Personnel Concepts and Doctrine Hardware and Infrastructure Verification and Validation			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
			\boxtimes	
Technical Objectives	The UK nuclear thermal hydraulics community has become sparse and fragmented with a high proportion of experts close to retirement. The limited and intermittent funding previously available for NTH modelling research and the mechanisms by which it is acquired have all worked to produce a competitive rather than a collaborative research environment. To enable the growth needed to support future UK participation in NPP design, it is essential that we consolidate what we know and both capture and share this knowledge and experience within the UK NTH community. Furthermore, a specific need has been identified in the area of sharing knowledge and experience regarding modelling best practice and uncertainty; something that can only be achieved via a collaborative effort. To this end this project aims to: Establish a framework for collaborative working in NTH modelling in the UK. Reach a consensus on and document co-working practices and procedures and provide tools to support the efficient implementation of current and future collaborative research. Develop and communicate best practice in nuclear thermal hydraulic modelling and specific 'lesson learned' information to the UK community to supplement and illustrate the most up to date international nuclear safety best practice. Assess the need and remit for future collaboration, knowledge capture and R&D management within UK nuclear modelling.			
Benefits			to create an intern ort term benefits c	•

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- More industry focused and better co-ordinated planning for all NTH modelling R&D projects (including all those carried out under Phase 2 of this programme).
- Knowledge dissemination sharing of 'lessons learned' leading to increased efficiency in UK nuclear thermal hydraulic modelling in both research and industry environments.
- Increased visibility of the complete scope of UK NTH expertise to the international community.
- The consolidation of the current UK skills base to give sound foundations on which to grow expertise.

The longer term benefits will be:

- Increased collaboration within UK NTH modelling, reversing the trend of fragmentation and loss of skills.
- ▶ Enhanced knowledge capture and efficient skills development.
- A more co-ordinated and exploitable approach for all UK NTH R&D (both inside and outside of this programme).
- A focus for NTH modelling activity in the UK in the absence of a national body (e.g. CEA in France).

Scope & Approach

For this project to be successful it is important that the initial collaborations be well focused around achieving specific aims in areas of common interest.

An area of considerable interest to industry is best practice and uncertainty evaluation in CFD. While nuclear safety specific publications exist to inform the development of highly accurate CFD solutions, there is (understandably) little information in these sources regarding the fast and economically efficient use of CFD in a NTH environment and little CFD tool specific guidance. The code vendors provide training in the use of their tools in a more generic sense, but it is left largely up to the user to develop the most efficient and effective ways of using them for a specific application.

Therefore, a gap exists where there is little information available. Skilled NTH CFD practitioners develop this knowledge over years of experience and many are keen to share what they know. Two of the recommended projects have been identified as strong areas for initial collaboration. However, if the framework proves valuable in the first year it should be expanded to encompass additional R&D projects and potentially other nuclear modelling research areas.

The scope of the work proposed is:

- 1. Establish or identify projects where collaboration is an essential component. Projects P1_C and P2_A proposed under this programme consider aspects of best practice and uncertainty respectively have all the right attributes to both promote and benefit from UK collaborative working, with the first likely to require primarily industry resource and the second likely to be dominated by academic contributions.
- 2. Develop co-working procedures/guidelines and forums/platforms for supporting collaborative projects and organise/run

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	forums/platforms for the duration of the 3 year project. As a minimum this should include an electronic means of exchanging information and disseminating results (e.g. website and/or the platform under development within WP1 - Virtual Engineering Project) and a working group to consolidate the information from the various collaborators and establish procedures for the dissemination of the outputs of the selected projects to the relevant communities (could include written or verbal communication and input into training). 3. Demonstrate the value of the framework via the capture and dissemination of best practice and uncertainty experience relating to the selected projects. 4. Review the potential benefits of the framework to all funded NTH R&D projects. Investigate if any of the findings or lessons learned could be used to benefit/influence these programmes. 5. Develop a vision (and potentially a business case) for the future
	of the UK NTH collaborative working environment.
Validation Requirements	The specific information disseminated could be validated via reference to international publications or collaborative bodies. 'Lessons learned' information would gain value from the peer review possible under a collaborative working environment.
Output	Documentation capturing any valuable information relating to best practice or uncertainty in CFD from the selected collaborative projects and dissemination of this information via the forums established under this project. Documented working guidelines, procedures/policies and framework objectives.
	Appropriate forums established.
	Virtual tools developed, as applicable.
	Documented business case and future vision.
Existing Research & Body of Knowledge International Programmes	Consideration of methods of collaborative working used in the UK in other/related industries e.g. 'UK Collaborative Computational Projects'.
	Consideration of mechanisms for collaborative working used internationally e.g. US national labs, CASL, participation in CFD and TH standard committees etc.
	UK Fluids Network Nuclear Thermal Hydraulics SIG (Special Interest Group) currently serves as a forum for the presentation and discussion of NTH research and has helped to build relationships in the UK NTH community. However, it fulfils a different purpose and only has funding for one more year. This project should build on these foundations to develop a more specific collaboration framework. Current best practice and uncertainty documentation for example:

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"Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Applications – Revision", NEA/CSNI/R(2014)11.
"Review of Uncertainty Methods for Computational Fluid Dynamics Application to nuclear reactor Thermal Hydraulics", NEA/CSNI/R(2016)4.
Forums are poorly supported/attended; interest in this area depends on a reasonable number of active UK participants. The success of this enterprise depends on the willingness of the NTH community to share information regarding both failure and success. This may be politically and/or commercially challenging in
some cases. Depending on the funding arrangements there is a risk that industrial participants from smaller organisations could be effectively excluded on grounds of the cost.
Needs a number of relevant collaborative projects to be in place and development of the collaborative working framework needs to be co-ordinated with the delivery timescales of these projects.
Approximately 1 FTE of effort in total split between a number of participants from both UK industry and UK academia. Skills required would include a lead engineer and engineer with IT skills for the creation of relevant platforms/tools. Additional funding for workshops and dissemination events including T&S allowance for participants.
This project should be exploited to provide a fundamental part of the management, co-ordination and successful exploitation of Phase 2 of the programme. Specific lessons learned regarding uncertainty and best practice could be exploited across a wide range of projects and initiatives. In the longer term, better co-ordinated research would enable more targeted funding by clarifying the areas of highest value to NPP design and operation.

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Project Title		Sensitivity and Uncertainty Analysis of a Reduced-Order Model for Simulating BWR Dynamics		
Topic	Best practice a	Best practice and uncertainty evaluation		
Reference	P2_C			
Source	Dan Cacuci, S	er Cymru Chair F	Professor at Bangor	University
Location on Capability Map	Concepts and	Validation and Verification Concepts and Doctrine Modelling Tools		
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
Technical Objectives	predictions of industry. The I use of such to caused by an 'wrong' the mois to changes to 'bounding' appropriate and in practical for the highly complete always clear. Improved method uncertainty in development of corresponding sensitivity and research, with project looks to and reduce unbehaviour. This current UK new area of model uncertainty wood to an extant remonlinear dynatic compute exact functional derivational derivation of the modern of the sure of the modern of the modern of the modern of the modern of the sure of the modern of the	modelling tools is imitations experied ols for nuclear satinability to robustly odel predictions may be or uncertainty in the or uncertainty in the prediction of track TH phenomena and the odologies for the nuclear modelling of mathematical at the (forward puncertainty analy excellent potentials of further developmental of the project and prediction, where outly an allow both economic project goals are adjoint uncertainty and efficiently and efficiently ovatives) of system actor power, tempodel's parameters	nsitivity and uncertary a key objective for a key objective for a kenced by current UK fety related applicating a nawer questions and how sern inputs or properties approach is also ansient effects in the where what is 'consequent and numerical adjoint rediction) multiphysical to deliver these becamed apply these memulation of dynamical day as representative the understanding of an ABWR. Then usuall of the 1st-order sequences of interest erature, delayed near test once parameters etc.	a high regulated industry in the ions is often about how estive an answer as. A simple ds to large often not presence of servative' is not at models, it is models, it is models for a area of enefits. This thods to quantify a ABWR ing pertinent to a of a challenging of sensitivity and safety benefits. All corresponding ating the cuse this model to rensitivities (i.e., est (e.g. time-utron fractions coefficients,

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demonstrating the proof-of-principle for performing exhaustive sensitivity analysis of large-scale models.

- (2) Perform the above pioneering sensitivity analysis under: (a) stable (normal) ABWR-operating conditions; (b) oscillatory ("limit-cycle") ABWR-dynamic conditions; (c) chaotic, worst-case scenario, ABWR-dynamic conditions. Use the above sensitivities to perform and demonstrate the complete/exhaustive path for performing paradigm quantification of uncertainties in the model predictions due to the model parameters.
- (3) Use the sensitivities quantified in (1) and the uncertainties quantified in (2), to perform and demonstrate the path for performing "predictive modelling" [1], including data assimilation and model calibration, aimed at obtaining optimally predicted values for the responses and parameters described in (1) and (2), above, while reducing the predicted uncertainties in these model parameters and responses. Perform pioneering "predictive modelling" to reduce uncertainties for (a) stable (normal) ABWR-operating conditions; (b) oscillatory ("limit-cycle") ABWR-dynamic conditions; (c) chaotic, worst-case scenario, ABWR-dynamic conditions.
- (4) Use the conceptual paths established in (1) to (3) above to prepare the path for the conceptual design of a natural circulation loop that would fill gaps in extant experimental data needed for validating further model developments for reducing uncertainties in the long-term operational stability and safety of ABWRs.

Medium-term (3 years) project goals are to apply the concepts underlying the "predictive modelling" path (including exhaustive sensitivity analysis, response uncertainty quantification, data assimilation, model calibration and validation) demonstrated in (1) to (3) above to extant coupled multiphysics codes that are both validated and accepted for reactor design and analysis by the US Nuclear regulatory Commission. This would provide, in a timely manner, tools beyond the state-of-the-art for the UK industry, while using these tools for the design of a unique-in-the-world natural circulation loop at Bangor University.

Longer-term project goals (i.e. 3+ years and beyond the timescale of this project) are to contribute towards:

- (1) Establishing a "LWR predictive modelling validation centre" at Bangor University, to provide (for use by the UK nuclear industry and academia) validated and regulator-accredited modelling tools, going beyond the current state-of-the-art, aimed at reducing uncertainties in operational and safety margins, thereby improving the overall economics and safety of LWRs.
- (2) Constructing a natural circulation loop for producing experimental data that would fill in current gaps in the data base that would be needed for predictive model validations of future high-fidelity simulation tools aimed at reducing uncertainties in operating and safety margins of BWRs, thereby improving significantly the economic competitiveness of the UK nuclear industry.

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	(O) Federal the applicability of the allowance of the left of the
	(3) Extend the applicability of the above-mentioned high-fidelity validated simulation tools to all (large and/or small modular) LWRs.(4) Extend the use of adjoint sensitivity and uncertainty evaluation to other NTH modelling tools and analysis methods.
D (1)	
Benefits	 Benefits to the UK nuclear industry are: Short-term: Quantify the uncertainties in results predicted by extant coupled multiphysics codes that are both validated and accepted for reactor design and analysis by the US Nuclear regulatory Commission thereby enabling well informed use of the tools by UK industry. Demonstration of the use of advanced sensitivity and uncertainty quantification methods in an NTH context and dissemination of findings will increase awareness and take-up of these methods by the UK nuclear industry. Medium-term: Reduce the uncertainties in results predicted by extant validated coupled multiphysics codes thus extending their validation domain while using these tools for the design of a unique-in-theworld natural circulation loop at Bangor University. Longer-term: Reducing uncertainties in operational and safety margins of LWRs, thereby improving the overall economics and safety of LWRs.
	 Extend the applicability of the above-mentioned high-fidelity validated simulation tools to all (large and/or small/modular) LWRs.
Scope & Approach	The approach to the work will be to build on the existing Bangor University expertise to apply, develop and exploit advanced sensitivity and uncertainty analysis in the context of ABWR dynamic behaviour analysis.
	Specific tasks envisaged for the project include: Task 1: Based on Bangor's reduced-order model of BWR-dynamics, conceive, derive and implement numerically the corresponding adjoint sensitivity model by applying Cacuci's "adjoint sensitivity analysis method (ASAM)" (see References 2 to 11). Task 2: Use the adjoint sensitivity model constructed in Task 1 to compute efficiently and exactly all of the 1st-order sensitivities of important model responses (neutron population, power, delayed precursors, fuel temperature, and coolant temperature) to all model parameters (reactivity, cross-section effects, feedback, etc.). Use these sensitivities to rank the parameters' importance in contributing to the various response variations due to variations in these
	parameters. Investigate the effects of parameter variations on the onset of the various bifurcations and chaos.

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	Task 3: Use the 1st-order sensitivities obtained in Task 2 to propagate parameter uncertainties deterministically to quantify the uncertainties (standard deviations) they induce in the respective model responses [11] Task 4: Using Cacuci's 2nd-Order Adjoint Sensitivity Analysis Methodology [11], construct the 2nd-Level adjoint sensitivity system to compute exactly and efficiently all of the 2nd-order sensitivities of the responses mentioned in Task 2 to all model parameters. Task 5: Use the 2nd-order sensitivities computed in Task 4 in conjunction with the uncertainty propagation formulas presented in [11] to compute the skewness and kurtosis of each of the responses described in Task 2 (pioneering work), which would enable the quantification of non-Gaussian features of the afore-mentioned responses. Also use the 2nd-order sensitivities computed in Task 4 to investigate deeper the nature of each of the bifurcation points, including the (worst-case scenario) transition-to-chaos displayed by Bangor's reduced-order model of BWR dynamics. Task 6: Use the results obtained in Tasks 1-5 to demonstrate the application of the predictive modelling methodology proposed by [1] to BWRs exhibiting oscillatory (limit-cycle) dynamics. Task 7: Use the results obtained in Tasks 1-5 to initiate the conceptual design of the natural circulation loop at Bangor. Task 8: Use the results obtained in Tasks 1-5 to initiate application of Cacuci's ASAM to the state-of-the-art code system TRACE/PARCS, which is sanctioned by the US Nuclear Regulatory Commission for performing BWR-analyses.
Validation Requirements	Task 9: Disseminate the methodologies and results obtained in Tasks 1-6 to UK nuclear industry, thus providing new tools and know-how towards reducing uncertainties in operational and safety design margins of LWRs. There is adequate extant validation data available for the completion of the first three years of this project. Moreover, the proposed work will identify gaps in extant experimental data (by assessing the
_	relevant OECD benchmarks), which would contribute towards establishing the design parameters of the proposed future TH loop(s) at M-SParc.
Output	Tasks 1, 2 and 3: Refereed journal articles presenting the results and consequences of the adjoint sensitivity & uncertainty analysis of Bangor's reduced-order model for simulation BWR dynamics. For each of the Tasks 4 to 9: Refereed journal article; dissemination of results to UK nuclear industry & ONR
Existing Research & Body of Knowledge International Programmes	Bangor University already possesses a reduced-order model that simulates the dynamic behaviour of a BWR based on the pioneering works cited in References 12 to 15. The above-mentioned model has been incorporated in BWR-simulators after the LaSalle (Illinois, USA, 1988) reactor incident,

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	because it qualitatively simulates the complete possible dynamical behaviour of a BWR, from the normal, steady-state operating state, through the onset of a limit-cycle oscillation, to the worst-case of chaotic dynamics. Several types of dynamic oscillations are possible in a BWR, as has been demonstrated experimentally (e.g. Ringhals, Oskarshamn, etc). Such oscillations can be modelled qualitatively by several coupled multiphysics code systems. In addition to its reduced-order model of BWR dynamics, Bangor University works with a system code (TRACE/PARCS) developed and sanctioned by the US Nuclear Regulatory Commission for investigation of BWR dynamics, and currently collaborates internationally in this domain with the Nuclear and Industrial Engineering (NINE) company in Italy, as well as several leading universities in the USA.	
Risks	Detailed knowledge and experience in this area in the UK is limited to Professor Cacuci; he is essential to successful completion of the work. Under the CAMP agreement there are limitations on the use of TRACE/PARCS coupled code by UK industry, which may limit its application. However, the methodology employed by the work and its findings will still be of considerable value.	
Timeline and Prerequisites	The outputs/deliverables from Tasks 1 to 3 are expected in Year 1. The outputs/deliverables from Tasks 4 to 6 are expected in Year 2. The outputs/deliverables from Tasks 7 to 9 are expected in Year 3.	
Resource/Costs	2 FTE researchers (at Bangor University) for three years +1 FTE industrial specialist for 2 years, to apply the modelling results produced by this project to design instrumentation for control aspects of the envisaged natural circulation loop at Bangor University.	
Exploitation Recommendations	 The outputs/deliverables from Tasks 4 to 6 (Year 2) will provide the proof-of-principle and illustrate the path for reducing uncertainties in predicted operating and safety margins for BWRs, and also for initiating the preliminary design of a natural circulation loop at Bangor. The outputs/deliverables from Tasks 4 to 6 (Year 3) will be directly applicable to extending the applicability and validation domain of industrial tools for reducing uncertainties in operational and safety margins, and (hence) economics of ABWR operation. 	

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Project Title	M-SParc Centre for Predictive Modelling and Validation of LWR Analysis and Design Tools			
Topic	Best practice and uncertainty evaluation			
Reference	P2_D			
Source	Dan G. Cacuci,	Ser Cymru Chair I	Professor at Bang	or University
Location on Capability Map	Verification and Validation Modelling Tools Personnel Concepts and Doctrine			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes	\boxtimes	\boxtimes
Technical Objectives	The validation of predictions is an essential component of nuclear thermal hydraulic modelling. It is required to support nuclear safety and also plays a key role in the development of new modelling techniques and tools. The new nuclear thermal hydraulics test facility proposed for the M-SParc site in Bangor gives the UK NTH community the opportunity to generate and use validation data in the UK along with opportunity to develop UK benchmark tools. The project aims at establishing a Centre for Predictive Modelling and Validation for LWR Analysis and Design Tools to be located in M-SParc, adjacent to the planned National Nuclear Thermal Hydraulics Centre. This Centre will maximise the value of the proposed test facility and serve the UK nuclear industry, academia, and research centres model validation needs.			
Benefits	The proposed Centre will enable the UK nuclear industry, academia, and research centres to validate their own computational models against the Centre's validated tools, as well as to employ the validation tools to be developed by the Centre in conjunction with data to be provided by the envisaged thermal hydraulics experimental loops to be located at M-SParc.			
Scope & Approach	The approach for this work will be to: acquire internationally established and validated codes to be used for the purpose of providing benchmarking for any new or developed UK codes; to further develop UK codes and models to advance the UK capability; to provide validation of these codes via the experimental facilities located at the M-SParc site. Task 1 (Year 1): Through the CAMP Agreement, obtain the validated state-of-the-art tools available from the US Nuclear Regulatory Commission (NRC), including the fuel behaviour codes (FRAPCON-3, FRAPTRAN), reactor kinetics code (PARCS), thermal hydraulics codes (TRACE, RELAP, SNAP), severed			

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	accident codes (MELCOR, SCDAP/RELAP5, IFCI, VICTORIA) and install them on the Bangor University servers and Welsh supercomputing Centre. These codes will serve as the state-of-the-art benchmarks for comparison to UK codes. Task 2 (Year 1): Negotiate with CEA/France permission for use of the French suite of codes (APOLLO, FLICA, CATHARE, NEPTUNE, etc.) for use as additional benchmarks/references for the comparisons with the future UK-based codes envisaged to be developed under Task 3, below. Professor. Cacuci served for 10 years (2002-2012) as Director of Research and Scientific Director of CEA's Nuclear Energy Directorate, so it is not inconceivable that it would be possible to successfully negotiate obtaining these codes for benchmarking purposes. Task 3 (Years 1-3): Initiate the establishment of an independent UK-based suite of coupled multiphysics codes for LWR analysis and design, advancing beyond the current state-of-the-art, to be validated using experimental data in conjunction with Cacuci's newly developed "Predictive Modelling for Coupled Multiphysics Systems (PM-CMPS)" Methodology ("Predictive Modeling of Coupled Multiphysics Systems: I. Theory," An. Nuc. En., 70, 266–278, 2014). Consideration will be given to the UK's developing needs and to the best available codes or platforms for development and could include current industry codes, open source codes requiring development for UK application or codes currently used in an academic
Validation Possiromente	environment, for example FETCH (3-dimensional neutron transport) and FLUIDITY (multiphase fluid flow). This work is envisaged to serve as the foundation for developing a UK-based capability.
Validation Requirements	The US-NRC and CEA/France code systems are already validated against state-of-the-art experimental data (from OECD benchmarks and national experimental facilities). For the duration of this project (3 years), the UK-based computational tools envisaged to be developed under the auspices of the proposed Centre will not need additional experimental data for the initial (3 years) development stage. In the longer-term, the UK-based computational tools will be validated against additional experimental data to be produced by the envisaged thermal hydraulics experimental facility to be located at M-SParc.
Output	The proposed Centre will provide an independent, UK-based, suite of coupled multiphysics codes for LWR analysis and design, advancing beyond the current state-of-the-art, to be validated (during the 3 years duration of this project) using extant experimental data.
	The Centre will also provide the ability to compare these and other UK-produced codes against the US-NRC validated codes and, possibly, CEA-validated codes. Beyond the timescales of this initial work the Centre aims to
	Beyond the timescales of this initial work the Centre aims to develop and provide experimental validation data and validation

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	expertise to all UK industry and researchers with regard to LWR NTH codes. The specific outputs for the first three years will be published in reports and peer-reviewed papers.
Existing Research & Body of Knowledge International Programmes	The extant research is too vast to be listed here. International collaboration, particularly with US and French institutions, is envisaged. Possible EPSRC/DOE-NEUP joint projects can be proposed based on specific work to be performed within the envisaged Centre.
Risks	There are risks associated with the ability to acquire all of the French and US codes. Some are open source, but others are less readily available.
Timeline and Prerequisites	Tasks 1 and 2 are expected to be completed within 1 year. Task 3 is envisaged to continue well beyond three years. After 3 years, the output of this Task will be a suite of coupled multiphysics (comprising neutron kinetics, core and plant thermal-hydraulics) codes advancing the current state-of-the-art for the analysis of LWR reactors (large and small)
Resource/Costs	1 FTE researcher responsible for setting up and running the US NRC (and possibly CEA) codes +3 FTE researchers responsible for coupling/developing the ("beyond-the-state-of-the-art") UK-based code system + 0.5 FTE industrial consultant all for 3 years.
Exploitation Recommendations	Through the envisaged Centre's personnel, the UK industry, ONR, academia and research groups will have access (while respecting various NDAs, CAMP agreement, etc.) to comparisons of their own computational tools to the US-NRC codes. The suite of UK-codes to be developed under the auspices of this proposed Centre could be used by ONR, UK industry, academia, and other research centres. Ultimately, through the envisaged Centre's personnel, the UK industry, ONR, academia and research groups will be invited to participate to the further development and validation of the "beyond-the-state-of-the-art" UK-based code system.

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Project Title	Improving the Prediction of Heat Transfer by Fundamental Multi-Scale Modelling of Bubble Growth Processes			
Topic	Boiling and condensation			
Reference	P3_A			
Source	Workshop Group	o 2		
Location on Capability Map	-	Physical understanding Physical/empirical mathematical models		
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		
Technical Objectives			e methods could r nuclear vast numbers sent the boiling chanistic need to be a single-bubble and departure surement but in fect of the herefore do not isms. In recent the level where attribute to the nicroscopic formation scale)	
Benefits	boiling models we Being able to preplace within the example:-	vould benefit nucle edict where, and v core would have o ediction of surface eby improving rea	more reliable come reactor analysis with what intensity considerable bene heat transfer in totor performance	s and design. , boiling will take fits. For he presence of

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- ▶ Improved ability to predict CRUD formation on nuclear fuel and an ability to investigate design options to eliminate it.
- Improved ability to predict the amount and disposition of steam within the core of a water-cooled reactor, thereby improving prediction of reactivity, power generation, and plant response.
- Understand the implication of accident tolerant fuels and advanced cladding on boiling mechanisms and therefore better predict heat transfer from the fuel under a wider range of conditions.

In the longer term these techniques could be used to develop component scale boiling models for Gen IV reactor technologies (e.g. liquid metals) where experimental data is even harder to acquire.

Scope & Approach

The approach to this project will be to build on existing microscopic CFD modelling work and the latest techniques to progress the highest priority areas affecting heat transfer. Modern interface-tracking CFD treatments will form the basis of this work [1]. These allow the discrete regions of liquid and vapour to be mechanistically modelled. Whilst work in this area is underway, there is much that still needs to be done.

The main activities under this project would be expected to include:

- ▶ Generation of good quality general-purpose models of the local heat transfer within superheated liquid towards a saturated bubble, where the length scales over which significant temperature gradients exist are tiny (of order microns). Coupling this with a reliable phase change model, to compute the mechanistic generation of vapour that goes on to inflate the bubble, will be a first and important challenge [2-4].
- ▶ The thermal interaction between a growing bubble and the heated surface on which it is growing is complex. Nominally steady heat fluxes actually more take the form of local transient cooling of the surface, with surface temperatures recovering during the quiescent period between bubbles. Transient conjugate heat transfer treatments need to be incorporated [5].
- ▶ Detailed analysis of the tiny "micro-layer" of water that can be left behind beneath the bubble as it grows [6-8]. Evaporation of this layer, at most perhaps 5 µm thick, but extending laterally some hundreds of microns, can be responsible for a big fraction of the early growth of the bubble. Understanding its formation and depletion requires both the solving of the equations for fluid flow within this fearsomely small body of water, and analysing the very local, very transient heat flux that is extracted from the surface by the rapid (almost explosive) evaporation of the layer. The differing behaviour of hydrophobic and hydrophilic surfaces needs to be properly incorporated. The development and validation of advanced microlayer modelling will be an important activity.

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	As a bubble departs from the wall nearby water necessarily flows into the region it previously occupied [9]. Such water, coming from a little distance from the heated surface, is relatively cool, and correspondingly high local rates of heat transfer from the wall are caused to take place. This phenomenon is responsible for a big fraction of the increased ability of boiling surfaces to convey heat to the fluid, and understanding and quantifying this near-wall liquid flow is very important. The detailed CFD models developed will be extended to take this into account.
Validation Requirements	Good quality public domain experimental programmes are underway in Korea (Kim [10]) and USA [11]. The generation of new validation data is not a requirement of this research project.
Output	Outcomes of the research will be published in academic papers, making the insights and quantifications gained available to component-scale boiling model developers. The understanding gained from the research will then feed in directly to the development of improved component scale boiling models and therefore into the advancement of practical modelling methods for the prediction of boiling and void distribution in reactors.
Existing Research & Body of Knowledge International Programmes	There is extensive published literature in this area. An accessible review is provided, with many references, by Giustini [1]. As noted, experimental programmes are underway in Korea (Kim [10]) and USA [11]. There are major modelling efforts in the UK (Imperial [1, 3-7, 9]), and PSI (Switzerland) [2, 4, 8, 9, 12], as well as some modelling work associated with the experimental programmes.
Risks	By its nature, with fundamental research like this, just what will be found, what will be found to be important, and what will turn out to be difficult to model, cannot be predicted in advance. (In this very area, the recently-appreciated need for quite mechanistic modelling of the microlayer, is a good example.) This is necessarily a risk.
Timeline and Prerequisites	3 years There are no prerequisites to this task but projects P3_D would benefit from the findings of this task.
Resource/Costs	1.5 FTE researcher for 3 years (The 1.0 academic, the 0.5 in industrial CFD, ideally)
Exploitation Recommendations	The outputs of this project can be directly exploited for the development of improved component scale boiling models by improving the accuracy of current assumptions regarding the wall heat transfer by the different mechanisms present in boiling flow. In the longer term, understanding gained from the research feeds into the fundamental body of knowledge regarding boiling flow and therefore supports efforts to improve the modelling of boiling in CFD and sub-channel codes.

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Project Title	Improved Two-Phase Flow Regime Transition Modelling					
Topic	Boiling and condensation					
Reference	P3_B					
Source	Workshop Group 2					
Location on Capability Map	Physical/Empirical Mathematical Models Modelling Tools					
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development		
		\boxtimes				
Technical Objectives	Two-phase flow regime transition for boiling flows is a key aspect of modelling the thermal hydraulic behaviour of BWRs in normal operating conditions and PWRs in fault conditions. Well established models exist for some two-phase flow regimes (e.g. dilute bubbles [1] and dilute droplets), however the modelling of transitions between these regimes is comparatively poorly developed.					
	In real light water reactors, multiple regimes are present and the often change with time under conditions of interest. To truly make best use of advanced NTH modelling methods in an LWR context the ability to predict and model these regime changes is an essential element.					
	The current methods, which rely on comparison against arbitrar defined void fraction set-points for the transition regions, are a significant contributor to the overall uncertainty of these models. The aim of this project is to develop improved models of two-ph flow regime transitions that can be implemented in CFD models.					
Benefits	Development of more detailed two-phase flow regime transition models for boiling flows is a vital part of improving the overall accuracy of multiphase flow CFD models (including boiling) employed in nuclear thermal hydraulics modelling. Improving the current models would lead to the following benefits: • Allow the full range of conditions in BWR normal operations and PWR fault studies to be modelled using CFD; • Enable modelling of large scale 3D effects in PWR fault conditions to improve the understanding of core cross flows, spacer grid effects etc. which cannot be captured in rod bundle					
	tests; Improve the accuracy of void distribution predictions which will enable improved understanding of neutronic feedback in BWRs. Furthermore, as this is an area of high international interest and activity, progress in this area would enhance the UK reputation and promote our involvement in current and future projects.					

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Scope & Approach	This project will focus on deriving improved methodologies for recognising flow regimes and modelling transitions between two-phase flow regimes in CFD. In particular the transition between modelling methods suitable for dispersed flow (i.e. bubbles in fluids) and interface tracking techniques [2], suitable for predicting the location of the boundary between phases will be investigated, demonstrated and validated. Specific activities will include: Implement interface detection and capture methods into a multifluid framework to enable either method to be used as applicable; Enable local selection of closure models depending on flow conditions and interfacial topology; Implement the improvements on a simple benchmark model (details to be chosen based on an investigation into the availability of validation data). Validate the improvements where possible (although it is recognised that this may be difficult across all regimes).	
Validation Requirements	Publically available validation data across all regimes is not likely to be available. A brief investigation is recommended as part of the scope and recommendations for the acquisition of any missing information should be considered part of the scope. Existing data is available for bubbly flows. Historical flow regime maps also provide a useful source of validation.	
Output	Outcomes of the research will be published in an academic paper A model will be developed as an output of the work which can be directly implemented in existing CFD codes. The model will be published in sufficient detail that it can be implemented in any capable CFD code rather than just the one used for the research project.	
Existing Research & Body of Knowledge International Programmes	TOPFLOW – GENTOP at HZDR, Germany Current CFD code two-phase modelling capability.	
Risks	Full validation may not be completed under this project. Whilst extensive experimental data is available for some flow regimes (e.g bubbly flows) similar experimental data may not be available for all of the flow regimes of interest.	
Timeline and Prerequisites	Good progress could be made in 3 years.	
Resource/Costs	1 FTE researcher and 1 FTE industrial specialist (CFD developer) for 3 years	

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A model will be developed as an output of the work which can be directly implemented in any existing multiphase CFD code and will be implemented into one as part of this project. As codes of this type are already used by the UK nuclear industry

 Colombo, M and Fairweather, M 'Accuracy of Eulerian-Eulerian, two-fluid CFD boiling models of subcooled boiling flows'. International Journal of Heat and Mass Transfer, Volume 103. December 2016, Pages 28-44

and their suppliers, there is a quick direct route to exploitation.

2. J. Feng, et al. 'Evaluation of bubble-induced turbulence using direct numerical simulation', International Journal of Multiphase Flow Volume 93, July 2017, Pages 92-107

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Project Title	Film Dry-out Mo	odelling in CFD				
Topic	Boiling and cond	Boiling and condensation				
Reference	P3_C					
Source	Workshop Group 2					
Location on Capability Map	Physical/Empirical Mathematical Models Modelling Tools					
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development		
			\boxtimes			
Technical Objectives	In normal operation the majority of the core of a BWR is cooled by the flow of a thin (~1/10 mm) film of water over the fuel, and essentially all design limits and set points stem from the requirement that this thin film does not dry out; a circumstance that would possibly lead to fuel melting.					
	Prediction of this dry-out, under the wide range of conditions that need to be analysed, is currently by a combination of expensive measurement augmented by one-dimensional essentially 'legacy codes [1, 2]. Exactly the same need, to model and predict film dry-out, arises fault studies for PWRs, and all of the issues and benefits noted below apply equally to this application. The objective of this project is to develop a three-dimensional representation of film dry-out within a modern CFD framework.					
Benefits	 A full three-dimensional CFD treatment will:- Provide higher fidelity dry-out predictions than current one-dimensional pipe-like models, with empirical representations of cross flow between sub-channels. Permit improved modelling of the response of the system to time-varying inlet flows, improving nuclear safety. (It is believed that just such a time-varying inlet flow was responsible for the recent dry-out event in a Swiss BWR.) 					
	 Contribute to the reduction of operational margins currently constrained by these modelling uncertainties, thereby providing economic benefits to operational and future NPPs. Allow much better representation of the complex effects of spacer grids enabling the development of improved designs. 					
	At a higher level, this project will provide valuable training and experience in an important BWR and PWR flow regime. As the UK prepares to operate these reactors growing this understanding is essential and potentially opens the door to our involvement in future design innovations.					

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Scope & Approach	High fidelity modelling requires analysis of the flow of the film; the flow of the vapour past the film; the flow of droplets entrained in the vapour; the deposition of these droplets onto the film, and the entrainment of droplets from the film by the high speed vapour flow. This project will use and develop 3D CFD modelling techniques to capture and predict these mechanisms, assembling them into a complete demonstration model of a BWR fuel channel. Specific activities include using: • Existing component-scale CFD boiling models will be used to analyse the lower ~1/3 of the core, up to the point of film flow. • Film flow 'sub-grid' models, developed for other industrial applications, will be extended to treat the conditions in the core • Eulerian, or Eulerian-Lagrangian models will be developed to treat the flow of entrained droplets in the vapour, and to predict their rate of deposition onto the film. • Empirical knowledge of rates of droplet entrainment from the film will be used to develop an entrainment treatment. • The overall conservation (of phases, fields, and mass and energy) will be handled within the CFD model. • Particular attention will need to be paid to modelling of the droplet flow around spacer grids, as the wide size distribution of the droplets will lead to a corresponding spread of behaviour.
Validation Requirements	The vast set of 'critical heat flux' data provides an excellent 'aggregate' validation capability. There is also much, more mechanistic, data that has been gained via the test facilities operated by all fuel / reactor vendors. Hitachi in Japan, and Westinghouse in Sweden, have particularly rich capabilities. Collaborative developments with such vendors would be valuable. Measurements of this kind or, even better, measurements to validate the modelling of individual phenomena such as droplet diversion, the disruption of film flows by spacer grids, and the rate of entrainment of droplets, would be good candidates for any new UK test facility.
Output	The principal output of the work would be the development of models to treat all of the phenomena noted above, and to assemble these models into a composite whole, observing all of the required conservation laws. These models would necessarily be developed at this stage in one selected CFD code, but would be intrinsically generic, and would be able to be implemented in other CFD codes in the future. Outcomes of the research will be published in academic papers, and presented at 'industry' conferences.
Existing Research & Body of Knowledge International Programmes	There is a vast body of prior work on film dry-out, from ~50 years back [3-5] to present times [6-9]; the references cited do not even scratch the surface. It overwhelmingly addresses wholly empirical, and semi-empirical one-dimensional phenomenological modelling.

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	The work proposed here would draw heavily on developments for other industries (for example, a major motivation for CFD film flow modelling has been automobiles in rain) Beside the 'vendor' measurement programmes noted, there are others, notably the Imperial College - Bhabha Atomic Research Centre (BARC) research under the Indo-UK Civil Nuclear Collaboration [1, 9].
Risks	Collaborative access to high quality vendor measurements would be desirable, and may not be forthcoming. Extant public CHF data provides a good backstop. Similarly, some access to new measurements of individual phenomena would be helpful; there is much older data which could be used, but naturally its accuracy is lower than modern measurement techniques would permit.
	Due to the challenging nature of the research, the successful completion of the technical objectives of the work is not without technical risk.
	Current UK CASL programme activities may already be covering this topic. This project should review this before commencement and modify the scope as appropriate.
Timeline and Prerequisites	3 years
	As film 'dry-out' represents one of the changes in boiling regime there is likely to be benefit in communication between this project and P3_B.
Resource/Costs	2 FTE researcher and 0.5 FTE industrial CFD specialist for 3 years
Exploitation Recommendations	As a more capable modelling tool, we would expect that the models and methods developed under this proposed programme would initially augment, and subsequently move to displace, the legacy methods used by reactor vendors.
	In the short term, the work could be exploited to reinforce safety cases, providing more detailed analyses of critical parameter sets for setting of operation limits, and helping with the continuing process of fuel design refinement and the understanding of necessary safety margins.

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Project Title	Improved Component-Scale Boiling Modelling				
Topic	Boiling and condensation				
Reference	P3_D				
Source	Workshop Group 2				
Location on Capability Map	Physical/Empirical Mathematical Models Modelling Tools				
R&D Spectrum	Basic Applied Early L Research Research Development Devel				
		\boxtimes			
Technical Objectives	Increased use of CFD to predict the flow of water within the core of light water nuclear reactors is vital to realise the improvements in economics, performance and safety that nuclear power must achieve. Even in PWR's (let alone BWR's) some boiling takes place quite deliberately during normal operation, as well, of course, as there being extensive boiling under fault conditions. To permit CFD to be employed usefully it is thus vital that it incorporates the capability to model boiling flows over "component scale" regions; that is, regions the size of a fuel sub-channel up to perhaps the entire primary vessel. The objective of this project is to conduct research and development to improve the way in which boiling is modelled within CFD, to allow such CFD treatments to achieve their full potential in contributing to the analysis of nuclear systems.				
Benefits	 Contributing to the analysis of nuclear systems. There are various respects in which an ability to predict boiling and the amount of vapour generated, where it is generated, and where it goes, is important for understanding reactor performance and thereby improving designs and reducing cost. A few of the most obvious include: In seeking to extract the greatest power output possible from a PWR core, it is routine that central, highly-rated regions of the core will be allowed to undergo a degree of nucleate boiling. Knowing the amount and the fate of the vapour so produced is vital to predict the neutronic behaviour of the core, as the presence of water vapour rather than liquid water has significant effects on the moderation absorption of neutrons. Such prediction, of the amount of vapour so produced, the bubble sizes in which it resides, and the subsequent transport and coalescence and breakup of these bubbles, is the fundamental task and output of the boiling models to be improved under this activity. The formation on fuel rods of CRUD is common in light water 				

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including increased risk of fuel failure and local reduction in neutron flux leading to reduced reactor power. The formation of crud is almost invariably associated with locations at which nucleate boiling is taking place on the surface of the fuel. Understanding where such boiling is likely to occur, why it occurs, and identifying means to mitigate it, are just the kinds of task for which a boiling-capable CFD model of the core would be extremely valuable.

- ▶ Essentially all fault conditions in a light water reactor will lead to some degree of boiling. Any increased use of CFD to predict the course of such accidents, to help design systems to mitigate them and by predicting them better to reduce margins imposed to cope with them, is reliant upon an adequate ability of CFD to deal with the generation and transport of vapour.
- Provide a significant UK contribution into an area of high international and domestic value.

Scope & Approach

At the component scale, boiling involves billions of bubbles and successful modelling therefore needs to employ an averaged, semi-mechanistic, semi-empirical approach. This approach relies upon experimental observations of quantities such as bubble departure diameters and frequencies, and nucleation site densities and incorporates these into the normal CFD wall treatment.

This incorporation into CFD treatments is very much a work in progress, and there is great scope for the development of high fidelity models, and the incorporation into these of the growing body of modern, higher fidelity measurement information, and of fundamental mechanistic predictions necessary to achieve a solution that is truly useful.

The specific activities of the this project are expected to include:

- ➤ Computational developments to minimise and possibly eliminate the sensitivity of the treatment to the degree of near-wall mesh refinement.
- ▶ Improvements of the modelling of the so-called "quench" process, where cooler water provides transient and local increased cooling of the wall, as it flows in to fill the volume previously occupied by a departing bubble. Here there is a current opportunity to replace a decades-old empirical model with understandings gained from recent microscopic modelling (including P3_A).
- Most measurement and most modelling to date has concentrated on boiling in stationary pools; understandably, as it is a much easier system both to measure and to model. Of course, reactor-relevant conditions are anything but, and further work in developing flow boiling modelling is required, and in particular in incorporating into the CFD treatment the effect of the sliding of bubbles before they finally lift away from the surface.

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	▶ There is a fundamental conceptual flaw within most CFD models of boiling, relating to the total neglect, by construction of the model, of the condensation of vapour at the upper reaches of a bubble where it protrudes into sub-cooled liquid. This has only recently been appreciated, and initial studies are suggesting ways in which it could be remedied, but more work is needed.
Validation Requirements	Note that for this project there are two very distinct requirements for inputs from measurements, only one of which is 'validation', and we address both here.
	There is a need for "validation"; measurements of macroscopic boiling behaviour under relevant conditions, against which predictions of such macroscopic behaviour can be assessed.
	There is also a need for input from smaller more fundamental measurements, not "validation", but rather to provide the data needed for the semi-empirical models that are fundamental to the boiling treatment.
	For both purposes a large body of extant public domain data is available, and progress can certainly be made based on this. More, and more focused, data would always be desirable for studies of this kind. In particular, measurements at more reactor-relevant conditions (high pressures, high temperatures, high heat fluxes and high coolant flow rates), with good instrumentation, would be helpful. This is certainly an area that we would urge be considered when assessing any possibilities for new thermal hydraulic measurement facilities in the UK.
Output	In general, leading CFD codes incorporate boiling treatments, and the intention would be that work under this project would be addressing the fundamental aspects of improving these. It would lead to the provision of improved models, and better parameterised models, which in turn could be incorporated into their own treatments by the CFD vendors. To facilitate this, outcomes of the research will be published in academic papers, and presented at more industrial, 'applied' conferences.
Existing Research & Body of Knowledge International Programmes	There is a large body of extant work on the development of heat flux partitioning boiling models for incorporation into CFD, and references we cite directly here can only really scratch the surface. The origins of the RPI stem from [1]. A more recent review is presented by Fairweather [2], and a typical 'nuclear' application by Lo is given in [3]. For more background the reader is directed to Walker & Lo [4], which in Chapter 5 provides a convenient exposition of the area (much more comprehensive than is possible here), along with more references. For a fuller discussion of possibilities for advanced modelling activities, as well as a very comprehensive review of the literature, the reader is directed to Thakrar [5].

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	This research will complement and extend research being undertaken by other international programmes such as the Indo-UK Civil Nuclear Collaboration, where BARC, Imperial and Leeds [6, 7] are working together on such developments, in a combined measurement and modelling programme. There have recently been installed at Culham (the UK fusion lab) facilities for making high heat flux boiling measurements at reactor-relevant conditions of flow, pressure and temperature, and a joint fission – fusion programme using it is under consideration. There is valuable potential symbiosis here. Such measurements would be right at the forefront of worldwide activity in the area. The UK already has significant expertise in the formation of CRUD, with NNL CRUD chemistry expertise (Henshaw and colleagues [8]) being in much demand worldwide, and particularly from the US. The NNL activity has expanded to include the support of associated thermal hydraulic and advection-diffusion modelling [9, 10] at Imperial, with a further PhD project presently underway. An increased ability to predict in-core boiling would be valuable, and would help keep the UK at the forefront of the area.
Risks	Further experimental results may not be forthcoming, which would force more reliance on extant data for validation.
Timeline and Prerequisites	This project would benefit from the work proposed in P3_A, P4_B and potentially P3_B. It may therefore be of benefit to schedule it for after these projects are well progressed. The scope of work is aimed at 3 years
Resource/Costs	2 FTE researcher and 1 FTE industrial specialist for 3 years
Exploitation Recommendations	A new extended and validated boiling model will be developed as an output of the work which can be directly implemented in existing multiphase CFD codes for industrial application. The very applied and NPP specific approach has been tailored to demonstrate the value to industry and the presentation of the findings at relevant conferences (as planned) will promote early exploitation.

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Project Title	Prediction of DNB using CFD				
Topic	Boiling and condensation				
Reference	P3_E				
Source	Workshop Group 2				
Location on Capability Map	Physical/Empirical Mathematical Models Modelling Tools				
R&D Spectrum	Basic Applied Early Late Research Research Development Development				
		\boxtimes	\boxtimes		
Technical Objectives	To a very good approximation, when a water cooled reactor remains cooled by water, very little harm will come to it. Conversely, when it becomes, inadvertently, cooled locally by only steam, the surface of the fuel is at a high risk of becoming hotter than design limits and may even fail or melt and release fuel and fission products. Boiling within a water cooled reactor varies between a primarily water environment with small bubbles of steam (nucleate boiling) to an environment where these bubbles coalesce, locally displacing the water and significantly reducing the heat transfer from the surfaces of interest. Predicting "Departure from Nucleate Boiling" (DNB) correspondingly lies right at the heart of nuclear thermal hydraulics and arguably represents one of its most challenging, but valuable goals for light water reactors. Identification of DNB is currently reliant on extensive experimental programmes. The current strategy comprises; "Measure DNB in as many circumstances as you can, and identify empirically the parameter space that the reactor designer must avoid." Inevitably, such identification embodies very wasteful margins to accommodate this empiricism and lack of mechanistic predictive capability. The objective of this project is to extend modern CFD tools for the prediction of boiling flows to enable their application to this rather extreme occurrence of boiling, "DNB".				
Benefits	 Developing CFD models that are capable of predicting DNB more mechanistically would have far reaching benefits including: Better understanding of fuel safety margins and the associated uncertainties leading to improved efficiency and reduce costs per MW for operators. Development of fuel, spacer grid and core designs with less reliance on expensive experimental programmes. Prediction of the impact of geometrical distortion such as rod and assembly bow on the safety of the reactor. 				

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	Extend the involvement of the UK in one of the most important (both economically and from a safety perspective) 'Grand Challenges' in nuclear thermal hydraulics.
Scope & Approach	Wall boiling CFD modelling is based on heat flux partitioning, which relies on a physically-based semi-empirical, semi-mechanistic treatment of the processes at work. In recent years the ability to incorporate wall-boiling into CFD analysis of component scale problems has improved markedly. Whilst this work has largely focused on nucleate boiling, with relatively low near-wall void fractions, the methods are now tantalisingly close to being able to be extended to allow their use as a predictor of bubble crowding DNB. The development of these methods to achieve this is a prime objective of this project. Previous work on the subject has aimed at introducing mechanistic modelling of departure diameter and bubble departure frequency. However, as for most current models, capabilities were limited to the isolated boiling regime where bubbles grow and depart without interacting with neighbours. By definition, this regime is typical at low-void fraction conditions. However, as soon as boiling is sustained and bubbles crowd the near-wall region, interactions between these can no longer be ignored. The approach for this work will be to initially examine DNB on a small scale with a view to extending the work to large scales in the future. The scope of this work is to: • Extend modelling capabilities to include bubble merging, during growth at the nucleation site or whilst sliding after departure. • Determine the effect on boiling wall heat transfer on the formation of larger (than a single bubble) vapour structures close to the wall.
Validation Requirements	A large body of extant validation data is available, in the form of Look Up Tables and correlations (built on thermocouple measurements), encapsulating the decades of effort in this area and a large body of experiments. However, the majority of these correlations are built for and limited to specific fuel assemblies. Additional measurements using modern equipment to provide flow visualisation (in addition to heat transfer) on a microscopic scale would be of value and could be the subject of testing in the UK.
Output	Outcomes of the research will be published in academic papers Developments to the boiling models will be made available for industrial use, via their incorporation into CFD treatments by code vendors. This project will include implementation of any advancements in a single CFD code as an example.
Existing Research & Body of Knowledge International Programmes	The general development of CFD-based component-scale boiling models has a very large literature, and there are now beginning to be published attempts to use this to predict DNB, from initial use of

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	single phase models to assess 'where' [1], to full blown RPI implementations [2]. The work proposed here will build upon this. More locally, work [3-5] in this area has been taking place under the Indo-UK Civil Nuclear Programme (BARC, Leeds & Imperial), and this will complement a new research programme getting underway, which will generate validation data for the study.
Risks	Due to the value of the work, there is much activity in this area world-wide. This introduces the risk of effectively repeating work that has already been done elsewhere. However, the importance and magnitude of the challenge means that any successes will need to be repeated independently by different teams before they are of true value to industry. The international activity also presents further opportunities to be involved in international collaborations. The technical difficulty of the work means that it is unlikely to be feasible to develop a fully validated DNB model within the timescales of this research project. However, significant progress should be possible on one of the LWR industry's most important challenges.
Timeline and Prerequisites	3 years The project links closely with P3_A (there would be value in carrying out P3_A first or at least in parallel with this task). Similarly this project links closely with P3_B as DNB represents a key transition between phases of boiling.
Resource/Costs	1 FTE researcher and 1 FTE industrial CFD specialist for 3 years
Exploitation Recommendations	Developments to the boiling models will be made available for industrial use, via their incorporation into CFD treatments by code vendors. Incorporation into a single code will be included in the scope of this project.

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Project Title	Modelling of Fuel Clad Ballooning Following LOCA				
Topic	Large-scale multi-phase flows				
Reference	P4_A				
Source	Workshop Group 2				
Location on Capability Map	Modelling Tools Verification and Validation				
R&D Spectrum	Basic Applied Early Late Research Research Development Developme				
		\boxtimes	\boxtimes		
Technical Objectives	model the therm following a large A LBLOCA will r At elevated temp 'creep' in respon This phenomeno contact between be formed to whis a matter of co regulator. The technical ob predictive capab	The objective of this project is to provide an improved ability to model the thermal and structural response of an LWR core following a large break loss of coolant accident (LBLOCA). A LBLOCA will result in a largely voided core and overheated fuel. At elevated temperatures the clad becomes more ductile and may 'creep' in response to the high net internal pressure of the fuel pins. This phenomenon is known as 'clad ballooning' and could result in contact between adjacent ballooning pins. A blocked region could be formed to which coolant would be unable to gain access and this is a matter of concern to fuel and reactor designers and the UK regulator. The technical objective of this project is to develop a better predictive capability for clad ballooning, underpinned by experimental validation.			
Benefits	 A better, and validated, predictive capability would: provide evidence to improve robust LBLOCA safety cases: reduce associated excessive margins thereby increasing reactor efficiency and reducing costs: and provide the evidence needed to support safety cases for increased fuel burnup. Furthermore, providing an advanced modelling complement to the existing international experimental data would constitute a major UK contribution to an area the UK was largely responsible for identifying originally, and to which it made major early contributions. 				
Scope & Approach	The approach will develop a coupled multiphysics model of clad ballooning in PWR fuel assemblies during LOCA, exploiting 3D CFD methods and two-way coupling to mechanical models. Advanced open source models are now available (e.g. the US code BISON [1, 2]), and these provide a very powerful platform for such advances. The scope of this project will encompass:				

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 A 3D CFD model of a PWR fuel assembly will be developed including the complex flow paths of the superheated steam as it is diverted by growing blockages. The model will be further developed to include the saturated water droplets entrained in the steam, and, vitally, the trajectories these follow, and their consequent evaporation into and cooling of the steam. The flow model will be coupled to a mechanical model of the ballooning fuel, so the changing geometry modifies the predicted flow field, and the modified flow field in turn modifies the cooling of the fuel and its further ballooning. The final model predictions will be validated using currently available test data.
Validation would be based on the PERFOI experimental programme currently being completed in France. Data is also available from older UK test programmes such as ACHILLES and REBEKA.
The prime output would be an improved ability to predict the course of events following a LBLOCA, and in particular to predict the likelihood / extent of clad failure and core melting. The specific output from this work will be a documented modelling approach supported by a validated example. All of the models and techniques developed will be published in sufficient detail that they can be implemented in any capable CFD code rather than just the one used for the research project.
Albeit it is from some years ago, previous UK work (Ammirabile [3-5], Jones [6]) probably represents the state of the art in modelling in this area. HSE- & BE-supported programmes led to the development of such coupled models, based on the then best available tools (one-dimensional system codes, and 'classical' 1½ dimensional fuel codes.) The body of worldwide experimental and modelling programs on this topic is summarised in Walker [7], as part of recent studies in this area by ONR. The modelling developments proposed here would be very timely. A major current IRSN experimental programme PERFOI [8, 9], with German involvement, is just beginning to generate important experimental results.
Access to data from PERFOI programme is desirable for the full benefits of the work to be realised, albeit the availability of various earlier published experimental results provide good insurance against this eventuality.
3 years
2 FTE researchers for 3 years

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	HPC resources
Exploitation Recommendations	The models and techniques developed can be exploited industrially through commercial CFD codes based on the published research.
	Potential for more detailed 3D models to inform the development of systems codes for LOCA studies, as the models can be used to run extensive sensitivity studies to support the data obtained from test programmes.

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- 2. Williamson, R.L., et al., *Multidimensional multiphysics simulation of nuclear fuel behavior.* Journal of Nuclear Materials, 2012. **423**(1-3): p. 149-163.
- 3. Ammirabile, L. and S.P. Walker, *Multi-pin modelling of PWR fuel pin ballooning during post-LOCA reflood.* Nuclear Engineering and Design, 2008. **238**(6): p. 1448-1458.
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- 6. Jones, J.R. and M. Trow, *Multi-Pin Studies of the Effect of Changes in PWR Fuel Design on Clad Ballooning and Flow Blockage in a Large-Break Loss-Of Coolant Accident*, in *International LWR Fuel Performance Meeting*, 2007: San Francisco.
- Walker, S.P., Review of the established good practices in development of clad ballooning and embrittlement models for higher burnup PWR fuel. ONR-RRR-014, 2016
- 8. Repetto, G., et al., The R&D PERFROI project on thermal mechanical and thermal hydraulics behaviours of a fuel rod assembly during a loss of coolant accident, in NURETH-16. 2015: Chicago, IL.
- 9. Repetto, G., et al., Core coolability in loss of coolant accident: the COAL experiments, in NURETH-16. 2015: Chicago, IL.

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Project Title	CFD Modelling of Macroscopic Convective Boiling Flows in NPP			
Topic	Large-scale multi-phase flows			
Reference	P4_B			
Source	Current Phase 1	development wo	rk	
Location on Capability Map	Physical/Empirical Mathematical Models Modelling Tools			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		
Technical Objectives	Two-phase flows can be present in a variety of flow configurations ranging from bubbly, where gas (or vapour) bubbles are distributed throughout a liquid, to disperse, where liquid droplets are interspersed within a flow of gas. The complexity and variety of flow patterns which arise in gas-liquid flows are predominantly caused by the deformable nature of the gas-liquid interface, which can adopt any shape, and the interphase transfers of mass, momentum and energy. This increased physical diversity within the flow means that there is a much broader range of modelling methodologies that can be used to construct viable numerical models. Accurate numerical prediction becomes of critical importance to the development, uptake and ultimate acceptance of CFD within the NPP community. Current two-phase CFD modelling approaches can be broadly divided according to the way in which the flow field of each phase can be described.			
	For dispersed flows, the dispersed phase (particles, bubbe droplets, for instance) is usually thought of as being imme within a continuous carrier phase. The latter typically invit Eulerian description of the flow. For the dispersed phase both Eulerian and Lagrangian approaches can be employ the Lagrangian description a number of individual fluid/so 'particles' are identified and their positions, velocities and properties are tracked and computed throughout time. Sin trajectories have to be computed for each particle include approach can quickly become computationally expensive highly dispersed phases, which thus require a large number of particles.			eing immersed bically invites an ed phase itself, be employed. In the invites and other at time. Since the included, the expensive for
	If an Eulerian description is applied to the dispersed phethen the approach is usually termed Eulerian-Eulerian and number of different modelling strategies arise depending how the governing equations are formulated. These included two-fluid approach, where the phases are treated as interpenetrating with separate sets of governing equations.			

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	each phase, the <i>one-fluid</i> interface tracking or capturing approach, where one set of governing equations is solved and a discontinuous change in material properties across the interface distinguishes the phases, and the <i>one-fluid</i> homogenous or mixture approach, where an assumption that the two-phases are strongly coupled negates the need to solve separate transport equations. The wide variety of approaches, sub-models and formulations within those sub-models serves to illustrate the difficulties in modelling multi-phase flows; disagreement is even present over which equations should be solved. The objective of this work is to consider the available CFD methodologies at a high level and specifically test these methodologies on boiling flows relevant to NPP to assess their effectiveness and identify possible routes for improvements in predictive quality.
Benefits	 The output will include a documented study evaluating the available methods in an NPP context. This type of output is valuable to provide both guidance and confidence enabling increased uptake of methods by industry. This research is intended to enable: More accurate predictions of boiling heat transfer at reactor design conditions (BWR) and at off design conditions (BWR and PWR). The above will lead to improvements in reactor efficiency and also reactor safety. Build on UK expertise in this area and grow knowledge of two-phase flow modelling relevant to Gen III+ and SMR reactor design and operation.
Scope & Approach	Off-design conditions in a LWR reactor may lead to loss of coolant circulation. Heat continues to be generated by the fuel rods; this will eventually cause the water to boil. Exposed rod surfaces experience dangerous increases in temperature. The two-phase mixture front develops and travels down the bundle; accurate modelling of this process is crucial. Arai et al. [1] reported boil off experiments for a 5x5 rod bundle at atmospheric pressure. Hence the boil off process makes a highly appropriate starting test case (highly relevant to reactors but not the most complex). Convective boiling cases can then follow.
	The approach for this work will be to start with this publically available test case and to explore both Eulerian-Eulerian approaches of different degrees of complexity, and also novel SPH (Smooth Particle Hydrodynamics) approaches.

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	The scope of work is envisaged to be:
	 Build on existing published work to investigate and demonstrate the current state-of-the-art in CFD boiling prediction and compare findings with initial test case data.
	 Investigate the potential for SPH approaches to predict two- phase boiling processes relevant to NPP (SPH is largely intended to model multi-phase flow and so may offer advantages).
	 Perform a literature review to identify additional suitable validation test cases for macroscopic convective boiling relevant to NPP.
	 Extend investigation of methods to additional model complex test cases where possible.
	 Following evaluation of methods, identify areas where further enhancements/extensions to model may be of value.
	 Plan and execute model development work to improve the state-of-the-art in the prediction of boiling with CFD.
	The first two tasks are being progressed as part of Phase 1 of this project.
Validation Requirements	One of obstacles in the development of two-phase CFD capabilities has always been the lack of sufficiently detailed data for validation and also for the development of more generic empirical functions, used to characterise the boiling process, such as rate of bubble generation, nucleation side density etc.
	While the data from Arai et al. [1] provide a starting point, a further review of the scientific literature will be needed.
Output	Phase 1 output will be an academic publication describing findings of the work
	Phase 2 outputs are envisaged to include:
	Development in open source codes:
	While two-phase models are included in major commercial codes (Fluent, Star-CCM+) and also in major open source codes like Code_Saturne and OpenFOAM. Further refinements/extensions of some models are expected to be necessary, which will extend the capabilities of current codes. The specific outputs of this project will include implementation of new developments in an open source CFD code to maximise wider exploitation.
	Demonstration of benefit and fidelity:
	The most important contribution will be a documented set of recommendations of which models can be used for which boiling flow applications.
Existing Research & Body of Knowledge International Programmes	As mentioned above all major codes include two-phase models and empirical functions for the different aspects of the boiling process. There have also been a number of attempts to evaluate the effectiveness of these approaches, [2] to [5] for example which

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	point to the need for more extensive validation and indeed for more detailed and wide-ranging data. The new UK test facility may provide an opportunity to produce this data. The boil-off case of Arai [1] is currently being investigated at the University of Manchester using both conventional Finite Volume
	(FV) methods and also smoothed particle hydrodynamics (SPH).
Risks	Reliance on existing data may not enable sufficient progress.
Timeline and Prerequisites	Phase 1: 1 year Phase 2: 3 years In the longer term (i.e. towards the end of Phase 2), this project would likely benefit from the work proposed in P3_A. This project would benefit from working with P3_B.
Resource/Costs	Phase 1: 2 FTE academic researchers for 1 year. Phase 2: 1.5 FTE academic researchers and 0.5 FTE industrial specialist for 3 years.
Exploitation Recommendations	The modelling of a number of boiling flows highly relevant to NPP will be investigated leading to better understanding and also to recommendations on how they can be more effectively modelled. Generic improvements in the modelling of two-phase flows will benefit the wider nuclear thermal hydraulics community and indeed other industrial sectors.

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- 4. Thakrar, R., J. Murallidharan, and S.P. Walker, "An evaluation of the RPI model for the prediction of the wall heat flux partitioning in subcooled boiling flows.", in ICONE, Prague, Czech Republic, 2014.
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Project Title	Dissolved Gas Transport In Molten Metals and Molten Salts			
Topic	Advanced fluids			
Reference	P5_A			
Source	Workshop Group	3		
Location on Capability Map	Physical Unders Physical/Empiric	tanding al Mathematical N	/lodels	
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
	\boxtimes	\boxtimes	\boxtimes	\boxtimes
Technical Objectives	Liquid metal and molten salt reactors can have pool type configurations with a free surface. The gas from the space above the pool can either diffuse into the coolant, or can be entrained at vortices near to surface piercing components or other disturbances. The dissolved gaseous species that are introduced into or be evolved within the coolant at any stage can re-emerge as gas bubbles mostly close to solid surfaces through a process similar to boiling. This is of relevance because a positive reactivity event (a transient power increase) can occur if a large accumulated quantity of gas crosses the core. The presence of gas bubbles in the primary circuit can also cause problems for pump behaviour and for ultrasonic measurements. This project aims to provide improved predictions of gas bubble nucleation and departure mechanisms within the coolant to be used as boundary conditions and sub-models for gas transport in a component or system level evaluation tool.			
Benefits	Improved system level design validation, particularly design substantiation of performance under thermal transients.			
Scope & Approach	on: the composite which evolve temperature, quantity of di heat and more nucleating but surface orient. This modelling is rate of departure.	ion and morpholo s during reactor o pressure and cor ssolved gases; mentum transport ubble; itation, to account s intended to allow of evolved bubbl	e from solid surface gy of the nucleating peration; mposition of the color in the fluid layer a for the effect of b of the prediction of es into the adjace mposition and surface	ng surface, colant and adjacent to a uoyancy. a macroscopic nt flow, as well

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	The details of the mechanisms for gas transport at gas/liquid and liquid/solid interfaces will be studied with a combination of:
	theoretical models, assessing the underlying physical processes, such as those described in:
	Meloni,S., Giacomello, A. and Casciola, C. M. Focus Article: Theoretical aspects of vapor/gas nucleation at structured surfaces, The Journal of Chemical Physics, Volume 145, 211802 (2016), https://doi.org/10.1063/1.4964395 to guide the form and parameterisation of models and boundary conditions
	 detailed continuum mechanics (DNS-like) simulations of individual bubble growth and dynamics (this links to project P3_A);
	 assessment of and comparison to available experimental data; definition of additional experiments to provide validation data
	and further physical insight;
	The models developed could then be used as an input to a larger scale CFD simulation, in the form of boundary conditions or source terms, or as a submodel of a system code.
	This is a complex topic, the results will be coolant dependent, and so it is expected that only a small subset of the possible physical effects and conditions will be tackled, and the details of the modelling tasks chosen to suit. The choice of whether to apply the modelling to liquid metals, molten salt, or both will also depend on the details of the research tasks undertaken.
Validation Requirements	Agreement between small scale experimental evaluation of density fluctuations, by ultrasonic means or similar. Necessary for understanding of bubble nucleation and gas diffusion mechanics.
Output	Boundary conditions and sub-models for inclusion in CFD or system codes to provide more accurate predictions of gas transport at a component or system level.
Existing Research & Body of Knowledge International Programmes	Active research is being undertaken by: Chuck Weber – ORNL. Diffusion chemistry and vapour mechanics. JaeYoung Lee – Handong Global University South Korea. Interest in advanced coolant multi-phase flows. Shuisheng He – University of Sheffield. Data on gas entrainment from cover gas in Sodium Fast Reactors (see project P5_F). VERA. Ben Collins/Cole Gentry – ORNL. Modelling fission product phenomena in MSRs. SALIENT. Jan Kloosterman – EU JRC. In-reactor testing of molten salt fuel to correlate fission product behaviour.
Risks	Instrumentation and measurements for high fidelity quantitative analysis may be hard or only able to be conducted by a limited number of institutions.

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Timeline and Prerequisites	t is expected that this project would be able to produce useful advances in three years.	
	For molten salts, depending on their composition, it may be necessary for some inputs, such as the behaviour of gas/liquid interfaces, to be able to be derived by molecular simulations (project P5_B). A similar approach could be applied to liquid metals depending on the availability of data.	
Resource/Costs	The modelling aspects require a researcher and a PhD student for 2 to 3 years. The costs for experimental aspects have not been able to be estimated at this stage.	
Exploitation Recommendations	Evaluation methods for these phenomena can support safety case development or design improvement upon baseline system solutions – improved heat-exchanger design could be a particular exploitation route.	

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Project Title	Molecular Dynamics Capabilities for Thermophysical, Thermogravimetric Phase Equilibrium Prediction Over Lifecycle			
Topic	Advanced fluids			
Reference	P5_B			
Source	Workshop Grou	o 3		
Location on Capability Map	Modelling Tools Inputs			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes	\boxtimes	
Technical Objectives	Nominal thermophysical and phase equilibrium characteristics of a small number of well-known candidate molten salts are established experimentally, however there are 1000s of salt compositions possible during MSR operation. Lifecycle and degradation factors require characterisation for licencing evidence. This could be achieved with a Molecular Dynamics (MD) derived library of candidate molten salts suitable to support safety case development.			
Benefits	The development and design optimisation of MSRs can be expedited by knowledge of a wider range of salt properties.			
Scope & Approach	An initial exploratory and validation phase is needed, which is required to confirm the prediction accuracy of the MD methods. A gap analysis of current data available on each parameter, and the degradation mechanics seen in reactor environments, would identify where further data are required. Thereafter, use well established and mature MD tools (such as LAMMPS, DL_POLY or GROMACS) to automate the creation of the properties of a given salt/series of salts. This could be used to build a database and appraise new compositions on-demand. A database library may consider influences from: Variation in salt species due to soluble contamination, activation			
	products or f electrochem	salt species due to ission product acc ical state to deterr s influence phase	cumulation and eq nine the valency c	uilibrium of species.
	thermogravir points). In addition to insoluble cor thermophysic conductivity,	netric properties (the above, atmost an al cal properties. Pre heat capacity, exposulusility, surface	vapour pressure a spheric contamina so contribute to va edicting variability pansion coefficien	and liquidus ation and ariation in in viscosity, t, absorption

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	 Energy/electrochemical potential, are all beneficial characteristics for determining evolution and degradation over time of molten salt fluids. The database can use existing knowledge for verification where available, but can be expanded to capture a broader range of candidate salts, with better understanding of their lifecycle and degradation and potentially to waste stream design considerations for the future design improvement.
Validation Requirements	Comparison is needed between a derived method and previously verified known and verified nominal data (ITU, NIST, MIT etc.), to validate extension to degradation regimes and new candidate molten salt fluids.
Output	A data library and/or service to support initial design evaluation and graded approach to licencing evidence, based on initial verified candidate salt data, and then expanding to a prediction tool for wider salt candidates.
Existing Research & Body of Knowledge International Programmes	There are similarities to the Virtual Materials Market Place (VIMMP): Horizon 2020 funded project with substantial UK involvement for non-nuclear applications. Many of the best MD tools are open-source and highly scalable on high performance computers. The UK has internationally leading expertise in this area. Existing research on this topic is well summarised in: Molten Salt Chemistry Workshop, Technology and Applied R&D Needs for Molten Salt Chemistry, April 10–12, 2017, Oak Ridge National Laboratory Existing phase data is available from the Institute for Transuranium Elements of the Joint Research Centre of the European Commission fissile salt database.
Risks	The method requires computationally intensive MD simulations, and is not a proven approach. Classical Molecular Dynamics methods may not be sufficient to predict some properties and <i>ab initio</i> (first principles quantum mechanical) methods may be necessary, which may make the computational cost prohibitive.
Timeline and Prerequisites	It is expected that this task would be able to be significantly progressed in three years.
Resource/Costs	One researcher and one PhD student for 2 to 3 years.
Exploitation Recommendations	This could be developed into a saleable or tradable service for supporting reactor and safety case development worldwide for MSRs.

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Project Title	Heat Transfer Correlations for Mixed Convection and Transitional Flows in MSRs			
Topic	Advanced fluids			
Reference	P5_C			
Source	Workshop Group	o 3		
Location on Capability Map	Physical Unders Physical/Empiric	tanding al Mathematical N	Models	
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		
Technical Objectives	heat transfer cor (Pr) number (Pr number for force Grashof (Gr) nur development wo both forced and during progress between laminal Heat transfer by similar effects as under considera thermal radiation	There is knowledge in the industry at applied research stage for heat transfer correlations in candidate salts, as functions of Prandtl (Pr) number (Pr which varies with temperature) and Reynolds (Re) number for forced convection or with Prandtl and Rayleigh (Ra) or Grashof (Gr) numbers for natural/buoyant convection. Little development work has been conducted on mixed convection (with both forced and buoyant effects) and the prediction of heat transfer during progress of reactor faults where flows in the transition region between laminar and turbulent are often encountered. Heat transfer by mixed convection in molten salts is influenced by similar effects as in more conventional fluids (e.g. by the geometry under consideration), but also by participating in the exchange of thermal radiation and the potential for strong variation in thermophysical properties (which need to be modelled).		
Benefits	Heat transfer correlations in mixed convection and transitional flow are important to demonstrate, for prediction of molten salt cooled reactor faults. It enables more reliable claims and design substantiation of fault progression and stability of events.			
Scope & Approach	 The project tasks will be: Determine the appropriate form and parameterisation (in terms, of Re, Pr(T) and Ra or Gr) for heat transfer correlations for mixed convection and transitional flows. Assess the available experimental data for the salt compositions of interest. This will need to consider distinguishing between flows that are buoyancy affected and those that are not. The body of existing experimental data is not expected to be extensive. Perform high resolution CFD (e.g. LES) simulations for mixed convection including radiation in prototypical or simplified geometries to address gaps in the experimental evidence. 			

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	 Perform high resolution CFD for transitional flows. Reynolds numbers are low by definition, so DNS becomes practical to use rather than LES.
	 Curve-fit the available data and CFD results to create correlations.
	 Specify more experiments for exploration of phenomena and for validation.
	Determining the form of correlations and separating out buoyancy affected flow data is part of project P5_G, and similar methods or approaches may be able to be applied here.
	The thermofluid properties of the salts of interest may not be available in the existing literature, but may be able to be generated under project P5_B.
Validation Requirements	Any relevant existing available data is required, and the project will define what additional validation experiments are most useful.
Output	Identifying and filling gaps in understanding of heat transport mechanisms in molten salt. Creating correlations for use in system codes and other low fidelity methods.
Existing Research & Body of Knowledge	Active research is being undertaken by: G. Yoder at ORNL
International Programmes	V Di Marcello at Milan Poly/ITU.
	R. Scarlat E. Baglietto under the US DoE Nuclear Energy University Programs - Radiative Heat Transfer.
Risks	Decoupling radiative transport from other experimental factors may be difficult, and require, for example, careful control of corrosion.
Timeline and Prerequisites	It is expected that this project would be able to produce useful advances in three years.
Resource/Costs	Estimated as a researcher and a PhD student for 2 to 3 years plus HPC resources.
Exploitation Recommendations	Collaboration with vendors at initial development phase, of value in capability growth outside of North America/China.

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Project Title	Supercritical CO ₂ Power Cycles			
Topic	Advanced fluids			
Reference	P5_D			
Source	Workshop Group	o 3		
Location on Capability Map	Physical Unders Modelling Tools	Physical Understanding Modelling Tools		
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		
Technical Objectives			national research i wledge and skills i	•
Benefits	Improved thermal efficiency (to ~47 – 48%) Reduced plant size giving lower capital cost. Wide applicability (Nuclear, Solar, Conventional, CCS) Particularly advantageous for LMFRs, especially sodium because it removes the possibility of a dangerous reaction of sodium with water.			
Scope & Approach	Conduct an investigation of the state of research internationally (especially in the EU and USA) to form a gap analysis. Identify existing involvement of UK Partners (especially in field of heat exchanger technology – Heatric). Investigate potential UK contributions in turbomachinery (e.g. Rolls-Royce, Siemens). Identify UK capabilities and knowledge of supercritical flow and heat transfer modelling in, for example, heat exchanger and turbomachinery components and experience with the behaviour of and heat transfer from supercritical fluids. This can exploit or utilise aspects of project P5_G. Build an offering of interested UK parties, and make contact in the EU or USA to offer to join research, with an idea of the modelling capabilities and other tools/knowledge/facilities or funding that could be offered.			
Validation Requirements	Significant validation is likely to be necessary, but also likely to be available through collaboration with international partners.			
Output	Initial output: Review of status of technology developments and development needs. Leading to: elaboration of a specific proposal for UK involvement.			
Existing Research & Body of Knowledge	Review papers are available (UK and US centric) and a Book Chapter written by Professor Derek Jackson.			

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International Programmes	There are two current EU Horizon 2020 projects in this topic, for nuclear and conventional power applications:
	http://www.sco2-flex.eu
	http://www.sco2-hero.eu
	There is good UK knowledge of key actors in US (e.g. lead partner is University of Wisconsin).
	International collaboration available through US National Labs and DoE.
	Contacts can be made with:
	▶ Professor Jeong Ik Lee (KAIST – S. Korea).
	 Professor Václav Dostál (Czech Technical University, Prague). Steve Wright, Sandia National Lab Chief Engineer of SC CO2 power conversion loop.
Risks	Strong evidence that the technology offers significant benefits over steam cycles and could be applicable across a range of energy system applications. The risk is that UK misses an opportunity to contribute and develop IPR – becomes just a customer with no ability to influence direction or derive value.
Timeline and Prerequisites	Review should be completed in less than 1 year with a further proposal issued within a few months. Target involvement of UK organisations with 18 months.
Resource/Costs	This is a medium-sized consultancy technology road-mapping project.
Exploitation Recommendations	Several UK organisations would exploit the technology and capability: Manufacturers of turbomachinery and heat-exchangers
	(potentially Rolls-Royce, Heatric, Siemens)
	 Engineering consultancies and designers (for example Frazer- Nash, Wood, Atkins)
	► Academia.
	The UK's involvement could be much greater than just in the area of thermal hydraulics. For example, in advanced materials or manufacturing.

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Project Title	Liquid Metal He	eat Transfer Mod	elling	
Topic	Advanced fluids			
Reference	P5_E			
Source	Workshop, Group 3			
Location on Capability Map	Physical Understanding Physical/Empirical Mathematical Models			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		
Technical Objectives	A major feature of all LMFRs (SFRs and LFRs) is that the heat transfer characteristics of liquid metal is very different from that of the conventional fluids (air and water). For example, the Prandtl number is several orders of magnitude smaller than that of the water. As a result, conventional turbulence models are not valid and new models are needed. In addition, experiments for liquid metals are significantly more difficult than for air or water and hence data for validation is sparse. Consequently, developing better modelling and producing more datasets (experimental or by high fidelity numerical modelling) are ongoing efforts in the current international and EU programs. The objectives of this project are: • Creation of database of DNS/LES data for liquid metal test cases • Improvement to turbulent heat transfer models considering low Prandtl number. • Improved understanding/correlations for sub-channel mixing. • Improved modelling of natural circulation and mixed convection relevant to the hot/cold plena of LMFR.			
Benefits	 Supports the development of liquid metal reactor designs. Numerical 'experimental' data for further development of RANS models – there is limited physical experimental data due to difficulty in working with/measuring in liquid metal. Confidence and accuracy for low Prandtl (Pr) fluids heat transfer – 'conventional' turbulence models are based on Reynolds analogy which is not valid in low Pr condition. 			
Scope & Approach	The code is scal for resolved CFI validate/apply it	able, high-order, on the control of	Argonne National open source solve rk has been done Rs in NEAMS, a knethods and need	er and is suitable to ey US program.

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	expertise and knowledge to make good use of it. The scope of this project is to develop UK capability in Nek5000 and make innovative use of it in simulating chosen LMFR components, with which new low-Pr heat transfer models are developed. Key approaches: Develop UK Nek5000 capability for advanced and innovative use of this powerful tool. Select key components to perform resolved (LES) modelling. Develop turbulent heat transfer and near-wall models (CFD) for low-Pr fluids using the DNS/LES data, considering natural/mixed convection when applicable. Develop mixing coefficients for sub-channels – considering large flow structures and flow instability.
Validation Requirements	Following validation and verification (through comparison using simple configurations for example), the Nek5000 LES models and simulations can be considered as reliable source data, which will be used as benchmark data for RANS and URANS model development.
Output	DNS/LES models and results A publically available benchmark case (similar to ORNL wirewrapped case). Correlations for RANS model improvement and validation.
Existing Research & Body of Knowledge International Programmes	The topic is huge and fundamental to LMFRs, so there is already research underway in Europe and the US. Despite extensive effort worldwide, this is the 'mainstream', key research field for LMFR and as such there is plenty of scope for the UK to contribute, especially through making use of its advanced modelling expertise. E-SCAPE is a 1/6 th model of MYRRHA, currently under commissioning at SCK·CEN. This is a pool-type reactor with lead bismuth eutectic (LBE) as primary coolant. As part of Phase 1, the University of Sheffield is developing a high fidelity CFD model of E-SCAPE. It is expected that this will be validated against the E-SCAPE data when it has become available.
Risks	Some preliminary work is being done as part of the current BEIS project, but this is a relatively small part and hence existing experience is limited. Nek5000 is known to require a high level of expertise to use correctly.
Timeline and Prerequisites	A large part of the scope described above can be achieved in a three-year project.
Resource/Costs	One post-doctoral researcher and one PhD student for three years plus HPC resources.

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Exploitation Recommendations	UK should aim to join international/EU consortia and can make its contribution using its expertise in advanced modelling.

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Project Title	Modelling of Co	over Gas Dynami	cs in SFRs	
Topic	Advanced fluids			
Reference	P5_F			
Source	Current Phase 1 development work			
Location on Capability Map	Physical Understanding Physical/Empirical Mathematical Models Modelling Tools			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		
Technical Objectives	SFRs above the vessel getting in above the sodium roof of the core in behaviour of the the components surface is a major becomes particular under the presson which leads to go more/stronger vestronger vestronger vestronger circulator pumps below Develop multimass transfer of a sodium of the sodi	sodium pool to procontact with sodium pool. The heat is of significant into reactor, whereas may be a safety of source of argorularly strong as the ure of the reduction reater free surface ortices generated of which lead to so of gas entrainment increase), followers. The objectives of tiphysics modelling and aerosol dynocooled fast reactorularly scale model for	argon gas cover revent any leakage um, which creates transfer from the serest in understand the deposit of soconcern. Converse gas entrainment e cover gas space in the overall size velocity/disturbation around structures stronger gas entraient is the possible ed by adverse important in the possible gament of this project are: If methods to preclamics occurring in under simple control the cover gas reg	e air into the a free surface surface to the ading the overall dium aerosol on ely, the free to sodium. This is reduced are of the reactor, naces and protruding the ainment. The positive pacts on the dict the heat & a the cover gas an figurations.
Benefits	sections of a Exploitation of international international maintaining of the complex hears.	n SFR. of currently under- ly valuable UK tes UK's leading posit ethods for the mod t transfer mechan	of the behaviour of cused and potential t data. Developing ion in this area. delling of large volutions, including the oral range of reactors	ally g and umes with e influence of
Scope & Approach	· ·		describing the key	

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	vapour generation and migration, natural circulation and radiation through opaque medium for simple configurations. a) Use a RANS CFD approach for wider application (real system modelling). b) Use an LES CFD approach for investigation to complement experimental data and to improve understanding of the essential physics involved and the influence of the design parameters. 2. Validate models against available experimental data. 3. Expand models to address reactor conditions in a reduced geometry. 4. Develop a full scale model (based on RANS) for the cover gas region for a chosen SFR design. 5. Further develop the full-scale model by coupling it with modelling of the sodium free surface to investigate and develop a better understanding of gas entrainment (linking to project P5_A). Note: Preliminary work is being carried out in Phase 1 of the current BEIS project, which aims to cover a large part of points 1(a), 2 and 3. The new project is to consolidate that work and extend it to address points 1(b), 4 and 5.	
Validation Requirements	The experimental data of Manchester Nuclear Research Lab in 1990's retrieved as part of Phase 1 are comprehensive and at near reactor conditions. These data are expected to be sufficient for validation for the initial models.	
Output	 Multiphysics models for heat and mass transfer and aerosol dynamics that can be incorporated into simulation tools. A full-scale model for the cover gas region for a typical SFR. 	
Existing Research & Body of Knowledge International Programmes	Validation data from previous University of Manchester experiments are available. Current US, European and other international SFR reactor programmes are underway.	
Risks	Existing data may not be sufficient, and relevant experimental facilities no-longer exist. To mitigate the risk and complement the experiments, resolved LES modelling has been included in the proposed project, which is able to produce 'computational experimental' data.	
Timeline and Prerequisites	First phase - 2 years to create initial models and test feasibility of approach (scope/approach – points 1(a), 2 and 3, currently underway in Phase 1 of the BEIS program). Second phase – 3 years to develop the models to an exploitable state (scope/approach – points 1(b), 4 & 5).	
Resource/Costs	2 researchers (with CFD code development experience) for phase 2. Input/support from industry and HPC organisation (e.g. STFC).	

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Exploitation Recommendations

Relatively little research has been conducted on this important topic. This is a relatively weak area in the current European and US consortium projects, therefore there will be opportunities to collaborate with European and US partners with the UK's historic data and new modelling capability to be developed.

Exploitation to be achieved via

- Publication of methodology in reports and papers.
- Demonstration of models implemented in open source code to remove financial barriers to exploiting the advancements.
- Present preliminary (Phase 1) results at the EU Consortium SESAME final workshop in 2019 to publicise UK capability (having already been invited by the organiser to present and an abstract has been prepared and sent).

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Project Title	Predicting Heat Transfer to Supercritical Fluids			
Topic	Advanced fluids			
Reference	P5_G			
Source	Workshop, Group 2			
Location on Capability Map	Physical Understanding Physical/Empirical Mathematical Models			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
	⊠	\boxtimes		
Technical Objectives	The key advantages of the supercritical water-cooled reactor (SCWR) design is its high efficiency and the availability of operation experience of existing conventional (gas/coal powered) supercritical reactors. There are however challenges in the design including the strong variations of properties of the coolant in the reactor core – for example, the density increases by seven times in the fuel channel even though the fluid does not change phase. A major concern is the so-called heat transfer deterioration, which may lead to significant increase in fuel temperature, especially under some transient/fault conditions. Reliable predictions of the flow and heat transfer under such conditions are a challenge that has been the subject of international R&D programs. Most methods deal with different effects separately (e.g., buoyancy, flow acceleration, strong variation of thermal properties). This project aims to develop a holistic approach to deal with the various factors in a single framework. The objectives are: • Develop a mechanistic model considering the various physical processes occurring in supercritical fluid heat transfer in combination to underpin models and correlations. • Develop new datasets to complement existing data. • Create improved heat transfer correlations parameterised and fit using the physically derived models.			
Benefits	validated to deal addressing only correlations do n supercritical fluid water nuclear resimultaneously). The ability to cap physically me	with heat transfe one physical effect not adequately acc I heat transfer pro- actor TH (i.e. whe oture: eaningful dimension of properties are	been previously der of supercritical flat at a time. Such count for the full rate cesses relevant to en various 'complication confess groups; ound the pseudo-	uids, often heat transfer ange of supercritical cations' occur

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	 heat transfer deterioration; within this parameterised framework would be a substantial improvement on current capability.
Scope & Approach	The approach for this work will be to build on existing data and then apply a logical and rigorous process to improving the current state-of-the-art.
	Specific tasks are envisaged to be:
	Collate and analyse existing datasets.
	 Separate out data influenced by different mechanisms (buoyancy, acceleration or other thermal properties) using recently developed methods (see 'Existing Research', Jackson 2017).
	 Identify missing information and perform simulations (DNS/LES) and/or experiments to consolidate dataset.
	 Develop improved engineering correlations using a holistic approach.
Validation Requirements	This project is expected to be data-rich, and will have access to sufficient validation data.
Output	Published parameterised heat transfer correlations that can be implemented in system codes or coarse grained CFD.
	Published new supplementary data generated using DNS/LES.
Existing Research & Body of Knowledge International Programmes	Supercritical fluid heat transfer is available from IAEA CRP Programmes 2008-2012 and ongoing (2014-2019). Professor Shuisheng He is the UK representative on the current CRP and participating in generating a database for model/correlation development as well as for use for benchmark exercises.
	Lawrence Leung at CNL can be contacted for access to additional Chinese and Canadian datasets
	Professor Derek Jackson has published methods for identifying and separating, acceleration and buoyancy effects.
	J. D Jackson, 2017, Models of heat transfer to fluids at supercritical pressure with influences of buoyancy and acceleration, Applied Thermal Engineering, Volume 124, 2017, Pages 1481-1491.
	Sheffield University has a unique in-house DNS/LES code (CHAPSim) capable of flow simulations at supercritical pressure, and has been involved in international collaboration research using both DNS and RANS sponsored by IAEA, EPSRC and the Royal Society.
Risks	Only a limited number of UK based academics have sufficient knowledge to make this successful. The UK has no current experimental facilities.
Timeline and Prerequisites	3 year research programme. No additional prerequisites.
	1

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Resource/Costs	3 years full time PhD student. 3 years full time post-doctoral researcher.
Exploitation Recommendations	Exploitation of this work will occur by allowing continued UK engagement with international expertise. This work allows us to keep "seat at the table", maintaining reputation and capability for the DNS and correlation development in the supercritical fluid domain.

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Project Title	Coupled Tool S	Coupled Tool Selection			
Topic	Multi-physics				
Reference	P6_A				
Source	Workshop Group 3				
Location on Capability Map	Personnel Physical/Empirical Mathematical Models Modelling Tools				
R&D Spectrum	Basic Applied Early Late Research Research Development Development				
		\boxtimes	\boxtimes		
Technical Objectives	Basic Applied Early Late Research Research Development Developmen				

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	This could either be achieved using their own staff, or an external resource (for example a university or consultancy firm).
Benefits	Adoption of a coupled approach to reactor analysis allows more accurate and detailed simulations, resulting in the reduction of conservatism and uncertainty and the increased understanding of phenomena.
Scope & Approach	Organisations already engaged in reactor design have an existing toolchain and work-flow that allows the analyses they require to be produced. Moving to an improved set of tools represents an investment of time and resources with uncertainty in the outcome. For a new reactor designer in early-stage design, investing in an appropriate toolchain for detailed analysis may not represent the highest priority activity, but could speed up and improve the design. The specific tasks undertaken will depend on technology that the tools are applied to and the stage of development of the reactor design. It will generically require: The definition of test cases for evaluation. The selection and acquisition of a candidate toolchain. Training and familiarisation, including repeating validation or benchmark cases. Simulation of the test cases and evaluation of the results.
Validation Requirements	The tools to be considered would be those that are currently in use elsewhere, and would be already validated and accepted. The main validation requirement would be to show the applicability to the technology in question.
Output	The organisation requiring the tools would obtain an increase in capability. A publically disseminated report on the tool evaluation findings to aid other UK organisations in choosing whether to follow a similar route.
Existing Research & Body of Knowledge International Programmes	Making connections to International programmes are the focus of this project, especially the extensive existing European and US toolsets. The Virtual Engineering Project critical review will also be a starting point for this task.
Risks	The organisations that have developed the most appropriate tools may not make them available, or access to currently available tools (or support or upgrades) may be withdrawn in future.
Timeline and Prerequisites	Obtaining access to some codes may need partnership agreements at a national agency or government level. An evaluation could take approximately six months to two years, depending on the tool availability and problem difficulty.

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Resource/Costs	A medium-sized consultancy project depending on the scope, to be able to evaluate and report. Some tools may have a license cost, or require an ongoing contribution to ongoing R&D and maintenance.
Exploitation Recommendations	Involvement with International programmes becomes easier if there is increased UK capability in the more commonly applied tools. This is particularly relevant because many of the component tools and methodologies originated, or have been already used and developed, in the UK.

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Project Title	Tritium Genera Coolants	Tritium Generation and Migration in Advanced Reactor Coolants				
Topic	Multi-physics	Multi-physics				
Reference	P6_B					
Source	Workshop, Grou	ıp 3				
Location on Capability Map	Physical/Empirion Modelling Tools	cal Mathematical I	Models			
R&D Spectrum	Basic Research					
			\boxtimes			
Technical Objectives	and connected p	power or process ated (for example	bution throughout plant. as a ternary fissionstructural compo	n product) and		
Benefits	This is a key issue for advanced reactors (all high temperature reactors: gas-cooled, salt, metal for example) and is a must-have for making the safety case.					
Scope & Approach	 Choose a HTGR reactor design to apply the modelling to. Develop a model for the tritium source term in the reactor under consideration. Create component scale tritium transport models (through clad, or heat exchangers for example) as a function of operating conditions, using physical models from existing literature as a starting point (e.g. see TPAC in "International Programmes"). Implement the component models within a system analysis code (for example CATHARE) to predict the tritium distribution through the system. Consider the extension of the approach to other high temperature reactor types as a follow-on task. 					
Validation Requirements	The accuracy of the models of tritium generation will be guided from nuclear fission data, and should be able to be validated as part of developing the source models. Validation of the component transport models will be required to ensure that the dependence on temperature and the balance of diffusion and advection in a flowing system is correct. The availability of this data is currently unknown and will need to be determined by the project. Transport of a trace gas species within a system code is part of the validation of the system code for other applications and has no additional requirements.					

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Output	A validated component within a system code.
Existing Research & Body of Knowledge	Knowledge of tritium generation and permeation through structural materials is available in the literature.
International Programmes	INL produced the Tritium Permeation Analysis Code (TPAC) in MATLAB SIMULINK to analyse tritium distributions in a VHTR including integrated hydrogen production systems.
	https://inldigitallibrary.inl.gov/sites/sti/sti/4591810.pdf
	This is comparable to the THYTAN code from Japan. These tools are not integrated within system codes.
	The Russian HYDRA-IBRAE/LM code has capabilities to simulate the production and transport of tritium in liquid metal reactors. doi:10.1088/1742-6596/899/5/052008
Risks	Technologies involving tritium are sensitive from a security and export control perspective, which a project will need to comply with.
Timeline and Prerequisites	This should be able to be progressed within 3 years.
Resource/Costs	One researcher for 2-3 years
Exploitation Recommendations	If the process followed by this project is successful HTGR reactor technologies, then it is likely to be extensible to others. Fusion reactors also have tritium transport issues, and the methods are transferrable.

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Project Title	Coupled 3D Neutronics and CFD Thermal Hydraulics Applied to BWR Fuel Channels				
Topic	Multi-physics				
Reference	P6_C				
Source	Professor Ali Tui	ran			
Location on Capability Map	Physical Understanding Physical/Empirical Mathematical Models Modelling Tools				
R&D Spectrum	Basic Applied Early Late Research Research Development Development				
		\boxtimes	\boxtimes		
Technical Objectives	The simulation of a nuclear reactor core combines the modelling of neutronics and coolant flow. The power distribution in the reactor core is strongly coupled to variations in local operating conditions, such as fuel temperature and coolant density, which in turn depend on heat production in the nuclear fuel. Due to this strong coupling, the thermal hydraulic and neutronic physics cannot be separated from each other without impairing the accuracy of the results. In the past, the complexities of the coupled problem and the limits of computer capacity have necessitated an approach based on simplified models and approximations. Only recently has sufficient computing power become widely available to tackle the coupled problem in detail. This project aims to create a design and development capability for coupled two-phase CFD and 3D Monte Carlo neutronics simulations. It will be developed and validated in the context of studying flow and instabilities in fuel bundles relevant to ABWRs.				
Benefits	The ability to carry out coupled 3D neutronics and thermal hydraulics will help to improve reactor design and enable an increase in the reliability and economic efficiency of a variety of safety case justification activities. This is relevant to all reactor types. Furthermore, insight into a number of operational issues or potential accidents for BWRs will be gained, including hydrothermal instabilities, LOCA and the prediction of critical heat flux.				
Scope & Approach	The Serpent (http://montecarlo.vtt.fi/) continuous energy Monte Carlo (MC) neutron transport code will be coupled to a general purpose CFD code (such as ANSYS Fluent, Code_Saturne or OpenFOAM) by writing the appropriate code to exchange temperature, void fraction and fission heat output data. This will then be used to perform detailed simulations of flows and instabilities in simplified ABWR fuel bundle geometries. These will be validated against experimental data and then a range of				

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Validation Requirements	simulations performed across a representative range of reactor conditions. These detailed and CPU intensive computations will be captured in the form of a reduced order model representing the various flow regimes. This capability can be used to inform the reactor operational map in larger scale, lower fidelity simulations of a whole BWR core.
validation Requirements	Validation experiments are available in the literature concerning critical heat flux, LOCA, and hydrothermal instabilities for simplified configurations. The coupling of neutronics and multiphase thermal hydraulics that have been developed in the past have extensive databases that might be partially available via DoE labs including Argonne, Oak Ridge and Idaho. Depending on the specific data requirements, existing capability in the EU (e.g. Finland) might also be able to be employed along with
	the proposed new UK nuclear thermal hydraulics facility.
Output	 The outputs of this task will be: An improved tool for efficient coupled 3D MC/CFD simulations. Research relevant to the operation and control of ABWRs primarily focussed on LOCA, prediction of hydrothermal instabilities in fuel channels, CHF, and material durability and integrity issues arising as result of nucleonics, such as induced hydrogen embrittlement.
Existing Research & Body of Knowledge International Programmes	Serpent has already developed a multiphysics interface and existing projects have been performed coupling it to OpenFOAM in Finland, Switzerland and France. The emphasis of this project is therefore on refinements to the efficiency and flexibility of the coupling methods and the application of the coupled toolset to the target application. Code_Saturne has already been coupled with the OpenMC (Monte-Carlo) neutronics by STFC.
Risks	This programme is reasonably ambitious in terms of the engineering goal to provide a validated design and development capability. Although elements of the proposed effort have previously been partially researched, implemented and reported elsewhere, the optimisation of the coupled approach with the aim of creating a validated engineering tool has not yet been accomplished.
Timeline and Prerequisites	It is expected that valuable progress can be made in approximately 3 years.
Resource/Costs	Estimated to be of the order of 2 researchers for 2 to 3 years.
Exploitation Recommendations	The improved coupling methods are relevant to detailed simulations of all current future reactor types. The ABWR research adds to the UKs capability in the domain of the Wylfa Newydd project.

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Project Title	State of The Art CRUD Deposition Models and the Effects on Heat Transfer Mechanisms				
Topic	Multi-physics				
Reference	P6_D				
Source	Workshop, Grou	p 3 with further de	evelopment by the	core team	
Location on Capability Map	Physical/Empirical Mathematical Models Modelling Tools				
R&D Spectrum	Basic Applied Early Late Research Research Development Development				
		\boxtimes			
Technical Objectives	of the best availa CRUD, and its e	able modelling ap ffect on heat trans	opt and contribute proaches for the design series.	leposition of	
	The UK has world leading expertise in this area, with NNL CRUD chemistry capabilities:				
	Henshaw, J., et al., <i>A model of chemistry and thermal hydraulics in PWR fuel crud deposits</i> . Journal of nuclear materials, 2006. 353(1-2): p. 1-11.				
	This niche capability is in much demand worldwide, and particularly from the US. NNL's activities have expanded to include the support of associated thermal hydraulic and advection-diffusion modelling at Imperial College:				
	Cinosi, N., et al., The effective thermal conductivity of CRUD and heat transfer from crud-coated PWR fuel. Nuclear Engineering and Design, 2011. 241(3): p. 792-798.				
	Haq, I., et al., Modelling heat transfer and dissolved species concentrations within PWR crud. Nuclear Engineering and Design, 2011. 241(1): p. 155-162				
		ility to predict in-cont of this valuable	ore boiling would area.	help keep the	
	US researchers are developing tools for coupled simulations including neutron transport, thermal hydraulics, fuel performance, and coolant chemistry. The recent report:				
	U-2017-131	0-000 casl.gov/sites/def	on Assessment fo		
	demonstrates the prediction of the deposition and effect of CRUD across a whole fuel cycle, but also highlights areas of improvement necessary in the toolsets.				
		•	, MAMBA-BDM (P e MOOSE framew		

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Benefits	Improvement to UK understanding of CRUD modelling, which is of use to current and future LWR technology, and potentially to the SCWR Gen IV technology. Greater contact with and collaboration with US researchers at the forefront of advanced modelling development. The opportunity for improved collaboration with the US Nuclear Energy Advanced Modelling and Simulation (NEAMS) projects.
Scope & Approach	 The project tasks will be: Obtain and gain capability in using the CASL toolsets with CRUD prediction capabilities. Review of chemistry and boiling heat transfer models implementations and apply the UK's expertise in these area to identify improvements and development that could be made. Implement improved modelling within the CASL toolset, revisiting existing validation cases where possible. Apply the tools to a reactor scale problem, preferably to help understand or solve a current reactor operational issue. Define further programmes of model development and reactor studies.
Validation Requirements	Validation programmes for the tools in question are already well developed within the CASL VERA project.
Output	Improved models implemented in the CASL toolset, and proposals for further model development and reactor research projects.
Existing Research & Body of Knowledge International Programmes	The substantial development in the US programs described above.
Risks	Access to US codes and information, documentation and data may not be granted, or access could be withdrawn.
Timeline and Prerequisites	This should be able to be progressed within 3 years.
Resource/Costs	One or two researchers for 2 to 3 years, plus access to substantial high performance computing resources.
Exploitation Recommendations	Research projects aimed at embedding UK expertise within a more powerful predictive framework to allow operational improvement in current and future UK and worldwide PWR plant. The ability to gain experience in the use of the MOOSE framework and other US tools, which can then be used in other modelling R&D areas.

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Project Title	Modelling of Air Ingress Accidents in HTGRs				
Topic	Multi-physics				
Reference	P6_E				
Source	Workshop, Grou	p 3			
Location on Capability Map	Modelling Tools				
R&D Spectrum	Basic Applied Early Late Research Research Development Developmen				
		X	×		
Technical Objectives	including chemic	al kinetics) to des	(mainly thermal h cribe the fluid mix emperature gas c	ring and thermal	
Benefits	Understanding the extent and consequences of air ingress accidents is a fundamental design and safety requirement for gascooled reactors.				
Scope & Approach	 The approach must address the following phenomena: Convective and diffusive mixing of multi-component gas mixtures (predominantly He and air). Rates of oxidation of fuel and structural graphite (depends on composition and temperature). Interaction between temperature field and heat generation (from both nuclear heating and exothermal oxidation). Heat transfer from the core to the environment over long time periods (many 10s of hours). Approach: Review of existing capabilities; Identification of gaps/needs; Development of integrated model addressing fluid mixing, heat transfer, chemistry and nuclear effects. 				
Validation Requirements	A large amount of validation data exists from tests conducted at FZ-Jülich (Germany), JAEA (Japan) and in the USA. Some additional validation covering gaps in the data may be necessary.				
Output	A validated calculation scheme (code or network of codes) that can be used to analyse a range of postulated faults in gas-cooled reactors.				
Existing Research & Body of Knowledge International Programmes	See above. Good opportunities for international collaboration: US National Labs (especially INL-NGNP project).				

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	JAEAGeneration-IV Forum
Risks	No significant risks, except loss of UK involvement and IPR opportunities if the capability is developed outside the UK.
Timeline and Prerequisites	Would need to be available in 3 years to be useful to the development and licensing of the U-Battery.
Resource/Costs	Estimated to be of the order of 2 to 3 researchers for 3 years. Would benefit from the involvement of current gas cooled reactor developer.
Exploitation Recommendations	Would significantly assist development and exploitation of UK IPR related to the U-Battery Project.
	Could facilitate UK collaboration with international VHTR development projects.

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Project Title	Improved Prediction of Flow and Thermal Development in Fuel Pin Cooling Passages				
Topic	Turbulent heat transfer				
Reference	P7_A				
Source	Current Phase 1	development wo	rk		
Location on Capability Map	Modelling Tools Physical and Empirical Mathematical Models Personnel				
R&D Spectrum	Basic Applied Early Late Research Research Development Development				
			\boxtimes		
Technical Objectives	Research Research Development Development				

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	 Improve understanding of the forced and mixed convection processes involved. Enable reliable parametric modelling for alternative designs.
	 Fully test the capabilities of (SPH) to predict mixed convection in complex internal passages.
Benefits	The primary benefit of this work is the development and demonstration of methods that are genuinely useable in industrial timescales (rather than just those that are of research value), based on both established Finite Volume (FV) and novel SPH approaches. The specific benefits of a successful outcome to this work would be: More accurate predictions of fuel operating temperature – Fundamental to both NPP performance and safety.
	Support to reactor design by enabling the developer to ensure that that the design can operate efficiently in a stable area of the design envelope.
	 Support to the assurance of nuclear safety by demonstrating improved confidence in important claims.
	In addition, the advances that will result from this effort are generic enough to be of benefit to most other sectors in which heat convection phenomena are influential. They include the gas turbine sector, solar power generation and HVAC applications.
Scope & Approach	The approach for this work is very much building on existing tools and research to produce a specific and exploitable advancement. For the more established FV approach, this research is suitable for a highly parallelisable code, like EDF's Code_Saturne, but other open source codes like OpenFOAM are also suitable.
	Novel SPH methodologies can achieve considerable speed-up by running on multiple GPU nodes.
	The specific activities are envisaged to be:
	Starting with a simple geometry with good extant validation data, investigate a wide range of CFD (and other) modelling techniques to investigate the prediction of unsteady flow and heat transfer in fuel pin sub-channels (LES, RANS, and Hybrid RANS/LES approaches should be explored).
	From this investigation identify the most promising physical models needed to reproduce the correct flow and thermal development in the fuel pin sub-channels, the presence of flow instabilities, and most critically the correct temperature variation within the reactor core.
	 Expand the work to including additional, more complex test cases.
	Expand this work to the investigation of the effects of mixed convection.
	 Provide well documented, referenceable test cases to provide both guidance and validation evidence which can be used by industry.

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Validation Requirements	Detailed local flow and thermal data are essential for the validation of the outputs of this task. However, there is a lack of thermal data in the open literature. Experimental and now increasingly DNS studies provide local flow data at low to moderate Reynolds numbers, so far limited to forced convection cases. DNS may provide the most promising route for data suitable for mixed convection flows. The new UK thermal hydraulics test facility could provide valuable additional information if a suitable test rig could be included, noting that the instrumentation required to provide measurements of sufficient detail, would need to be given careful consideration.
Output	Development in open source codes: While most of these models are included in major commercial codes (Fluent, Star-CCM) and also in major open source codes like Code_Saturne and OpenFOAM. Further refinements/extensions of some models will probably be necessary, which will extend the capabilities of current codes. The specific outputs of this project will include demonstration of new developments in open source CFD codes, FV and SPH, to maximise wider exploitation. Demonstration of benefit and fidelity: The most important contribution will be a set of recommendations of what modelling practices are needed to reliably simulate fuel cooling flows and advances in our understanding of the physical processes involved.
Existing Research & Body of Knowledge International Programmes	This work builds on extensive and world leading research performed in the UK. The University of Manchester group in particular, which has recently led the critical review of the subject [7] and been involved in an initial evaluation of the effectiveness of RANS models for sub-channel flows as part of this project, has a long-established and internationally acknowledged activity in the development of refined turbulent models [8] and [9], and their application to the simulation of internal cooling flows [10] and [11], and also in the use of LES and DNS in the simulation of practical engineering flows, [12] and [13].
Risks	The most critical risk is that no further validation data will become available. This can be mitigated by including a DNS study in the scope. There is also a risk that the methods tried, especially RANS and hybrid RANS/LES will not be as successful as expected, especially in capturing the mixed convection effects. However, the knowledge of how effective different modelling approaches can be and at what cost, will be of considerable value to UK industry.
Timeline and Prerequisites	1 year to complete initial investigations using a simple, forced convection test case (completed under Phase 1 of this programme).

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	A further 3 years to extend the work to more complex and mixed convection test cases and to produce clear guidelines and recommendations. This work would likely benefit from, and be of benefit to, that proposed in projects P7_B and P7_E.
Resource/Costs	1 FTE researcher for 4 years (1 year Phase 1 + 3 years Phase 2). Additional FTE for 18 months to generate DNS data for validation. Access to HPC resources for the DNS analysis.
Exploitation Recommendations	The work can be exploited by means of dissemination of the study to industry, enabling it to be used for both educational purposes and as a reference supporting the use of specific modelling techniques for NTH applications.
	Code that is developed, and knowledge and understanding gained, can be used to support future collaboration or involvement in international programmes.

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Project Title	Improved Accuracy of RANS Models for Turbulent Heat Convection			
Topic	Turbulent heat transfer			
Reference	P7_B			
Source	Workshop Group	o 4		
Location on Capability Map	Physical/Empiric	al Mathematical N	Models	
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
Technical Objectives	Basic Applied Early Late Research Research Development Development			

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Benefits

The main benefits of this project are in improving state-of-the-art modelling tools in a way that is both targeted at the needs of the civil nuclear industry and realistically exploitable by the same. Specifically:

- Higher fidelity CFD modelling without computational cost of LES will mean that analysis can be incorporated into a robust design process and a larger design envelope can be covered.
- Demonstration and evaluation of advanced turbulence models in NTH applications will remove barriers to their use by industry practitioners.
- The evaluation aspects of the project will deliver output of benefit to the training of NTH modelling engineers.
- ▶ The specific scope of work is key to developing industry tools for the modelling of passive flows and is an enabler to more reactor specific investigations proposed in related projects.
- The advances that will result from this effort are generic enough to be of benefit to most other sectors in which heat convection phenomena are influential. They include the gas turbine sector, solar power generation, heat exchanger design, cooling of electronic components and HVAC applications to name but a few.

Scope & Approach

An assessment of RANS models in the prediction of forced, natural and mixed convection phenomena relevant to nuclear thermal hydraulics will provide real benefit to industry, especially with the emphasis on passive cooling involving natural and mixed convection for both fault recovery and some cases normal operation in new NPP.

Given the flow complexities involved, the approach chosen for this project will be to focus on non-linear eddy-viscosity and second-moment closures as these are considered to give the best chance of success [ref. critical review]. While most of these models are included in major commercial codes (Fluent, Star-CCM) and also in major open source codes like Code_Saturne and OpenFOAM further refinements/extensions of some models will probably be necessary, which will extend the capabilities of current codes.

The scope of the work will involve:

Selection of a minimum of 3 benchmark test cases, For the initial stages of the project these could be relatively simple, but the work should move on to complex three-dimensional (and where possible reactor specific) test cases for which either detailed experimental data for both the dynamic and thermal fields are available, or cases for which there are high quality DNS or LES flow and thermal data. It is recommended that forced convection, natural convection, mixed convection and internal shear flow phenomena are included, due to their particular relevance to NPP. Steady and unsteady phenomena are of relevance and both should be investigated.

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	 The testing and refinement of non-linear effective-viscosity and stress transport models. Assessment of their predictive effectiveness and comparison with the predictive performance of more widely used linear effective-viscosity models, such as the k-ε and k-ω SST, will identify superior RANS models that in many circumstances can be used instead of LES. Implementation and demonstration of improved models in open source code. Documentation and dissemination of the study to the UK NTH community.
Validation Requirements	Test cases should be chosen such that there is validation data available. This may be very challenging in the area of natural convection and the generation of high quality experimental data in this area should be considered in the development of test rigs for the UK nuclear thermal hydraulics test facility. The availability of DNS data should be considered as an alternative, although experimental validation would ultimately be needed.
Output	Development in open source codes: The specific outputs of this project will include implementation of new developments in an open source CFD code to maximise wider exploitation. Demonstration of benefit and fidelity: The most lasting and valuable contribution to both the topic and the industry will be a clear and definitive demonstration of the capabilities of advanced turbulence models in thermal simulations. This information will enable nuclear engineers to select the most reliable and cost-effective model for each application. This project will provide clear, referenceable documentation of the study. The outputs from the project will be reported in academic papers.
Existing Research & Body of Knowledge International Programmes	This work builds on extensive and world leading research performed in the UK. The University of Manchester group in particular, which has recently led the critical review of the subject [1] within this project, has a long-established and internationally acknowledged activity in the development of refined turbulent models [2], [3], [4], and their application to the computation of turbulent heat convection [5],[6],[7] and [8]. Such activity provides a base and a starting point for a research project focused on the use of refined RANS models for heat convection.
Risks	There is a technical risk that the methods tried will not be as successful as expected (as is often the case with research activities). Especially regarding the capturing of buoyancy effects in non-linear eddy-viscosity models. However, the knowledge of where such models do not provide good predictions is also information of considerable value to industry and providing this guidance will save much wasted effort.

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	There is a risk that appropriate validation data will not be available in all cases.
Timeline and Prerequisites	For the complex cases, approximately 1-2 FTE years per case including further model development to realise the full benefits. This project follows from work carried out under Phase 1 of this
	project and described in P7_A.
	The findings of this project would be of benefit to project P7_E especially with regard to the complex natural convection test case.
	This project could be expanded beyond the 2-year timeframe by the incorporation of the outputs of P7_D to enable a more complete validation to be carried out (including detailed consideration of heat transfer to the walls of any test rig to reduce distortions). This could be done in combination with the use of a rig in the new UK test facility.
Resource/Costs	1 FTE researcher for 3 years with industry collaboration (0.2 FTE industry) for selection of test cases and potentially assistance with the provision of validation data.
Exploitation Recommendations	The work can be exploited by means of dissemination of the study to industry, enabling it to be used for both educational purposes and as a reference supporting the use of specific modelling techniques for NTH applications.
	The work can be directly exploited by other research programmes considering passive flow.
	Code that is developed, and knowledge and understanding gained, can be used to support future collaboration or involvement in international programmes.

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Project Title	Improving the Ability to Predict Structural Vibration in Reactor Design			
Topic	Turbulent flow			
Reference	P7_C			
Source	Workshop Group	o 7 and subseque	nt development by	y the core team
Location on Capability Map	Concepts and D Modelling Tools Validation and V			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes	\boxtimes	
Technical Objectives				

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	The first technical objective of this project is to take the current state of the art in FSI prediction from across industry (aerospace, gas turbines, wind turbines and automotive are all expected to have value to add in addition to civil nuclear design) and investigate/demonstrate how they might be applied to NTH. The second objective is to develop and improve these methods to better meet the needs of NTH analysis and design.
Benefits	The benefits of improved FSI prediction methods are:
Selicino	Ability to identify and possibly eliminate potential resonance issues early in the design thereby reducing risk and the subsequent cost of achieving a successful design.
	Improvement in predictions of component vibration and consequent through-life wear (e.g. grid-to-rod fretting). This will help inform design and operating limits for reactor components and potentially reduce maintenance costs.
	To make a valuable contribution to modelling applicable across a range of industries.
Scope & Approach	The approach to the work is to collate the tools and experience available from across multiple industries and build on these to develop the state-of-the-art in FSI modelling in NPP. This approach has been chosen as it is perceived that other industries are likely to have more developed methods than NTH and therefore a better outcome may be reached more efficiently in this way
	Specific activities are expected to include:
	 Review and collation of current FSI modelling methods, empirical correlations, test data and codes of practice for dealing with FSI in industrial design.
	 Investigate the application of different methods to typical NPP FSI examples.
	 Develop and improve the modelling methods, starting with a simple geometry to confirm principles and requirements.
	Development and, if possible, validation of improved methods using an NPP example such as part of a fuel bundle with vibration data, or idealised validation cases involving axial flow- induced vibrations of a single fuel pin.
	Challenges that need to be taken into consideration include:
	Mesh movement and deformation. The way this is handled is crucial. Large movement of the solid boundary can lead to deterioration in the quality of the mesh in the fluid domain strong enough to result in numerical divergence. Use of sophisticated re-meshing, or sliding meshes is essential [1].
	Method of integration/coupling/interpolation between fluid and structural solutions. This is especially critical in unsteady FSI cases, such as flow-induced vibrations. Interface interpolations resulting from different data structures for the fluid and solid regions can lead to inaccuracies which increase with successive

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	time steps. Use of separate codes for the fluid and solid analysis can also result in unacceptably high computational overheads in time-dependent analysis. The use of integrated FSI codes is certainly one obvious remedy (although the development of such a code is likely beyond the scope of this project). Capturing of the fluid driving mechanisms in a successful but efficient way. An obvious and crucial requirement is that the flow model should be able to reproduce the large-scale flow fluctuations which generate the vibrations. LES is definitely one option, but its mesh and time step requirements may well make it prohibitively expensive. Unsteady RANS has been shown to be able to capture large-scale unsteadiness [2], [3], [4] for a range of flows, especially when used with some of the more advanced models of turbulence. Their effectiveness in capturing flow instabilities in NPP applications needs to be investigated. Laminar rigid-body FSI cases with strong coupling between the
	flow field and the solid body motion, like the case of a vibrating cylinder in laminar cross-flow [5], can be used to validate the numerical coupling between the fluid and solid motions.
Validation Requirements	The availability of publically available NPP specific vibration data may be sparse as such data is often proprietary. Potential sources of data could be experienced NPP designers and fuel designers e.g. Hitachi, Westinghouse, AREVA. This may be mitigated by starting with a simpler 'benchmark' case where data is available.
Output	Documented review of FSI methods available from other industries with regard to their potential applicability to NPP analysis. Academic papers presenting work undertaken and innovative methods developed. A model demonstrating the methodology and best practice applied.
Existing Research & Body of Knowledge International Programmes	One of the reasons for the slow progress in this field has undeniably been the lack of suitable experimental data to drive model validation. There are very few experimental studies on FSI in general, and most of them, like Steriopoulos et al [6], are for steady state FSI phenomena, for which the coupling of existing CFD and solid mechanics codes is a realistic option. Moreover, unsteady FSI experimental studies such as [5], [7] and [8] only provide displacement data such as amplitude and frequency of oscillations. Emerging experimental research from the University of Manchester [9] is now trying to remedy this by combining surface tracking techniques with phase-averaged PIV measurements. Test data for drag and lift coefficients for not moving and not deforming bodies under the fluid flow stream influence might be used as the first step in validating fluid solvers and turbulent modelling capabilities.

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Risks	There are lots of different methods and tools with potential to add value. It may be difficult to ascertain the most appropriate early in the project. Availability of NPP specific validation data is a risk (see Validation section above).
Timeline and Prerequisites	2-3 years depending on extent of model development following findings of initial review.
Resource/Costs	1.5 FTE, academic PDRA requiring specific experience with FSI 0.5 FTE industry partner with specific experience of FSI in NPP design and access to validation data if possible.
Exploitation Recommendations	The developed methodology could be applied within a state-of-the- art digital reactor design environment, reducing risk and streamlining the need for experimental data.
	Initial findings could be exploited at an earlier time by raising awareness of methods available and their potential for application to NPP FSI analyses.
	Dissemination of the findings at an appropriate UK forum is essential to maximise early exploitation.

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Project Title	Predicting and Assessing Thermal Fatigue in NPP			
Topic	Turbulent flow			
Reference	P7_D			
Source	Workshop Group	o 4		
Location on Capability Map	Physical / Empirical and Mathematical models Validation and Verification			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
			\boxtimes	
Technical Objectives	Thermal fatigue is an issue affecting reactor designs based on a number of different technologies. Welds in the vicinity of junctions where fluid streams of different temperatures mix are particularly vulnerable. Failures of NPP components due to thermal fatigue have occurred and, despite considerable effort, the prediction of this failure mechanism still represents a significant challenge. The driving mechanism for damage is transiently fluctuating fluid temperatures adjacent to a solid component, causing fluctuating thermal stresses within the solid, shortening the life of the material. Depending on the precise geometry and operation of the system and the details of the flow, the frequency of the temperature fluctuation can vary considerably (and randomly!). Currently 'coded' methods based on previous experience and experimental data are used to identify high risk areas, but detailed analysis is often restricted to computationally expensive methods that are not currently realistic for extensive industry use. The challenge of controlling damage by thermal fatigue is a combination of thermal hydraulics, stress analysis and materials science. This project aims to contribute to improving the state-of-the-art by investigating potential methods for the prediction of high and low frequency thermal fatigue fluid driving mechanisms found within NPPs and, vitally, the conjugated heat transfer to the solid component. A key objective is to produce recommendations regarding methods appropriate for industry use along with relevant NTH examples.			
Benefits	such that the de Enable a more a reducing the und expense of exte	sign can be modi analysis based mo certainty in more on nsive experiment	fied to reduce the ethodology to be u generic methods v	risk. used by industry, vithout the
	important to NP	P design and ope	ration, the developer modelling has the	oment of

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improve numerous predictions. Additionally the heat transfer to and from the solid surfaces of a test rig can be extremely important in understanding and using the experimental results. Scope & Approach The approach for the work will be to make use of a range of CFD modelling approaches along with thermal stress prediction tools to develop a method for the prediction of thermal fatigue in NPP components. This work is intended to build on and combine existing methods, developing and demonstrating the extent of their capabilities for this application (rather than performing any new basic research). The scope of the work will comprise: • Review methods used in other industries e.g. oil and gas, gas turbines. • Identify specific examples of NPP components at risk of thermal fatigue (include consideration of both high and low frequency driving mechanisms). • Investigate the use of CFD modelling (including URANS, second moment closure models, LES) to predict the temperature fluctuations and wall heat transfer important to thermal fatigue. The use of LES involves extending the same time steps used for LES simulations in the fluid, to the solution of the instantaneous temperature field in the solid, which is rather expensive. The use of URANS is certainly more affordable, but it involves introduction and validation of transport equations for the temperature variance and its dissipation rate, as described in [1]. Further development of the URANS approach will likely be necessary. • Investigate the potential for creating a combined fluid and structural model to predict the transient temperature variation in and resulting thermal stresses in the solid component. Note that the further development of the Structural response of the solid component is outside of the scope of the 3 year timeline, but could be considered for a later phase. • Create at least one DNS analysis for validation purposes. • Create at least one DNS analysis for validation purposes. • Create at least one DNS analysis for validation purposes.		
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Identify specific examples of NPP components at risk of thermal fatigue (include consideration of both high and low frequency driving mechanisms). Investigate the use of CFD modelling (including URANS, second moment closure models, LES) to predict the temperature fluctuations and wall heat transfer important to thermal fatigue. The use of LES involves extending the same time steps used for LES simulations in the fluid, to the solution of the instantaneous temperature field in the solid, which is rather expensive. The use of URANS is certainly more affordable, but it involves introduction and validation of transport equations for the temperature variance and its dissipation rate, as described in [1]. Further development of the URANS approach will likely be necessary. Investigate the potential for creating a combined fluid and structural model to predict the transient temperature variation in and resulting thermal stresses in the solid component. Note that the further development of the structural response of the solid component is outside of the scope of the 3 year timeline, but could be considered for a later phase. Create at least one DNS analysis for validation purposes. Create at least one DNS analysis for validation purposes. Create a number of documented examples to demonstrate the strengths and weaknesses of the different approaches applied. Validation Requirements Due to the difficulties involved in setting up experiments suitable for conjugate heat transfer data, DNS offers the best chance to acquire data suitable for CFD validation, especially for the penetration of temperature fluctuations into the solid region. DNS studies of conjugate heat transfer can be found in the scientic literature like [1] to [6], but these for the most part are confined to fully developed channel flows. A notable exception is the recent work of Wu et al	Scope & Approach	modelling approaches along with thermal stress prediction tools to develop a method for the prediction of thermal fatigue in NPP components. This work is intended to build on and combine existing methods, developing and demonstrating the extent of their capabilities for this application (rather than performing any new basic research). The scope of the work will comprise:
moment closure models, LES) to predict the temperature fluctuations and wall heat transfer important to thermal fatigue. The use of LES involves extending the same time steps used for LES simulations in the fluid, to the solution of the instantaneous temperature field in the solid, which is rather expensive. The use of URANS is certainly more affordable, but it involves introduction and validation of transport equations for the temperature variance and its dissipation rate, as described in [1]. Further development of the URANS approach will likely be necessary. Investigate the potential for creating a combined fluid and structural model to predict the transient temperature variation in and resulting thermal stresses in the solid component. Note that the further development of the structural response of the solid component is outside of the scope of the 3 year timeline, but could be considered for a later phase. Create at least one DNS analysis for validation purposes. Create a number of documented examples to demonstrate the strengths and weaknesses of the different approaches applied. Validation Requirements Due to the difficulties involved in setting up experiments suitable for conjugate heat transfer data, DNS offers the best chance to acquire data suitable for CFD validation, especially for the penetration of temperature fluctuations into the solid region. DNS studies of conjugate heat transfer can be found in the scientific literature like [1] to [6], but these for the most part are confined to fully developed channel flows. A notable exception is the recent work of Wu et al		► Identify specific examples of NPP components at risk of thermal fatigue (include consideration of both high and low frequency
structural model to predict the transient temperature variation in and resulting thermal stresses in the solid component. Note that the further development of the structural response of the solid component is outside of the scope of the 3 year timeline, but could be considered for a later phase. • Create at least one DNS analysis for validation purposes. • Create a number of documented examples to demonstrate the strengths and weaknesses of the different approaches applied. Validation Requirements Due to the difficulties involved in setting up experiments suitable for conjugate heat transfer data, DNS offers the best chance to acquire data suitable for CFD validation, especially for the penetration of temperature fluctuations into the solid region. DNS studies of conjugate heat transfer can be found in the scientific literature like [1] to [6], but these for the most part are confined to fully developed channel flows. A notable exception is the recent work of Wu et al		moment closure models, LES) to predict the temperature fluctuations and wall heat transfer important to thermal fatigue. The use of LES involves extending the same time steps used for LES simulations in the fluid, to the solution of the instantaneous temperature field in the solid, which is rather expensive. The use of URANS is certainly more affordable, but it involves introduction and validation of transport equations for the temperature variance and its dissipation rate, as described in [1]. Further development of the URANS approach will likely be
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	Validation Requirements	conjugate heat transfer data, DNS offers the best chance to acquire data suitable for CFD validation, especially for the penetration of temperature fluctuations into the solid region. DNS studies of conjugate heat transfer can be found in the scientific literature like [1] to [6], but these for the most part are confined to fully developed channel flows. A notable exception is the recent work of Wu et al
Output This Project will result in: ▶ DNS studies which will provide validation data for conjugate heat transfer and will also further advance our understanding of	Output	DNS studies which will provide validation data for conjugate

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Existing Research & Body of Knowledge International Programmes	the process. These data will be summarised and discussed in academic publications and will also be made publically available. Development/demonstration of URANS models capable of modelling the generation of temperature fluctuations within the fluid region and their advancement into the solid region. These will be reported through scientific publications. Existing guidance on the identification of areas at risk of thermal fatigue (e.g EPRI handbook on fatigue management). Existing research demonstrating the use of LES and DNS for the prediction of transiently fluctuating fluid temperatures in mixing streams. Existing models for the transport of thermal fluctuations and of their dissipation rate. Existing tools for the prediction of thermal stress. Both the IAEA and JAEA have investigated thermal fatigue in NPP [2 to 8]. Progress in this area in the UK would certainly be of international interest and has potential applications outside of the
Risks	civil nuclear industry. The area of highest technical risk is the multiphysics modelling, i.e. the coupling of the thermal hydraulics with the thermal (and ultimately the structural) response of the component. However, as there is considerable value in improving the prediction of the thermal hydraulic driving mechanism even without this direct coupling, the risk of the project as a whole not delivering a benefit is low.
Timeline and Prerequisites	 3 year timeline: Selection of cases and acquisition of existing validation data +6 months Initial CFD cases +12 months Development of CFD cases and investigation of coupling methods +24 months. Development of DNS validation data +24 months Final delivery +36 months
Resource/Costs	Involvement of at least one reactor designer to target the examples at areas of high industrial relevance and to provide input regarding the guidance that would be of most use to them. 1 FTE researcher for 3 years duration + allowance for industry guidance if work is carried out by an academic institution. 1 FTE researcher (DNS) for 1 year for the development of DNS benchmark case. HPC resources for DNS work.

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Exploitation Recommendations

The documentation of the process followed and the tools used, plus availability of demonstrated examples moves beyond the usual outputs from research work and is explicitly included in this project to enable exploitation.

The recommended route is to make the project outputs available to a number of reactor designers with concerns regarding thermal fatigue to enable them to develop their own models in an efficient and cost effective manner.

- 1. T. J. Craft, H. lacovides, S. Uapipatanakul, "Towards the Development of RANS Models for Conjugate Heat Transfer", *J. of Turbulence*, **11**, 1-16, 2010.
- 2. N. Kasagi, A. Kuroda, M. Hirata, "Numerical Investigation of Near-Wall Turbulent Heat Transfer Taking Into Account the Unsteady Heat Conduction in the Solid Wall", *J. Heat Transf.* **111**, 385–392, 1989.
- 3. T.P. Sommer, R.M.C. So, H.S. Zhang, "Heat Transfer Modelling and the Assumption of Zero Wall Temperature Fluctuations", *J. Heat Transfer* **116**, 855–863, 1994.
- 4. A. Mosyak, E. Pogrebnyak, G. Hetsroni, "Effect of Constant Heat Flux Boundary Condition on Wall Temperature Fluctuations", *J. Heat Transf.* **123**, 213–218, 2000.
- 5. I. Tiselj, "Tracking of large-scale structures in turbulent channel with direct numerical simulation of low Prandtl number passive scalar", *Phys. Fluids* **26**, 125111, 2014.
- 6. C. Flageul, S. Benhamadouche, É. Lamballais, D. Laurence, "On the discontinuity of the dissipation rate associated with the temperature variance at the fluid-solid interface for cases with conjugate heat transfer", *Int. J. Heat Mass Transf.* **111**, 321–328, 2017.
- 7. C. Flageul, S. Benhamadouche, É. Lamballais, D. Laurence, "DNS of turbulent channel flow with conjugate heat transfer: Effect of thermal boundary conditions on the second moments and budgets", *Int. J. Heat Fluid Flow*, Special Issue, **55**, 34–44, 2015. [7] Z. Wu, D. Laurence, H. Iacovides and I. Afgan, "Direct simulation of conjugate heat transfer of jet in channel cross-flow", *International Journal of Heat and Mass Transfer*, **110**, 193-208, 2017.

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Project Title	Improved Predi Flows	ction of the Stall	ing of Natural Ci	rculation
Topic	Turbulent heat transfer			
Reference	P7_E			
Source	Developed by Core Team and Professor Walker based on requirements and Group 4 workshop initial ideas.			
Location on Capability Map	Physical Understanding Modelling Tools Physical and Empirical Mathematical models			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes	\boxtimes	
Technical Objectives	cooling within the as an important of complexity and so natural circulation large height to do Currently predict under these consuch as system. In many respects well predicted by However, fundar the entire cross and that it is suff developed and deffects, when difflows in different conditions (and significantly reductions) (and significantly reduction of idelity methods computational reductionally, the challenges to Reductionally, the challenges to Reductional resources. The findings of a the-art tools are, large-scale and safety of any suggestions.	e primary reactor safety feature of resize of full-scale resize of full-scale resize of full-scale resize of the flow raditions are largely codes. Is, natural circulation rentally, systems section of the pipericient to model flow ini-directional. Uniferent parts of the directions, are versioned or even stalled flarge natural circulations as CFD is his esources, even us flow phenomena and shall models, pote ence modelling are any natural circular therefore, subject expensive testing children design demonstrations.	culation loops to encircuit has long being reactor design eactors inevitably etrically complex and heat dissipated and heat display the property important under hormal operation) and flow. Sullation systems upon and flow an	een advocated as. The means that and of very ipation achieved idelity methods, as codes". bresumption that the same thing, it were fully ree-dimensional pipe could have ar NPP fault and can result in sing higher and can result in severe equiring more computational arrent state-of- uncertainty and at the nuclear copment of as is therefore

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In this project proposal we identify one particular instance of such buoyancy driven flow (further discussed under project approach) within an NPP for further investigation and development. It is chosen both because of its intrinsic, specific importance in the analysis of several reactor systems, including reactors under current development in the UK, and because in many respects it captures most of the difficulties in modelling these flows. It can be viewed as an archetypal problem, and thus developments under this project would have wider applicability to other instances of these flows.

The technical objectives of this project are to:

- Develop a better predictive capability for a specific instance of challenging three-dimensional flow directly impacting natural circulation flow rates in NPP.
- Provide valuable input that can be further developed into improvements (or at least a better understanding of the uncertainty) in existing lower fidelity tools for the prediction of overall natural circulation flow rates under normal operation and fault conditions.

Benefits

The overall benefit of this work is improved confidence and demonstration that passive safety designs work.

Specifically an improved, validated, predictive capability would:

- Allow a better understanding of the phenomenon, and provide a tool that would allow identification of circumstances under which it was of concern:
- Allow safety cases dependent on asserting reliable natural circulation flows in piping loops to be made more robustly;
- Add to the underlying capabilities within CFD to predict these complex flows;
- Potentially reduce the number of tests needed to validate a particular design, thereby reducing reactor development costs.

Scope & Approach

The detailed modelling and investigation of an entire reactor primary (or other) circuit 'loop' under natural convection conditions with a view to developing a thorough understanding of every aspect and improving the entire predictive capability is a scope that is too large for a single project.

The approach for this project is therefore to focus on a particular area of concern and use this to provide both an improved predictive capability of that area and fundamental learning that can be built upon to improve the prediction of natural circulation in many other areas.

A common concern that needs to be addressed in predicting slow natural circulation flow in piping is flow blockage, sometimes (but misleadingly) referred to as the formation of cold traps. Consider a slow upward flow of water in a vertical section of a pipe, driven by the modest density differences around the circuit, where that vertical section happens to be subject to external cooling. With

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	modest cooling, the small quantities of cooler water formed adjacent to the pipe walls will be swept upwards with the main flow. As the cooling increases, there will tend to a downwards-flowing sheath of cooler, denser water adjacent to the pipe wall, leaving a reduced passage for the rest of the water, and applying a downwards shear traction to the upwards flow. As the cooling increases the net flow can fall to zero. A focused study will be undertaken to identify where conventional CFD will struggle to give accurate predictions for this scenario. The scope of the work will include: An assessment of the appropriateness of the various RANS turbulence models available. Further model development, building on the understanding gained, with modified models and / or more appropriate model parameters incorporated (potentially taking value from P7_B at this stage). An assessment of the model performance against more highly resolved modelling methods (e.g. LES CFD). Validation using experimental data if possible. This work could be usefully extended to consider the influence of two-phase flow. The scope of this task should include the planning of a subsequent task to cover these aspects.
Validation Requirements	As noted above, validation by comparison with measurements is highly desirable. It is unlikely that any suitable existing data is available but appropriate initial experiments need not be extensive, or take place at difficult conditions of temperature and pressure, and as such should be relatively inexpensive. To prove applicability under prototypical fluid conditions, however, may ultimately be necessary and would be more expensive. There is certainly a case for a detailed experimental study of a large-scale natural convection loop and such a loop would be a valuable addition to the new UK nuclear thermal hydraulics test facility.
Output	Outputs will be reported in an academic paper and can be noted under two headings:- (i) A greater understanding of, and ability to predict, a specific problem that arises in many reactor systems. (ii) Generically, increased ability to predict this class of flow in multiple circumstances.
Existing Research & Body of Knowledge International Programmes	The literature on buoyancy-driven flows is vast, albeit much focuses on very 'academic' problems, such as the classical differentially-heated cavity. Two relevant references, within which a reasonably focussed literature review is to be found are Sebilleau et al., 2015b, Sebilleau et al., 2015a. [1] and [2].

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	Consideration of natural circulation phenomena and their relevance to passive cooling in light water reactors are published in a number of IAEA documents [3], [4], [5].
	Preliminary 2-D simulations in progress under Phase 1 of this program at the University of Manchester, shows that even under the 2-D restriction persistent instabilities are present which will result in thermal fluctuations. This suggests that a full study of such phenomena is most urgent.
	A PhD study is under way at the University of Manchester, but its focus is the natural circulation flow in small modular reactors.
	Work carried out by industry (e.g. EDF) to examine natural circulation in specific reactor designs.
	Relevant experimental work is currently being undertaken at BARC in India, as part of the Indo-UK Civil Nuclear Collaboration.
Risks	This is a difficult area, and finding suitably skilled researchers with the necessary understanding of CFD will not be easy.
	There is a risk that no directly-relevant experimental measurements are available to the project, either via measurements conducted under the project itself, or for example using those from India noted above. However, much progress could still be made by conducting the activities described, and using LES CFD as a basis for model development.
Timeline and Prerequisites	The scope of the work for single phase flow could be completed by 1FTE within 3 years.
	This project could benefit from the findings of P7_B and could also use the conjugate heat transfer model from P7_D to improve accuracy under validation.
Resource/Costs	1 FTE researcher for 36 months
Exploitation Recommendations	The models and techniques developed can be exploited industrially through commercial CFD codes based on the published research. Additionally, the results could be used to improve the modelling of 'cold traps' in lower fidelity codes.
	Results would be of direct relevance to the designers of reactors, and to those developing their safety cases. The findings could be used to enable industry to develop 'design specific' models to inform future passive cooling analyses.

- 1. SEBILLEAU, F., ISSA, R. I. & WALKER, S. P. 2015a. Analysis of Turbulence Modelling Approaches to Simulate Single-phase Buoyancy Driven Counter-current Flow in a Tilted Tube. Flow, Turbulence and Combustion, 96, 95-132.
- 2. SEBILLEAU, F., KANSAL, A. K., ISSA, R. I., WALKER, S. P. & MAHESHWARI, N. K. 2015b. CFD and experimental analysis of single phase buoyancy driven counter-current flow in a pipe. NURETH16. Chicago.
- 3. IAEA, 'Natural Circulation in Water Cooled Nuclear Power Plants', November 2005, IAEA-TECDOC-1474.

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- 4. IAEA, 'Passive Safety Systems and Natural Circulation in Water Cooled Nuclear Power Plants', November 2009, IAEA-TECDOC-1624.
- 5. IAEA, 'Passive Safety Systems in Advanced Water Cooled Reactors (AWCRs)', September 2013, IAEA-TECDOC-1705.

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Project Title	Improved Predi Volumes	ction of Passive	Cooling in NPP	Containment
Topic	Turbulent flow			
Reference	P7_F			
Source	Workshop Group and Professor W		bsequent work by	the core team
Location on Capability Map	Physical understanding Modelling Tools Physical/empirical mathematical methods			
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
			\boxtimes	
Technical Objectives	natural circulation removal. As an illustrative that a loss of coordinates.	e example, under solution to	de by reactor designed to be relied upon some circumstanche AP 1000 plant ops to the inner su	es it is asserted will be
	dimensional nate that will be present be by a combinate steam from the such circumstant difficult to claim frassive means difficult and expending that will be such circumstant difficult to claim frassive means difficult and expending that will be present that will be such circumstant difficult to claim frassive means difficult and expending that will be present th	ural circulation flowent within the contestion of heat loss for the the end of the ces extremely chall of the benefits of fault recovery.	ermal hydraulic phe e containment atm allenging, to the ex offered by this (an Experimental meand therefore impro	nd air mixture s to the wall will condensation of nenomena nosphere under extent where it is nd similar) assurements are ovements in
	The objective of challenges pose influenced convert is noted that the real PWR contains the presence of	this project is to ind by CFD simulatection in a large anis work initially comment has the adnon-condensable	re of particular values of particular values on a conditions of conditions of complex cavity on siders only singled ded complexity of gases, the work work to completely	dress the of buoyancy c. e phase flow. A condensation in would need to be
Benefits	an improved pre containment sys	dictive capability	tially to produce ar for passive heat re is of high value to pecially SMRs).	emoval from a

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However, as noted, the problem can be considered as a prototypical example of cavities within NPP design. Predictive techniques able to cope with this problem will then be able to be applied with confidence to what are perhaps less challenging circumstances in other reactor fault analyses.

The specific benefits of an improved, validated, predictive capability would be:

- More confident analysis of flow and heat transfer under fault or passive cooling conditions to support nuclear safety;
- Potential for improvement to existing empirically-based designs, allowing conservatism to be reduced and cost savings to be realised.

Scope & Approach

As the emphasis of the work is on the prediction of threedimensional buoyancy influenced flow, the approach will initially focus on the prediction of single phase flow within the containment volume.

There has of course been considerable work on the modelling of natural circulation flows, with much measurement and modelling, for example, of classic canonical problems such as the differentially-heated cavity. These works will be a starting point, but here the need is to go beyond the more abstract and simplified "test problems", to explore the application and necessary methods development in this highly applied context, where various phenomena come together.

The scope of the work will include:

- Identifying and understanding areas in which conventional commercial CFD treatments are less than ideal for these flows based on the phenomena of interest and the specific implementations/empiricisms in the CFD.
- ▶ Consideration of bulk-heating and cooling in this context, as radiation from either hot solid surfaces, or hotter regions of the gas, transfers heat, complementing the normal advection-diffusion processes otherwise at work.
- Identify advanced modelling methods available within a research environment and investigate their potential to improve predictions.
- ▶ Devising and implementing modifications to CFD to make these methods more suited to complex cavity flows.
- Comparison of modelling with experimental data (where possible) for improved understanding of any limitation and validation of any improvements. This is not anticipated to be straight forward and a focussed search for relevant data is expected to be needed as part of this project.
- ▶ If appropriate, plan experiments to investigate relevant combinations of phenomena.

Validation Requirements

Work carried out under Phase1 has identified a significant shortage of specifically relevant, freely available validation data in the area of

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The outputs of this project will be published in academic papers. A CFD modelling example of a PWR containment volume. Any modelling improvements will be documented in sufficient detail to enable implementation in any capable CFD code. Existing Research & Body of Knowledge International Programmes The general problem of modelling complex, interacting three-dimensional buoyancy-driven flows has received considerable attention, albeit it tends to focus on rather "academic" problems, in part a reflection of the difficulty of the area. Some application in industry is seen, but usually limited to double checking of the assumptions of lower fidelity tools and confidence in the detailed results is generally low. In addition to the information given in the modelling critical review, two further references [1] [2], provide a good literature review of the three-dimensional buoyancy-driven flow and heat transfer modelling that is to be found. NPP specific knowledge and experience of some relevance is given in a number of IAEA documents e.g. [3], [4], [5]. There are various measurement programs in different countries addressing the broad area of buoyancy driven flows e.g. work undertaken at BARC in India, as part of the Indo-UK Civil Nuclear Collaboration, addressing the three-dimensional flow aspects, and there will be some gain from interaction with this. This program does not, however, include the bulk heating, cooling and radiation issue. There have been various 'macroscopic' tests of mixing and circulation within containments. In principle these provide some opportunities for validation, but instrumentation would not have been adequate for detailed CFD modelling to be compared with observations [6]. Risks This is a difficult area, and there is a need for suitably skilled and experienced researchers with the necessary understanding of CFD. The availability of specifically relevant validation data may be limited.		natural convection. However, there are some good quality published measurements of simple natural circulation flows that include some of the characteristics that are important, that could be used as a starting point. The performing of a carefully focused search to identify measurements that had been made of relevant phenomena is an important part of the scope of the work. It would be desirable if carefully planned experiments were to be performed (although this is beyond the scope of the specific activity proposed here) to provide the detailed results needed for CFD validation of these combined phenomena. The new UK thermal hydraulics test facility could be used for this purpose.
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experienced researchers with the necessary understanding of CFD. The availability of specifically relevant validation data may be limited.		circulation within containments. In principle these provide some opportunities for validation, but instrumentation would not have been adequate for detailed CFD modelling to be compared with
Timeline and Prerequisites	Risks	experienced researchers with the necessary understanding of CFD. The availability of specifically relevant validation data may be
	Timeline and Prerequisites	Current scope could be completed in 3 years.

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	Work will likely benefit from turbulence modelling work carried out under P7_A and P7_B.
Resource/Costs	1 FTE researcher for 2- 3 years (see risks for further details). Involvement of PWR developer may enable access to additional validation data and/or enable the project to be even more focused on industry needs as well as providing a fast-track to exploitation.
Exploitation Recommendations	The models and techniques developed can be exploited industrially through commercial CFD codes based on the published research. Results would be of direct relevance to the designers of reactors, and to those developing their safety cases. The demonstration of the techniques used within an NPP application will promote early exploitation.

- 1. SEBILLEAU, F., ISSA, R. I. & WALKER, S. P. 2015a. Analysis of Turbulence Modelling Approaches to Simulate Single-phase Buoyancy Driven Counter-current Flow in a Tilted Tube. *Flow, Turbulence and Combustion*, 96, 95-132.
- 2. SEBILLEAU, F., KANSAL, A. K., ISSA, R. I., WALKER, S. P. & MAHESHWARI, N. K. 2015b. CFD and experimental analysis of single phase buoyancy driven counter-current flow in a pipe. *NURETH16*. Chicago.
- 3. IAEA, 'Natural Circulation in Water Cooled Nuclear Power Plants', November 2005, IAEA-TECDOC-1474.
- 4. IAEA, 'Passive Safety Systems and Natural Circulation in Water Cooled Nuclear Power Plants', November 2009, IAEA-TECDOC-1624.
- IAEA, 'Passive Safety Systems in Advanced Water Cooled Reactors (AWCRs)', September 2013, IAEA-TECDOC-1705.
- J. Woodcock and M. B. Dzodzo, "APPLICATION OF LARGE SCALE CONTAINMENT DATABASE TO AP600 LOSS-OF-COOLANT-ACCIDENT INTERNAL CIRCULATION AND STRATIFICATION EVALUATIONS," Proceedings of ICONE 8 - 8th International Conference on Nuclear Engineering, ICONE-8488, April 2-6, 2000, Baltimore, MD USA

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Project Title	Investigate the Modelling Pred	-	Surfaces on NTH	l Heat Transfer
Topic	Turbulent heat to	ansfer		
Reference	P8_A			
Source	Workshop, Grou	p 4 and subseque	ent core team worl	k.
Location on Capability Map	Physical underst Physical/empiric Validation and ve	al mathematical n	nodels	
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes		
Technical Objectives	that solid walls a especially after sassumption. Wall roughness (clips, wires, boliwith time such a This roughness along a channel to/from the surfal Modern CFD comeans of a numequivalent 'sand thickness of the high degree of eturbulence mode the surface of indefine the mode well represented Numerous specito better underst components. However, the generally well unconsider this aspaplication than The objective of surfaces on the an improved unconsidences so the surfaces surfaces so the surfaces s	may occur due to the rivets etc.) or dependent the potential thand, even more some in the potential thand, even more some in the effect of suffice thand the effect on present the project is to us the project is to us the effect on present the project is to us the effect on present the effect of the effect on present the effect of	mal hydraulic modally smooth, in readeration, this may not small scale surfacture to mechanisms to sition (e.g. CRU to affect both the programment of the determs/coefficient, by modifying (readerstand grain' appropriate of the complete of	or be a correct ce features sthat develop D in PWRs). bressure drop eat transfer bughness by the to define an ducing) the ver, there is a the near-wall ed knowledge of appropriately all surfaces are bach. other industries cicular ing employed in in available. at transfer is not tries only rarely and for their bact of rough lar value will be luced by surface ered through

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Benefits	The prediction of surface heat transfer is absolutely key to the most important aspects of reactor design and safe operation.
	The benefit of this project will be better informed predictions of surface heat transfer to support reactor design and nuclear safety applications.
	Specifically:
	 More accurate fuel temperature predictions and an improved understanding of the uncertainty in predictions;
	▶ More accurate predictions of system pressure drops;
	 Improved understanding of plant aging and the effect on performance;
	More generic models of turbulent flow over rough surfaces which can be used in a wide range of applications (i.e. beyond NPP).
Scope & Approach	The initial approach for the work will be to understand the effect of surface roughness on NPP heat transfer with single phase turbulent flow, although there may be considerable value to extending the study to two-phase flow in the future.
	Activities are anticipated to be:
	 Determine the nature of surface roughness that may occur within an NPP and select a diverse range of test cases.
	Review the most recent work in the modelling of rough surfaces in CFD for studies where heat transfer was an important consideration. This should include identification of sources of experimental validation data.
	Perform high fidelity (LES or DNS), detailed modelling of the surfaces to understand the interaction of the surface with the boundary layer and the effect on heat transfer relative to a hydro-dynamically smooth surface.
	Investigation of the 'sand grain roughness' CFD approach and the available wall heat transfer methods to determine the extent of their validity in the context of the test cases. Derive methods of evaluating the relevant modelling coefficients if appropriate.
	 Investigate alternative approaches to simplifying the modelling of typical NPP rough surfaces and the resulting heat transfer in CFD.
	 Produce a plan for a further phase of work, potentially including experimental validation, extension to two-phase flow analyses and extension to consider surface treatments to enhance heat transfer.
Validation Requirements	Although the approach is primarily to use high fidelity modelling to investigate/validate common CFD simplifications, ultimately test data will be required for the final validation of any innovations.
	This project should endeavour to use existing data where possible (considering that produced from studies in other industries).

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	In the future, tests could be performed on a small scale to provide
	specifically relevant validation evidence.
Output	Academic publication of study including:
	Review of existing published work.
	 Assessment of accuracy of current correlations and an improved understanding/quantification of the uncertainty in these methods for various NPP applications.
	 High fidelity (DNS) simulations of flow over heated rough surfaces.
	Development and demonstration of new methods/models.
Existing Research & Body of Knowledge International Programmes	Extensive data is published on the micro-structure of reactor specific surface phenomena, such as crud. This can be used to define representative surfaces.
	Numerous 'one-off' studies on the effect of surface roughness for specific examples are published in the context of a variety of industries. These should be reviewed in detail and the value of these incorporated into this project.
Risks	There has clearly been considerable work in closely related areas in the past and there is a risk of re-treading old ground. The review task within this project is designed to mitigate this risk and, should sufficient previous work be found at that stage, the task should be re-planned to report the review in detail, in the context of application to NTH CFD analysis. Future areas for investigation, such as the impact of the surface roughness on two-phase flow could then be brought forward.
Timeline and Prerequisites	2-3 years, with review complete in first 6 months. This project has links with both P8_B and P7_D.
Resource/Costs	FTE academic researcher for 2- 3 years. Input from industry of specifically relevant surfaces to maximise short term exploitation value.
Exploitation Recommendations	The most direct and fastest exploitation will be in the quantification of uncertainties associated with CFD modelling. Methods to develop appropriate input parameters to existing CFD code methodologies could also be immediately exploited. In the longer term new modelling techniques could be incorporated into CFD codes to improve them. The work could contribute to a more ambitious, coupled (say CRUD accumulation) simulation to give a more accurate prediction of the impact of the deposits on surface heat transfer. This would provide future potential for international collaboration.

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Project Title	Improved Wall	Models for Accui	rate Heat Transfe	er
Topic	Turbulent heat to	ransfer		
Reference	P8_B			
Source	Workshop Group	o 4		
Location on Capability Map	Personnel Physical/Empirio	cal Mathematical N	/lodels	
R&D Spectrum	Basic Research	Applied Research	Early Development	Late Development
		\boxtimes	\boxtimes	
Technical Objectives	is fundamental to designs. For examination from solid fuel of the solid surface steam to achieve transfer is therefore design and safe. The modelling of transfer prediction presence of a solid layer adjacent to field. The rate of largely determining Standard detailed.	er between the soling the successful of the successful of ample, the heat ever and into the primares of a steam generation or error of paramount operation. If near-wall turbule on and is complexed to surface causes of the attention and also a strong the strong of the surface causes of the attention and the surface causes of the attention and also a strong the surface causes of the surface cau	peration of almost olved within the fully circuit fluid and for any from the rator and from the importance to such the fully and the formation of the formation of the tween the fluid at so of the viscous sidelling of near-wall	t all NPP uel must pass from there into ere into the of this heat ccessful reactor successful heat ows. The a thin viscous he turbulence nd the surface is ub-layer. Il turbulence can
	significant comp complex geome cost of solutions dimensionless the lower parts of the are thus insensite potential for inact (which resolve the applicability and range of conditional NPP predictions There is consequence of the comprehensive	ng that resolves the utational resource tries employ wall for a wall-function stransickness of the vise boundary layer (tive to changes in a courate results. Lone boundary layer) can produce reliations, but still have I	es and most indust unctions to reduce ategies prescribe cous sub-layer and it.e. the log-law distinction the main flow, lea w-Reynolds-numble predictions for imitations when a le scope for improat all levels and a	trial CFD of e this time and a fixed a shape of the stribution), and ding to the per models age of a broader pplied to real evement of the need for a

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	The technical objectives of this project are to improve the prediction of wall heat transfer in an NTH context and, crucially, to investigate and disseminate information regarding the strengths, limitations and ranges of applicability of approaches when applied to prototypical NTH scenarios and phenomena.
Benefits	The outcome will be more effective models of near-wall turbulence and also a clearer set of guidelines to the community as to what different models can achieve and at what cost. In particular to:
	 Develop improvements in wall model accuracy and robustness leading to improved prediction of key reactor parameters such as fuel temperature.
	Improve confidence and accuracy in heat transfer predictions using wall models, thereby supporting the uptake of advanced thermal hydraulic modelling by industry.
	While the use of wall models in RANS turbulence CFD represents an approximation compared with detailed prediction of the viscous sub-layer, it is currently necessary to enable use of CFD in industrial timescales. To maximise the potential for rapid exploitation of the research, the approach to this project will be to focus on the range of applicability and developments in the accuracy of wall models for NTH analysis.
	The reliable prediction of wall heat transfer is not a requirement exclusive to the nuclear industry. It is relevant to all other areas of thermal power generation, cooling of electrical and electronic components, HVAC applications and many others, all of which stand to gain from the proposed research.
Scope & Approach	▶ Identify suitable experimental or LES/DNS CFD benchmark test cases which have sufficiently high quality and well resolved heat transfer and flow-field data to enable high quality comparison to CFD results. These should include:
	 forced, natural and mixed convection heat transfer;
	 flows with separation, recirculation and reattachment;
	 flow including the impingement of jets;
	 variation in the temperature of the solid surface.
	 Assess the available wall models (including low-Reynolds number models) in the open source CFD tools Code_Saturne and OpenFOAM against the benchmark test cases.
	Identify the limitations of current models in terms of wall resolution, phenomena captured, and accuracy in an NTH context and address the reasons for them.
	Investigate and develop improved wall functions which do not need to prescribe the log-law distribution of the near-wall velocity in an NTH context.
	Implement the improved wall function models in Code_Saturne and OpenFOAM and test them on the benchmark cases.

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	 Write and disseminate a guidance document for heat transfer predictions with RANS CFD using wall models. Define further benchmark cases and their required measurement resolution to improve the validation evidence.
Validation Requirements	The validation requirements are the identified experimental data underlying the set of benchmark cases chosen. It is important that the work moves beyond 'text book' cases of constant heat flux or constant surface temperature to be industrially useful. However, there is a lower probability of finding publically available validation data. High fidelity CFD modelling should be used to form part of the validation, especially in the absence of detailed experimental data.
Output	Improved wall-function models implemented in open source CFD codes. A guidance document detailing the phenomena captured and accuracy that can be expected from the range of wall functions assessed, providing guidance in selecting a model for an NTH application.
Existing Research & Body of Knowledge International Programmes	Ongoing developments at the University of Manchester, which has a long track record on this topic. In the case of low-Re models, this goes beyond the work of Launder and Craft in the 90s on low-Re stress and non-linear models [1] and [2]. There have been subsequent studies on the implementation of non-linear models to recirculating and impinging flows [3], the use of length-scale damping terms in the dissipation rate equation [4] and the use of low-Re models in conjugate heat transfer analysis [5]. On the development of wall functions, two proposed alternatives are currently being developed [6] and [7], neither of which relies on the prescription of near wall velocity, one of which was subsequently extended to rough surfaces [8].
Risks	There are potentially many models to be evaluated and determining what each is capable of resolving and where its limits are may prove hard for some. Knowledge of Code_Saturne and OpenFOAM is needed to implement models, and also more detailed knowledge of the numerical implementation (compared to typical code users) of some aspects of the codes will be necessary.
Timeline and Prerequisites	It is expected that this can be accomplished within 2 years. The findings of this project are likely to be of benefit to projects P7_E and P7_F. This project has strong links with the development of conjugate heat transfer methods in P7_D.
Resource/Costs	0.5 industrial FTE and 1 academic FTE for 2 years. HPC resources required for high fidelity CFD.

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xploitation ecommendations	The development of more accurate and advanced models of near-wall turbulence and their introduction to the open source Code_Saturne and OpenFOAM CFD will maximise the availability of the benefits.
	The production of guidance will lead to their more rapid up-take by industry.

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ANNEX B - WORKSHOP INFORMATION

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B1 Workshop Briefing Pack

The following briefing pack was supplied to all attendees prior to the modelling R&D development workshop.

B.1.1 Introduction

The Department of Business, Energy and Industrial Strategy (BEIS) have tasked Frazer-Nash Consultancy and our partner organisations with delivering the first phase of a programme of nuclear thermal hydraulics research and development.

Phase 1 of the BEIS programme comprises two parts:

- The specification and development of innovative thermal hydraulic modelling methods/tools.
- The specification of a new UK thermal hydraulics test facility.

The work is intended to consider all future reactor technologies including Gen III+, modular light water reactors and advanced modular reactors (Gen IV).

The team carrying out Phase 1 is led by Frazer-Nash Consultancy and comprises: The University of Manchester; The University of Sheffield, EDF Energy R&D Centre UK, Westinghouse Electric Company and The Science and Technology Facilities Council, who have already completed a body of work including:

- A review of the state-of-the-art in nuclear thermal hydraulic modelling;
- The gathering of nuclear thermal hydraulic modelling requirements and challenges; and
- The development of the concept of what constitutes a thermal hydraulic modelling capability to help clarify where R&D activities can contribute.

As part of the development of the thermal hydraulic modelling specification, Frazer-Nash is organising a workshop to understand both the industry "pull" for solutions to known problems and shortfalls, and the Research and Development (R&D) community's "push" of promising areas of research and new development. The workshop will be a collaborative session, structured over two days, and represents a significant opportunity to shape the future direction of research funding in this area. The outputs of the workshop will be used to make recommendations for the specification which will be used as the basis for Phase 2 of the BEIS nuclear thermal hydraulic modelling programme.

B.1.2 Context

This work forms part of the six NIRAB research strands which together form a five-year integrated programme. The long term aims of the programme are:

- By 2020, establish the UK as a partner engaged in collaborative design projects for new reactors (including Generation IV and Small Modular Reactors), building on its existing and growing design expertise.
- By 2030, maturing R&D results in deployment of new plant with significant UK design content and manufactured parts.
- By 2050, R&D has facilitated UK industry to be a significant partner in the global deployment of Gen III+, Gen IV and SMR technologies.

The thermal hydraulics project forms part of the 'Digital Reactor Design' research strand.

The development of a specification for advancing the UK's nuclear thermal hydraulic modelling capability requires knowledge of the UK nuclear industry's reactor technology goals and

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development programme. It is not presently possible to clearly define the complete scope of future activity. Until recently, there had been no significant civil nuclear reactor design or development activities in the UK for many years. The nuclear thermal hydraulic modelling efforts undertaken have been focused on the safe operation of, and providing extended lifetimes for, the existing – mainly gas cooled - reactor fleet. Work on future reactor designs is now underway within a number of organisations and the UK Government has expressed an ambition for the UK to become more involved, as per the 2020, 2030 and 2050 aims.

B.1.3 Capability

Exploring the breadth of what should be considered within a 'nuclear thermal hydraulic modelling capability' is an important step in specifying the research that might support it. The project is focussed around the development of methods and tools. However, it is important not to forget other aspects of 'capability' that are equally important in delivering a solution that is industrially useful and acceptable to regulators.

A representation of a UK nuclear thermal hydraulic modelling capability is presented [in Figure 1].

B.1.4 Workshop Process and Objectives

The workshop will be used to elicit, record and understand the views of a range of stakeholders and subject matter experts in the nuclear thermal hydraulics domain, including you. You will be asked to consider the gaps and difficulties within industry and to extrapolate from the current knowledge and toolset to propose areas of promising research which could be exploited to drive progress and development. The contribution sought will start with the areas where the UK can contribute and where collaboration might add the most value and lead to the definition of research tasks to be undertaken in the next phase of the BEIS programme. The workshop will use discussion groups, guided sessions and structured decision making to prioritise the research challenges, grouped under the topics described in the rest of this document, and recommend projects, based on the benefits that they might bring to the UK's nuclear industry.

Using the input gained from the workshop, Frazer-Nash will produce recommendations and outline plans for research and development programmes. These will form the basis of years three to five of the "Digital Reactor Design - Thermal Hydraulics" programme; future years of the programme will involve developing the individual research strands in more detail. There is likely to be further opportunities for the stakeholders attending the workshop to deliver, contribute to or benefit from the recommended research and development activities.

B.1.5 Nuclear Thermal Hydraulic Research Topics

The number, breadth and scope of thermal hydraulic modelling challenges related to reactor design and operation is extensive. Many of the challenges have existed for a long time and considerable world-wide effort has been dedicated to making improvements. Because it is not possible to cover all potential areas for modelling improvement under the current research programme, and because the UK is not best placed to undertake research in every area of nuclear thermal hydraulic modelling, the following topics have been chosen to frame discussions at the workshop.

These are not intended to be exhaustive, rather they have been identified in the project's work todate as areas which the civil nuclear industry deem important and where the UK could make a valuable research contribution. There is, inevitably, a high degree of potential overlap between the challenges that will be addressed within each area, and so titles and descriptions should not be taken as firm boundaries, only as guidance.

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Multi-fidelity

The use of modelling methods across the full range of fidelities and scales, from DNS to system codes.

There are currently a wide range of thermal hydraulic modelling tools available to the civil nuclear engineer. These are applied at a range of different scales, from the whole reactor to specific components. They are used for different purposes; are aimed at achieving different levels of accuracy; contain different levels of empiricism; and involve a different level of effort and expertise to use.

This topic considers the use of the various different modelling tools available and considers how we can better use the range of tools at our disposal to address the specific challenges of scale and complexity posed by the thermal hydraulics of a nuclear reactor.

Specific areas for discussion could include: the embedding of high fidelity sub-models in lower fidelity methods; the use of high fidelity tools for benchmarking or validation; or the development of tools currently used in a research environment to something appropriate for industry.

The workshop will aim to decide what could be done in the UK to maximise the benefits of an intelligent combination of the range of thermal hydraulic modelling methods at our disposal.

Best Practice and Uncertainty Evaluation

Improving the confidence in and quality of model predictions.

All models are, by definition, an approximation of reality and will always differ from the real world in some respects. It is, therefore, of particular importance to the modelling engineer that they understand the implications of this in their predictions and nowhere is it more important than in a highly regulated industry such as civil nuclear.

Confidence in modelling predictions is developed by a combination of the rigor and consistency of the model developers and users and an understanding of the areas of uncertainty in the underlying tools and the specific analysis. The fast moving pace of model development, the complexity of some of the tools available and the difficulty of experimental validation make this a considerable challenge.

This topic considers how best practice and uncertainty evaluation methods might be further developed and exploited in the UK to expand appropriate and confident use of thermal hydraulic modelling by both industry and regulators.

Specific areas for discussion could include: how to gain confidence in highly flexible tools such as CFD; which modelling approach to choose; uncertainty evaluation at a reasonable cost; or improving understanding of commonly encountered approximations and assumptions.

The workshop will aim to define what the UK can do to enable more confident and informed use of modelling tools.

Boiling and Condensation

The application of and improvement to mechanistic modelling predictions.

Boiling and condensation are key mechanisms in defining the performance of light water reactors either under normal operation (in the case of BWRs) and/or fault conditions. Furthermore, they are of relevance to a wider range of technologies that incorporate a steam cycle secondary circuit. However, modelling these phenomena with confidence remains a challenging area.

This topic considers the challenges of mechanistic modelling of boiling and condensation processes at surfaces and interfaces with particular consideration given to heat transfer.

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Specific areas for discussion could include: The modelling of two-phase flow with CFD; the effects of surface roughness and deposit (e.g. 'CRUD'); the exploitation route for detailed microscopic models to reactor design; or engagement with the international two-phase flow modelling effort.

The workshop will aim to develop some specific research areas where the UK can usefully add value to the considerable international effort.

Large-scale Multi-Phase Flows

The prediction of the effects of complex, transient, multi-phase flows.

Many of the most onerous fault conditions considered within light water reactors are characterised by large scale, complex, transient, multi-phase flows. In the past these have necessarily been handled by means of empirical and often conservative methods. A number of codes exist to enable whole system models to be built of complex scenarios such as a Loss of Coolant Accident (LOCA). However, these are dependent on a large body of empirical data and cannot be reliably extrapolated outside of specific envelopes of operation.

This topic considers what might be done to improve the modelling of bulk, multi-phase flows and the associated heat transfer. Specific areas for discussion could include: heat transfer and pressure changes during 'flashing'; droplet laden flows; dynamic instability; two-phase naturally driven circulation.

The workshop will aim to identify research to move the state-of-the-art forward and promote international collaboration in this area.

Advanced Fluids

The additional challenges of molten metals, molten salts and supercritical water.

As with all tools, modelling methods are developed to achieve what is needed of them at the time of development. Many engineering processes (including existing reactor types) are concerned with the flow of gases, liquid water or steam, and so the majority of tools suitable for thermal hydraulic modelling are most comprehensively developed, validated and applied to these fluids.

For designs of reactors that use fluids other than gas or water as their primary coolant, the atypical material properties of these fluids make the use of readily available modelling methods either more challenging or impossible, as the underlying assumptions of the methods are invalid for the fluids under investigation.

The topic considers how to address the challenges posed by the modelling of the more unusual fluids present in Gen IV reactors; specifically liquid metals, molten salt and supercritical water.

Specific areas for discussion could include: modelling of fluids with Prandtl numbers that are not of order one; fluids with large density variation; free surface effects and gas entrainment; freezing and melting.

The workshop will aim to specify work that the UK can perform to improve the thermal hydraulic modelling toolset available to Gen IV reactor developers.

Multiphysics

The coupling of thermal hydraulics modelling with neutronics and chemistry.

Within a reactor, thermal hydraulic performance is one of many important interdependent aspects, and often has a strong feedback with other processes, such as neutronics. The modelling of interactions between physical processes is often simplified or idealised. This could be via the use of approximate or basic models or using one-way rather than two-way coupling.

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This topic considers the improvements in the prediction of aspects of the reactor performance by the improvement of coupling of thermal hydraulics with other relevant physics.

Specific areas for discussion could include: the challenges of predicting flow/structure interaction; the coupling of thermal hydraulics with neutronics; the coupling of thermal hydraulics with the coolant chemistry.

The workshop will aim to specify research tasks that can be used to draw together well established, but separate, modelling methods and tools, addressing the areas that make their integration challenging.

Turbulent Flow

The prediction of pressure drops, mixing and buoyancy driven circulation.

The prediction of single phase turbulent flow is the most common fluid modelling challenge in all engineering. Despite this, it still remains an area of difficulty, with a broad array of methods for accounting for turbulence available in CFD tools, from RANS approaches to the resolved turbulence LES and DNS methods. Within nuclear reactors the prediction of flow mixing and pressure drops through complex passages is vital for design, operation and plant longevity.

This topic considers the current state of modelling methods for the prediction of turbulent flow and the best ways forward for improving the quality of the predictions that can be made.

Specific areas for discussion could include: the prediction of mixing of flow streams of different temperatures; natural convection flows and stratification; the challenges of predicting flow in large plenums with multiple thermal hydraulic phenomena of importance.

The workshop will aim to specify research tasks that will improve single phase turbulent flow modelling in a nuclear context.

Turbulent Heat Transfer

The prediction of heat transfer and buoyancy influenced convection.

In the environment of a nuclear reactor, the prediction of surface heat transfer is vital for design and demonstrating safe operation. In a similar way to the prediction of turbulent flow in general, the modelling methods for the prediction of surface heat transfer often contain significant empiricism. The uncertainty in this area leads to the need for a large body of experimental data and often significant conservatism to ensure safe reactor operation.

This topic considers the potential for improvement in the methods and tools available for the modelling of heat transfer within turbulent flow.

Specific areas for discussion could include: the prediction of jet impingement heat transfer; thermal striping and drivers for thermal fatigue; improving the accuracy and applicable range of lower fidelity tools; buoyant and mixed convection.

The workshop will aim to specify research to improve the modelling of single phase convective heat transfer in the areas of most importance to nuclear reactors.

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B2 Workshop Agenda

Venue: Level 9, Technology & Innovation Centre, University of Strathclyde

99 George Street, Glasgow, G1 1RD, UK

Day 1 – Tuesday 1	0 April 2018
09:30 to 10:00	Arrival and registration
10:00 to 10:45	Day 1 Plan: Introduction of workshop aims, structure/process and topics
10:45 to 11:00	Break
11:00 to 12:30	Work Session 1 – Exploration of topics and identification of challenges
12:30 to 13:15	Lunch
13:15 to 14:45	Work Session 2 – Detailed investigation of topics and challenges
14:45 to 15:00	Break
15:00 to 16:00	Work Session 2 – continued
16:00 to 16:45	Nuclear Industry timeline discussion: research and development timescales
16:45 to 17:00	Arrangements for dinner and tomorrow
Day 2 – Wednesda	ay 11 April 2018
Day 2 – Wednesda 09:00 to 09:20	Keynote: The current UK nuclear industry context
09:00 to 09:20	Keynote: The current UK nuclear industry context
09:00 to 09:20 09:20 to 09:45	Keynote: The current UK nuclear industry context Day 2 Plan: Developing research activities
09:00 to 09:20 09:20 to 09:45 09:45 to 11:00	Keynote: The current UK nuclear industry context Day 2 Plan: Developing research activities Work Session 3 – Synthesis of potential R&D activities and outcomes
09:00 to 09:20 09:20 to 09:45 09:45 to 11:00 11:00 to 11:15	Keynote: The current UK nuclear industry context Day 2 Plan: Developing research activities Work Session 3 – Synthesis of potential R&D activities and outcomes Break
09:00 to 09:20 09:20 to 09:45 09:45 to 11:00 11:00 to 11:15 11:15 to 12:30	Keynote: The current UK nuclear industry context Day 2 Plan: Developing research activities Work Session 3 – Synthesis of potential R&D activities and outcomes Break Work Session 3 – continued
09:00 to 09:20 09:20 to 09:45 09:45 to 11:00 11:00 to 11:15 11:15 to 12:30 12:30 to 13:15	Keynote: The current UK nuclear industry context Day 2 Plan: Developing research activities Work Session 3 – Synthesis of potential R&D activities and outcomes Break Work Session 3 – continued Lunch
09:00 to 09:20 09:20 to 09:45 09:45 to 11:00 11:00 to 11:15 11:15 to 12:30 12:30 to 13:15 13:15 to 14:30	Keynote: The current UK nuclear industry context Day 2 Plan: Developing research activities Work Session 3 – Synthesis of potential R&D activities and outcomes Break Work Session 3 – continued Lunch Work Session 4 – Definition of recommended activities and plans

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DOCUMENT INFORMATION

Project: Project FORTE - Nuclear Thermal Hydraulics Research & Development

Report Title: Specification Supporting a UK Nuclear Thermal Hydraulic Modelling Capability

Client: Department for Business, Energy and Industrial Strategy (BEIS)

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G. Macpherson

Issue No.: 1 D. McNaught

Date: May 2019 Approved By: R. Underhill

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