Project FORTE - Nuclear Thermal Hydraulics Research & Development

Critical Review of State-of-the-Art Thermal Hydraulic Prediction Capability

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FRAZER-NASH CONSULTANCY

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:

FRAZER-NASH CONSULTANCY

The University Of Sheffield.

EDF ENERGY

Westinghouse

MANCHESTER 1824
The University of Manchester

Science & Technology Facilities Council

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

Executive Summary

Nuclear Thermal-hydraulics (NTH) is a key element of Nuclear Power Plant (NPP) design and safety. It is the study of engineering systems where energy from nuclear fuel is transferred by a coolant to a power generation turbine or to the environment, by heat transfer, phase change and flow processes.

Computational modelling of NTH is already a vital part of both the design and safety substantiation of modern NPP. State-of-the-art NTH modelling tools have the potential to enable a level of design and operational optimisation for future NPP beyond anything seen in the past, delivering both improved safety and economic benefits.

NTH shares modelling challenges and tools with many industries where fluid dynamics is important, but perhaps uniquely, has to deal with all of them simultaneously on a huge range of geometrical scales. Moreover, practical NTH computer codes cannot be completely based on first principles, so incomplete knowledge results in uncertainties that must be rigorously quantified and mitigated.

This review highlights a selection of underlying phenomena most important to NPP, including: turbulence; heat transfer; bubble and droplet thermodynamics and transport; flow induced vibration; surface effects and ageing of structures, together with the multiscale aspects linking of all the above. Current practice and procedures by designers, regulators and utilities are outlined, including consideration of uncertainty management and the challenges of scaling from experiments. Classical ‘whole system’ tools are briefly summarised followed by more detailed discussion on finer grained modelling by 3D Computational Fluid Dynamics (CFD). This review also includes sections summarising emergent technology and international benchmarks and projects.

This review found that, thanks to the exponential growth of computing power, previously unexploitable methods are shown to now be applicable to the research of real NPP components. For example, Direct Numerical Simulation (solving first principles equations avoiding any modelling approximations) is set to complement (and in some cases replace) experiments. This change in frame-of-mind and basic philosophy is supported by many experts and particularly by the US Department of Energy. “Conservative” safety margins can now be re-evaluated and placed in more likely accident scenarios with “best estimate plus uncertainty methods”. Raw computer power combined with mathematical advances have accelerated changes in risk management and decision making methods. This places additional complexity on top of existing complex processes, but “machine learning”, an established branch of Artificial Intelligence, can alleviate this, and is already being used to assist in turbulence modelling.

After 50 years of research and technology progress, NPP design and safety challenges still remain great enough that it is tempting to conclude that it is impossible or unreasonable to foresee major modernisation to the empirical and conservative methodology used in the industry. There is, however, a surprising extent of worldwide openness and collaboration (in open-source codes, forums and documentation), as well as improving ease of use of all kinds of mature software. Progress is accelerating at an ever increasing rate, perhaps reaching a “singularity” in technology progress speed, and now is the perfect time for the UK to invest to gain the full advantage of these advances. The UK was historically, and still is, well placed to harness a combination of engineers, mathematicians and computer power to tackle the hardest thermal hydraulic problems.

Preface

This review was assembled by academics at the Universities of Manchester and Sheffield, some of whom have up to 50 years' experience of continuous research in Nuclear Power Plant (NPP) flows. This is mostly related to refined modelling of turbulence, in collaboration with the likes of CEGB, EDF R&D, and more recently British Energy, EDF Energy, National Nuclear Laboratories, BNFL and Rolls-Royce. Nevertheless, the breadth of the prediction methodologies employed in nuclear thermal hydraulics proved a challenge even to our collective expertise. Even while limiting the search to the recent decade, an assessment of the online literature led to thousands of papers, as well as to mention thousands of documents from regulators and organisations more directly involved in tools for NPP design; US NRC, DOE and Nuclear related National Labs, OECD Nuclear Energy Agency and others.

While completing this review we discovered fresh books, reviews and action plans compiled by hundreds of international experts. The four below are essential vis-à-vis this project's objectives:

1. **Thermal Hydraulics in Water-Cooled Nuclear Reactors**, D'Auria, F.
2. **Grand Challenges of Advanced Computing for Energy Innovation Report**, Larzelere, A. et al. (2013). Technical Report, Pacific Northwest National Lab, Richland, WA.
3. **Handbook of Uncertainty Quantification**, Ghanem, R. et al. (Eds.), 2017.
4. **Scaling in System Thermal-Hydraulic Applications to Nuclear Reactor Safety and Design: A State-of-the-Art Report**, Bestion, D., D'Auria, F., Lien, P., Nakamura, H., 2016. Report (No. NEA/CSNI/R(2016)14). OECD-NEA.

The 2017 book on thermal hydraulics (D'Auria, 2017) in NPP by 14 world-leading senior experts with life-long careers in Thermal Hydraulics (TH) in conventional NPP, covers almost all aspects of our intended review. The extent of the task is best expressed in D'Auria's preface:

"This implies the consideration of a universe of topics which may need an encyclopaedia rather than a book. So, …[only] a window is opened"

"Thermal-hydraulic phenomena identification and characterisation, code development and validation, as well as scaling demonstration and prediction of errors of code calculations, i.e., uncertainty evaluation, may appear a matter for guru: rigorous procedures are not always applied or simply do not exist. This is also a consequence of some inadequate modelling of aspects in nature, behaviours like turbulence, and bubble motion and coalescence"

"The grown expertise, sometimes of guru-type, is going to be lost because of retirement of top scientists acting during the golden period,…the enormous research investment 1970-2000."

"The Book may resemble a description of a dynamic target rather than an archival product."

The 'silver lining' we discovered through this review exercise is that the "moving target" is in fact accelerating at an increasing pace! The computer power available at the beginning of our career has increased a million times and Artificial Intelligence (AI) is transforming all areas of engineering, from driverless cars to machine learning design of NPP. The US Department of Energy (Larzelere et al., 2013) "has no doubt" that safer, more efficient, NPP will be conceived through Nuclear Energy Advanced Modelling and Simulation (NEAMS), from "first principles simulations" to Uncertainty Quantification (UQ).

UQ (Ghanem et al., 2017a) in support of risk management and decision making has also progressed incredibly fast and is producing reliable and probability framed predictions to replace the "conservative" approach (a worst case single result plus a guessed safety margin) used for licensing, which has possibly ill-directed technical focus and introduced excessively costly safety measures. UQ is now applicable to very complex systems thanks to the combined efforts of mathematicians and physicists embracing full statistical approaches, but it is again thanks to the brute force of today's computers enabling 100's of simulations with Monte-Carlo inputs for each case, compared to the past where we used to produce just one solution.

The following review is inevitably incomplete and uneven. We give more details on issues that we are more familiar with and are relevant to plant operators, such as life extension, conjugate heat transfer and 3D CFD turbulent simulations of flow around fuel pins and heat exchangers. The areas less well covered here, such as historic developments, severe accidents and licensing, 1D systems' codes and experiments are well presented in the TH in water cooled nuclear reactors book (D'Auria, 2017). Its subject index is essential for any reader wishing more details, for example, on the 100's of concepts and phenomena we could only introduce herein. We also only briefly comment on the monumental cataloguing, evaluation and exploitation work by the OECD Nuclear Energy Agency on 100's of separate and integral test facilities which they revisited in the recent report on Scaling (Bestion et al., 2016a).

Another encouraging revelation from this review is the open dissemination and world-wide collaboration around TH for NPP, perhaps as a response to public wariness and subsequent pressure on decision makers. This openness should help acceptance of modern tools and UQ for NPP design and will likely also help the UK to be accepted into areas where we have not been active for some time.

Lead Author:

Professor D. Laurence	The University of Manchester

Authors:

Professor H. Iacovides	The University of Manchester
Dr T. Craft	The University of Manchester
Dr D. Wilson	The University of Manchester
Dr A. Cioncolini	The University of Manchester
Dr C. Moulinec	Science and Technology Facilities Council
Professor S. He	The University of Sheffield
Dr B. Liu	The University of Sheffield

Editors:

R. Underhill	Frazer-Nash Consultancy Ltd
Dr G. Macpherson	Frazer-Nash Consultancy Ltd
C. Howlett	Frazer-Nash Consultancy Ltd

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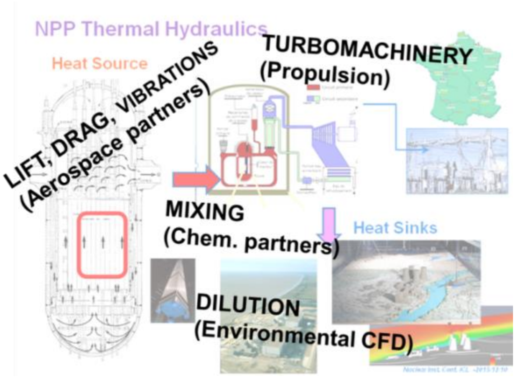

Thermal Hydraulics (TH) modelling for Nuclear Power Plants (NPP) is daunting as it encompasses almost all fields of Fluid Mechanics, but benefits from research progress that is driven and funded through many application areas such as aerospace, turbomachinery, chemical engineering, and environmental flows. To name a few baseline examples:

- Lift-drag-vibrations: the fixed flowrate through fuel cooling passages or across boiler tubes must be kept high enough to extract the heat released yet below a threshold where lift forces might retard the fall of control rods or increase vibrations of the very long and thin fuel rods or exchanger tubes.
- Turbulent Mixing: in hot-cold T-Junctions, downcomer, boron dilution, hydrogen/air concentration, atmospheric dispersion. These are all applications in which turbulent mixing controls the turbulent diffusion of mass, chemical concentration, momentum and thermal energy, all of which can be critical to the performance of reactor components.
- Rotating flows: strongly affecting turbulence in turbines, pumps, cyclone separators, but also in pipe bends or T-Junctions followed by persistent swirling motion as in “wing tip vortices”.
- Buoyancy: as in cold source dilution (river, hot water discharges and cooling tower plumes) borrowing and coupling methods from coastal / atmospheric modelling, but also cold fluid traps in e.g. lower U-Shaped pipes during transients. Horizontal stratified flows severely damp turbulent mixing. Horizontal penetrations provide another example of a reactor space where buoyancy can generate unstable flow and thermal fluctuations. Less obviously, buoyancy aided vertical flows, as in passive safety also impair heat transfer.

Perhaps no other sector tackles such a wide range of even baseline turbulent flows and this is without even mentioning the challenges of two-phase flows in many flavours: droplets, bubbles, nucleate boiling, film boiling, annular boiling in internal passages etc.

In addition, multidisciplinary issues are now attracting a lot of interest. These include fluid-solid interactions, conjugate heat transfer, deposition, corrosion, embrittlement, weld and materials ageing that need to be accounted for in the design of a near century-long investment; from planning, build, 60 years amortisement to decommissioning.

Severe accident management outside of the reactor is not even considered herein. Some consider that it “is so complex that it is always unpredictable to some extent. Instead, one should design systems that are not at all likely to lead to severe accidents and put the effort toward eliminating severe accidents rather than understanding, computing, analysing, managing, and/or mitigating them” (Yadigaroglu and Lakehal, 2016).

1.1 Objective

The main objective of this review is to produce an assessment of the capabilities of current prediction methods of thermal hydraulics phenomena relevant to nuclear power plants. This includes identifying the contributions these methods currently make to nuclear reactor design and innovation, their current levels of reliability across the range of thermal hydraulics phenomena present in nuclear power plants and the topics in which further development is most essential.

In order to achieve these objectives, we start by presenting the thermal hydraulics phenomena relevant to existing and proposed designs, we then review current practices in nuclear thermal hydraulics, the most widely used modelling packages, and the available resources. The detailed review of current prediction methodologies across a range of thermal hydraulics phenomena relevant to nuclear power plants is then followed by a look at emerging methodologies and explore their potential.

The above enable us to finally reach conclusions and recommendations for future research and development.

1.2 Report Structure

This review covers the following areas:

- Thermal hydraulic phenomena relevant to existing and advanced designs (Section 2);
- Practices (Section 3) and current (Section 4) and developing (Section 5) simulation and modelling employed by the industry and regulators;
- Emerging disruptive technologies and innovative advanced models being tested and used in a research environment (Section 6);
- Verification and Validation (V&V) resources, databases and outputs from national and international projects (Section 7);
- Outputs from international consortia and projects (Section 8).

2 Thermal-Hydraulic Challenges

The design and safe operation of nuclear power plants presents a number of signficant thermal hydraulic modelling challenges, often involving a combination of complex and interacting phenomena.

The level of understanding of these challenges and the phenomena involved varies with the level of maturity of the plant technology and the length of time for which development has occurred. For example, for the continuously developed, mature Light Water Reactor (LWR) technologies, the NEA's Committee on Safety of Nuclear Installations (CSNI) has produced test matrices for Separate Effect Tests (SET) and Integral Effect Tests (IET) and listed the thermal-hydraulic phenomena that they have categorised. The CSNI document also provides a wide and high level general description of the types of phenomena and physics that need to be modelled to capture the effects accurately.

> 'Separate Effects Test Matrix for Thermal-Hydraulic Code Validation: Volume 1 Phenomena Characterisation and selection of facilities and tests (OECD/NEA, 1994)'

This 680-page report on SET matrices classifies 67 thermal hydraulic phenomena providing a cross-reference to 2,094 experimental tests from 187 test facilities (1973-1993) in the LWR safety thermal hydraulics field. Some of the TH phenomena identified are basic fluid mechanics phenomena within a large range of useful parameters, for example: fluid to wall friction, heat transfer and critical flow, stratification in horizontal flow and phase separation in vertical flow. Other listed phenomena are more specific to LWR components or regimes such as: pressure drop at geometrical singularities, phase separation at branches, entrainment/de-entrainment, liquid-vapour mixing with condensation, condensation in stratified conditions, spray effects, counter-current flow, heat transfer and global multi-dimensional fluid temperature void and flow distribution.

CSNI also produced expert panel's evaluation of reports on:

- Separate effect tests[1] (SET) (Aksan et al., 1996);
- Integral Test Facility Validation[2] (Glaeser et al., 1996);
- Scaling[3] (Bestion et al., 2016a).

CSNI's SET database has been valuable in collecting best sets of open data for code validation on isolated components or physical phenomena. It recognised the value of exact computation of partial differential conservation equations and also provided a sound view of the nature of two types of correlation coefficients: the more naturally empirical coefficients such as friction and the ones due to the necessity (with limited computing power at the time) to introduce space and time averaging. This led to the need to empirically set "coefficients that appear as the ratio of the averages of products divided by products of averages" e.g. for turbulence or two-phase flow mixtures since microscales could not be resolved. Paul Durbin wittily summarised mitigation for similar loss of information through averaging non-linear equations as: "a model coefficient is the ratio of what you wanted to what you get" (about earlier near wall turbulence damping functions).

For NPP other than those employing light water as a coolant, the data available for validation and the understanding of the phenomena is less widespread. In other technologies most of the modelling challenges associated with Generation I and II gas cooled reactors remain, e.g.

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[1] https://www.oecd-nea.org/nsd/docs/1996/csni-r1996-16.pdf
[2] https://www.oecd-nea.org/nsd/docs/1996/csni-r1996-17.pdf
[3] https://www.oecd-nea.org/nsd/docs/2016/csni-r2016-14.pdf

turbulence, or even exacerbated as when natural convection (buoyancy) is replacing fixed flowrate pumps, others such as two-phase flows may be alleviated.

Far from being encyclopaedic, but with tools for design of future plants in mind, a selection of the most important thermal-hydraulic challenges seen in nuclear reactors are introduced below and revisited throughout the report in the context of specific modelling methods and tools.

2.1 Natural Convection

Natural convection is a mechanism of heat transfer where the motion of the fluid is driven by density differences (resulting in buoyancy forces) occurring due to temperature gradients. Natural convection, stratification (where the buoyant forces act to maintain temperature gradients) and mixed convection (where buoyancy influences fluid already in motion) are ubiquitous in Generation II and III reactor thermal hydraulics: cold trap transients in U-bends, severe accident conditions, hydrogen build-up in the reactor building, in vessel retention. All of these are also key to passive safety in Generation III+ and Generation IV reactor design and yet remain very challenging to model.

A vertical heated pipe is the simplest and most well documented example to illustrate the modelling challenge. Figure 1 compares the variation in the prediction of wall heat flux with increasing buoyancy for different modelling tools. Increasing buoyancy forces lead to the collapse of the turbulent activity which manifests as a sudden drop in the heat flux.

When the near wall layer is accelerated by buoyancy, the high velocity gradient region is pushed closer to the wall and, as a result, turbulence production due to velocity shear is restrained by wall proximity. Eventually, for a certain range of buoyancy parameter values, the flow re-laminarises. It is difficult for many modelling methods to account for interaction between the actual turbulence length-scale (size of large eddies), and the non-local turbulence damping influence of a solid wall. For example, the commonly used ‘k-omega’ Reynolds-Averaged Navier-Stokes (RANS) turbulence models (discussed further in Section 5.3.1) misses the collapse entirely. Only the most sophisticated turbulence models are capable of capturing this effect and therefore correctly predicting the resulting heat transfer.

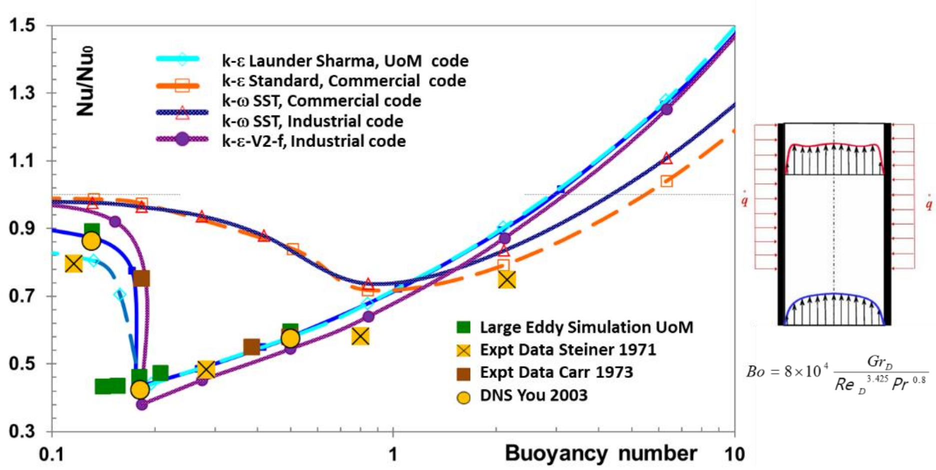


Figure 1: Vertical heated pipe heat transfer collapse: Nusselt number drops suddenly along with turbulent intensity (see Figure 17) as near wall flow accelerates in high buoyancy cases 0.1 < Bo < 1

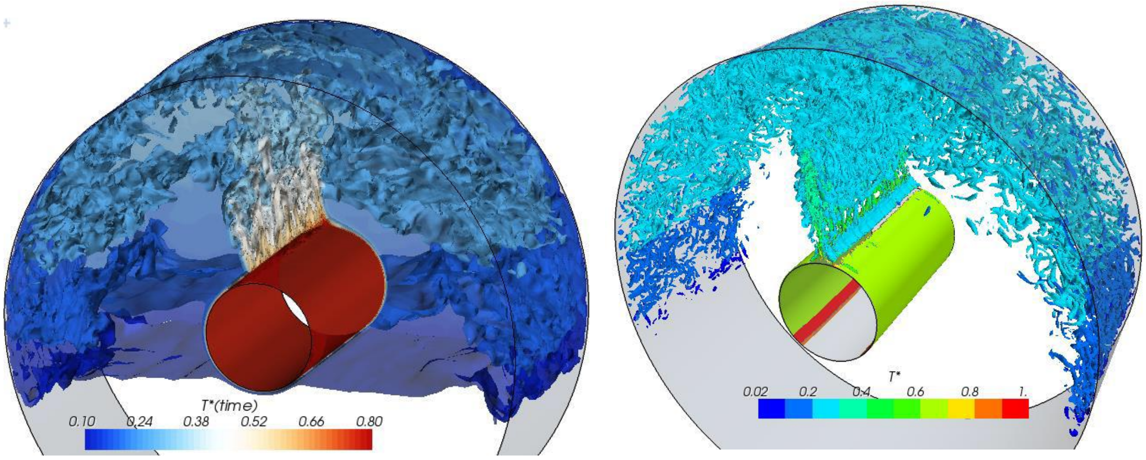


Figure 2: AGR feeder line stratification (Addad et al., 2015)

Buoyancy driven flows even in simple cavities bounded by co-axial horizontal cylinders present a more complex example. In Advanced Gas Reactors (AGR) for instance, there can be 'thermosyphons' in the penetrations running horizontally through the thickness of the Reactor Pressure Vessel (RPV), or in the spent fuel transfer cask neutron shields. There are complex flow patterns inside the annuli, the coexistence of turbulent and stagnation regions and a wide range of time scales, from boundary layer heat transfer to global cavity thermal equilibrium. Significant modelling challenges arise due to the geometry curvature and the impingement of the hot fluid on the walls as visible in Figure 2.

Research groups at the University of Manchester and EDF Energy in the UK (previously CEGB or British Energy) and in France have collaborated over 3-4 decades on the modelling of these buoyant cavity flows, i.e. entire careers of some authors of this report. Work was initially with simple rectangular cavity experiments, which are still challenging to model, producing well recognised databases *(*such as the ERCOFTAC database discussed later*)* for rectangular cavities (Boudjemadi et al., 1997) and some more complex flows such as a negatively buoyant jet (Addad et al., 2004). They extended the low Rayleigh number experimental data for the coaxial cavity using advanced modelling techniques such as fine Large Eddy Simulation (LES) (Addad et al., 2006) and recently Direct Numerical Simulation (DNS) (Addad et al., 2015) which remove most of or all (respectively) turbulence modelling hypotheses.

Readers unfamiliar with the turbulence models employed in CFD and their associated abbreviations may first browse Section 5.3.

Natural convection at NPP scales is among the most difficult single phase flows to model, it is therefore worth detailing further. Lab-scale dimensions and temperature differences of physical and then later DNS studies were limited to the lower Rayleigh number range ($10^4 < Ra < 10^9$). As Ra is roughly the square of the Reynolds number, Re varied between a few hundreds to a few thousands, i.e. onset of the laminar to turbulent transition. There is a wealth of environmental data available, but that is at the other (high) Ra-range extreme and does not provide the fluid to smooth-solid-wall heat transfer information needed. The RANS route was initially favoured in view of the slow and long transients that make the LES approach a four-dimensional multiscale problem, however, fine experimental data is very scarce for RANS validation. Measuring turbulent heat flux, i.e. the correlation between fluctuating velocity and temperature at the same location, was found to be all but impossible without large filtering and flow perturbation errors. It is now worth revisiting with modern non-intrusive data acquisition techniques.

Part of the validation problem also arises from the time taken to reach steady conditions. A laboratory experiment, of only 50 cm, with a cavity heated and cooled on opposite sides needs to be left running for hours before the turbulent contribution is established and mean temperatures stabilise. Starting from isothermal state there is no motion and only molecular diffusion slowly develops thin temperature gradients very near the thermally active walls. To reach fully developed state the following physical processes must take place:

1. Velocity gradients away from the wall need to be developed.
2. The resulting shear generates turbulence.
3. Turbulent mixing then enhances heat fluxes.
4. Increased wall heat transfer leads to faster development of temperature gradients.
5. The resulting stronger buoyancy forces away from the wall enhance velocity gradients which leads back to 1.

Only then does the coupling process speed up, through turbulence and wall layer renewal, as characterised by the Nusselt number typically of order 100. This is only at mean velocity and temperature level. There are further anisotropic convoluted coupling effects between Reynolds stresses, heat fluxes and turbulent kinetic energy and temperature fluctuation variance. As vertical temperature differences develop in the cavity, core stratification damps turbulence, slowing down the stabilisation of the temperature profile in the cavity but also allowing secondary natural convection cells and gravity waves to appear both with timescales ten thousand times larger than that of the boundary layer turbulence.

The DNS analysis of the AGR cavity in Figure 2 needed a millisecond fixed time-step to capture the small physical time scales and the simulation could only run for a physical duration of a minute, probably too short for gravity waves which are certainly most important for the ageing of the external steel casing and concrete, not to mention the transient regimes, which are totally out of reach of DNS.

The complexity of the phenomena involved in predicting heat transfer due to natural convection results in the use of empirical correlations by most industrial engineers. However, many currently used empirical methods are based entirely on experiments relating to specific geometries and quickly become inaccurate when applied more widely. This, in combination with the importance of this area to both current and future NPP designs, emphasises the potential benefits of improved prediction methods. The accurate prediction of the turbulent mixing is key for success and the modelling of turbulence using CFD is discussed further in Section 5.3. Advanced CFD methods have demonstrated that considerable improvement is possible, but the modelling of natural convection is still an area requiring development to realise the benefits of advanced methods. This is certainly an archetype of nuclear thermal hydraulics problems needing a joint physical and first principles simulation approach.

2.2 Conjugate Heat Transfer

The term ‘conjugate heat transfer’ is used to describe the combination of heat transfer within both fluids and solids where there is thermal interaction between them. The ability to predict the variation in the temperatures of solid components as a result of heating or cooling by a fluid is important in all NPP technologies. For example, materials scientists could use this information to assess whether a component will fail through high-cycle fatigue crack growth. Enhanced understanding of these issues will help design long life NPP which was essential for amortisation of classic plants and of course now mandatory for SMR’s to be loaded once and buried underground.

As mentioned in the TEE Junction problem considered later in Section 2.12.2, extending a CFD simulation to include temperatures inside solid walls is easy but there is no detailed validation data. It suffices to solve the same equation as in the fluid while setting the convective velocity and turbulence generation to zero. Alternatively the CFD code can be coupled to a structures code. Applied studies have so far only considered mean temperatures, with few extensions to predict fluctuating temperatures inside the solid.

Study of conjugate heat transfer including solid temperature (and subsequently stress) fluctuations using first principles DNS is very recent but promising. Figure 3 shows attenuation of small scale instantaneous temperature fluctuations at a TEE junction (Wu et al., 2017) while larger scale ones are traversing the wall.

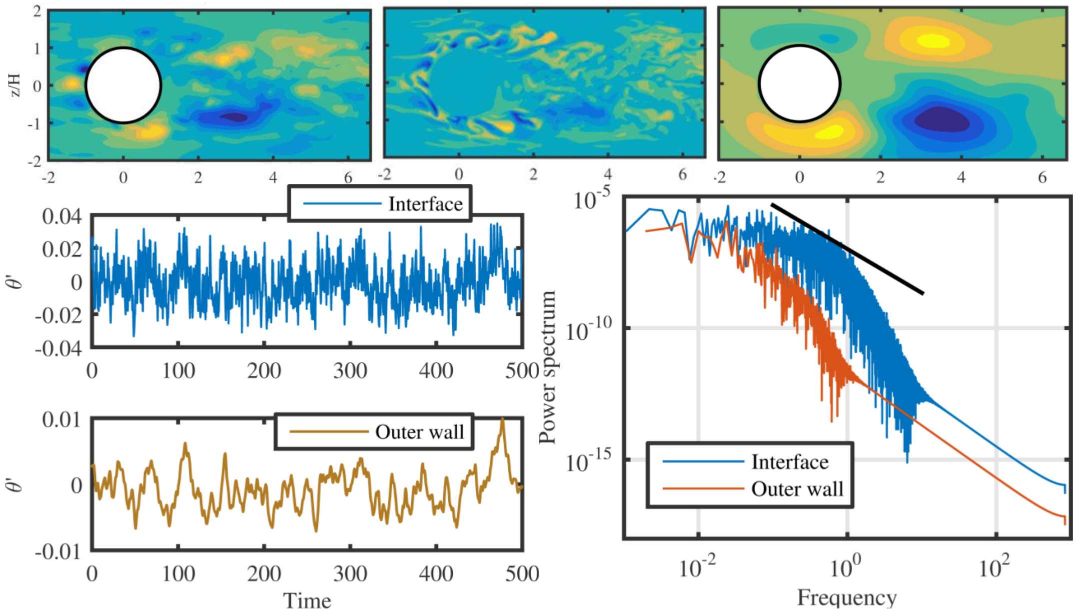


Figure 3: Instantaneous temperature fluctuations above and below a TEE junction
Top left in the fluid near wall layer ($y = +0.05$)
Top middle: on the fluid-solid interface ($y = 0$)
Top right: inside the solid wall ($y = -0.5$)
Bottom: time series and spectrum of temperature fluctuations

2.3 Turbulence

The term 'turbulence' is used to describe the chaotic variations in pressure and velocity that occur in fluids where the kinetic energy of the flow overcomes the fluid's viscous damping. In general terms it is the presence of unsteady vortices of a variety of scales which interact with each other changing important overall flow characteristics such as the drag and heat transfer.

The importance of the modelling of turbulence is therefore certainly not limited to nuclear thermal hydraulics. Much, although by no means all, turbulence model development over the past two decades has been primarily sponsored by the aerospace sector, with lift and drag forces, near-wall modelling and flow separation playing major roles. While much of this work is also relevant to thermal hydraulics, there are often further challenges to consider, including heat transfer and buoyancy effects, and the fact that, in closed circuit applications, the details of flow downstream of bluff bodies must be correctly captured (whereas for single aerodynamic body structures the far downstream behaviour is often not so crucial).

Thermal hydraulics problems frequently involve natural or mixed convection; adequately representing this requires not only accurate modelling of the near-wall flow and heat transfer processes, but also the subtle interactions between the buoyancy forces and turbulence structures and statistics in both the near-wall and outer flow regions. Many such flows can also be statistically unsteady, posing a further challenge for turbulence models.

Buoyancy influences on turbulence are typically very anisotropic in nature, and at the modelling level this means that schemes are required to adequately capture the interactions between the various Reynolds stress and turbulent heat flux components. Many of the simpler models that rely mainly on predicting the correct shear stress response to mean flow behaviour can fail in such flow situations, as can the simpler gradient diffusion representations for turbulent heat fluxes. Whilst more complex models, including full stress transport models, have been shown to perform more reliably in many buoyancy-dominated flows, their take-up in general purpose CFD codes has been rather limited often due to the perceived higher costs and longer timescales associated with both building and running the models.

A further challenge in many turbulent thermal hydraulics problems is the modelling of the near-wall flow layers, which are often crucial to accurate predictions because of their importance in heat transfer processes. Resolving these thin layers with very fine grids, and turbulence models designed to account for near-wall effects where turbulent eddies become very small and momentum or temperature mixing occurs on molecular scales increases computational costs drastically (both in RANS and LES modelling approaches, see Section 5.3). Alternatives such as “wall-functions” which bridge the viscous sub-layer thanks to correlations are widely-used, but most of the standard forms of these are based around log-law representations which are rarely appropriate for strongly buoyancy-influenced flows. More advanced forms of wall-functions have been developed, and applied with some success, although there is clear scope for further development and application to allow both advanced RANS and LES modelling approaches to be used in very large and complex industrial applications at a reasonable computational cost. A detailed discussion of the modelling of turbulence use in CFD methods is given in Section 5.3.

2.4 Turbulent Heat Transfer

The prediction of turbulent heat transfer within fluids and between fluids and solid surfaces is amongst the most important of all modelling challenges to both NPP design and safe operation. For most industrial applications relating to NPP this means turbulent heat transfer.

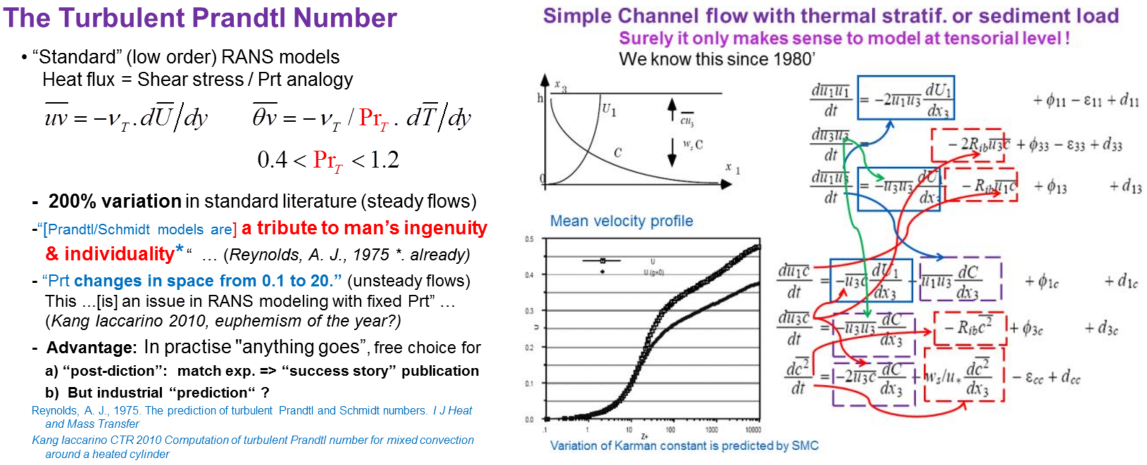
In lower fidelity modelling codes (such as the system codes described in Section 4) the overall heat transfer between fluid and solid walls is prescribed via solution specific empirical correlations. In most higher fidelity methods (i.e. classic CFD), this heat transfer is predicted by solving the energy equation together with the momentum equations with a user specified ‘turbulent Prandtl number’, the constant introduced to model the ratio between turbulent viscosity and turbulent thermal conductivity in effective-viscosity models.

The fact that a 30% variation of this turbulent Prandtl number (Pr_t) between 0.7 and 1.0, is widely accepted is perhaps by analogy to large changes of the molecular Prandtl number (the viscosity to diffusivity ratio) with temperature and type of fluid. There is no relation, however, between fluid properties and turbulent flow characteristics at high Reynolds numbers and leaving the choice of Pr_t up to the user’s whims or default code value is one of the weakest links in CFD thermal hydraulics predictions.

Unlike in pure aerodynamics, which is dominated by the exact pressure-inertia balance, while turbulent effects are weaker, temperatures depend only on convection and turbulent heat flux balance and thus predictions are much more sensitive firstly to the kinematic turbulence model chosen and secondly to how it is extended to heat fluxes. Much larger differences are observed in temperatures between simulations as a result of user choices which explain the wariness of decision makers in NPP thermal hydraulics compared to aerospace. This is in part due to the historic turbulent Prandtl number "fallacy":

> *'The Reynolds analogy leads to assuming that the ratio of turbulent momentum transfer over turbulent heat transfer is constant, in space and across applications and that this turbulent Prandtl number can be prescribed a priori by the savvy CFD user, or worse, by the code default value.'*

Already in 1975, Reynolds (1975) asserted that this approach "is almost certainly inadequate… the roles of intensity and of position within the flow must be separately accounted for", and this even for passive simple shear flows where the single mean temperature gradient and mean flow velocity gradient are aligned (e.g. boundary layers and jets). He tagged the 30 analytical models already on offer "a tribute to man's ingenuity and individuality" and accurately predicted that rapid progress was unlikely.



The Turbulent Prandtl Number

- "Standard" (low order) RANS models
  Heat flux = Shear stress / Prt analogy

$$\overline{uv} = -\nu_T . d\overline{U}/dy \qquad \overline{\theta v} = -\nu_T / \Pr_T . d\overline{T}/dy$$

$$0.4 < \Pr_T < 1.2$$

- **200% variation** in standard literature (steady flows)
- "[Prandtl/Schmidt models are] **a tribute to man's ingenuity & individuality***" … *(Reynolds, A. J., 1975 *. already)*
- "Prt **changes in space from 0.1 to 20.**" (unsteady flows)
  This …[is] an issue in RANS modeling with fixed Prt" …
  (Kang Iaccarino 2010, euphemism of the year?)
- **Advantage:** In practise "anything goes", free choice for
  - **a) "post-diction": match exp. => "success story" publication**
  - **b) But industrial "prediction" ?**

Reynolds, A. J., 1975. The prediction of turbulent Prandtl and Schmidt numbers. *I J Heat and Mass Transfer*

Kang Iaccarino CTR 2010 Computation of turbulent Prandtl number for mixed convection around a heated cylinder

Simple Channel flow with thermal stratif. or sediment load

Surely it only makes sense to model at tensorial level !

We know this since 1980'

$$\frac{d\overline{u_1u_1}}{dt} = \boxed{-2\overline{u_1u_3}\frac{dU_1}{dx_3}} + \phi_{11} - \varepsilon_{11} + d_{11}$$

$$\frac{d\overline{u_3u_3}}{dt} = \boxed{-2R_{ib}\overline{u_3c}} + \phi_{33} - \varepsilon_{33} + d_{33}$$

$$\frac{d\overline{u_1u_3}}{dt} = \boxed{-\overline{u_3u_3}\frac{dU_1}{dx_3}} \boxed{-R_{ib}\overline{u_1c}} + \phi_{13} + d_{13}$$

$$\frac{d\overline{u_1c}}{dt} = \boxed{-\overline{u_3c}\frac{dU_1}{dx_3}} - \boxed{\overline{u_1u_3}\frac{dC}{dx_3}} + \phi_{1c} + d_{1c}$$

$$\frac{d\overline{u_3c}}{dt} = \boxed{-\overline{u_3u_3}\frac{dC}{dx_3}} \boxed{-R_{ib}\overline{c^2}} + \phi_{3c} + d_{3c}$$

$$\frac{d\overline{c^2}}{dt} = \boxed{-2\overline{u_3c}\frac{dC}{dx_3}} + \boxed{w_s/u_*\frac{d\overline{c^2}}{dx_3}} - \varepsilon_{cc} + d_{cc}$$

Mean velocity profile

Variation of Karman constant is predicted by SMC

Figure 4: Turbulent Prandtl number fallacy
Slide on right shows in red effect of adding buoyancy to the tensorial Re stress and heat flux coupling for a simple 1D shear flow. These production terms are exact at second moment closure level.

It is disappointing that years later most applied thermal hydraulics studies are still based on a user prescribed turbulent Prandtl number despite the availability of entire books devoted to more general second moment closures (Hanjalić and Launder, 2011). As major CFD codes now start to seriously incorporate these there is at last hope they might be used, protracted certainly by the complexity of the theory of second moment closures where all six turbulent stresses and three heat fluxes are kept as independently computed variables (Figure 4 and Section 5.3.1.3).

It is easy to see that it is already a dramatic over-simplification to reduce these nine fundamental stresses and fluxes to just two scalars (an eddy viscosity forcing alignment of the stress tensor on the velocity gradient and an eddy diffusivity aligning the heat or concentration fluxes on the mean gradient). In Figure 4 right, the blue boxed terms are exact gradient production terms with arrows pointing to the tensorial level coupling. Red boxes indicate the additional production terms introduced by buoyancy effects. The introduction of the turbulent Prandtl number to define the eddy diffusivity as a rescaled eddy viscosity (left of Figure 4) is another drastic simplification. Its value or choice of correlation (“a tribute to man’s ingenuity and individuality”) is left to the whims of the CFD user.

The more advanced turbulence modelling methods that do not require the user-specification of a turbulent Prandtl number have been developed over decades, but are very seldom used in NPP TH studies due to the complexity of the theory and lack of fine enough validation data in this context. Recent breakthroughs in machine learning (Section 6.4) might resolve these issues regarding second moment closures. In the LES context, the so called “dynamic sub-grid-scale modelling” approach whereby the modelling of small scale turbulence is improved by observing interactions at slightly larger scales, while the simulation progresses in time, might already be considered as machine learning.

2.5 Two-Phase flow and Phase Change

The term two-phase flow refers to a mixture of a liquid and a gas or a vapour that flows simultaneously through a channel, and is a particular example of a multi-phase flow. These flows, or indeed those which are expected to undergo a change of phase, pose a serious challenge for numerical modelling owing to their increased complexity over their single-phase counterparts. The primary complication arises from the existence of discernible interfacial, or boundary, regions which separate the phases. As well as the challenge of how to actually represent the interface region in a numerical sense, the interfaces undergo continual topological change whilst simultaneously facilitating the exchange of mass, momentum and energy between the phases. This two-way coupling between the fields of the phases is one of the most difficult aspects of multi-phase flows to model.

Two-phase flows feature extensively within the context of nuclear thermal hydraulics and are expected to be present both during normal operations and off-design conditions. The most obvious occurrence of on-design two-phase flow is the process of boiling within the core of a Boiling Water Reactor (BWR), but subcooled nucleate boiling also usually occurs inside the top-third of a Pressurised Water Reactor (PWR) core (D’Auria, 2017). It is also relevant to LWRs under various fault conditions when, aside from the potential for significant vapour generation in the fuel channels, vapour bubbles in water, droplets in steam or other flow regimes in between may occur anywhere within the reactor.

Even in geometries limited to simple channels, two-phase flows exhibit a variety of flow regimes, or flow patterns, dependent on the relative concentration of the two phases, the total mass flow rate, the operating pressure and flow geometry of the channel. These range from *separated flows*, where the two-phases are almost entirely separated by a large interface, to *dispersed flows*, where one phase consists of discrete elements (such as bubbles or droplets) and those flows which are in a transition between the two. General types of two-phase flow (Figure 5) are described in Ishii and Hibiki (2011), but those of particular relevance to nuclear applications are:

- **Bubbly flow:** characterised by a continuous liquid phase with dispersed vapour bubbles, where the bubbles are notably smaller that the channel diameter;
- **Slug flow:** the vapour is concentrated in elongated bubbles whose diameter approaches that of the channel, interspersed by liquid slugs;
- **Annular flow:** a continuous liquid film flows along the channel wall surrounding a central vapour core that may carry entrained liquid droplets in suspension;
- **Mist flow:** characterised by a continuous vapour phase with dispersed liquid droplets in suspension;
- **Inverted annular flow:** a continuous liquid jet flowing in the centre of the channel with a vapour film located at the channel wall.

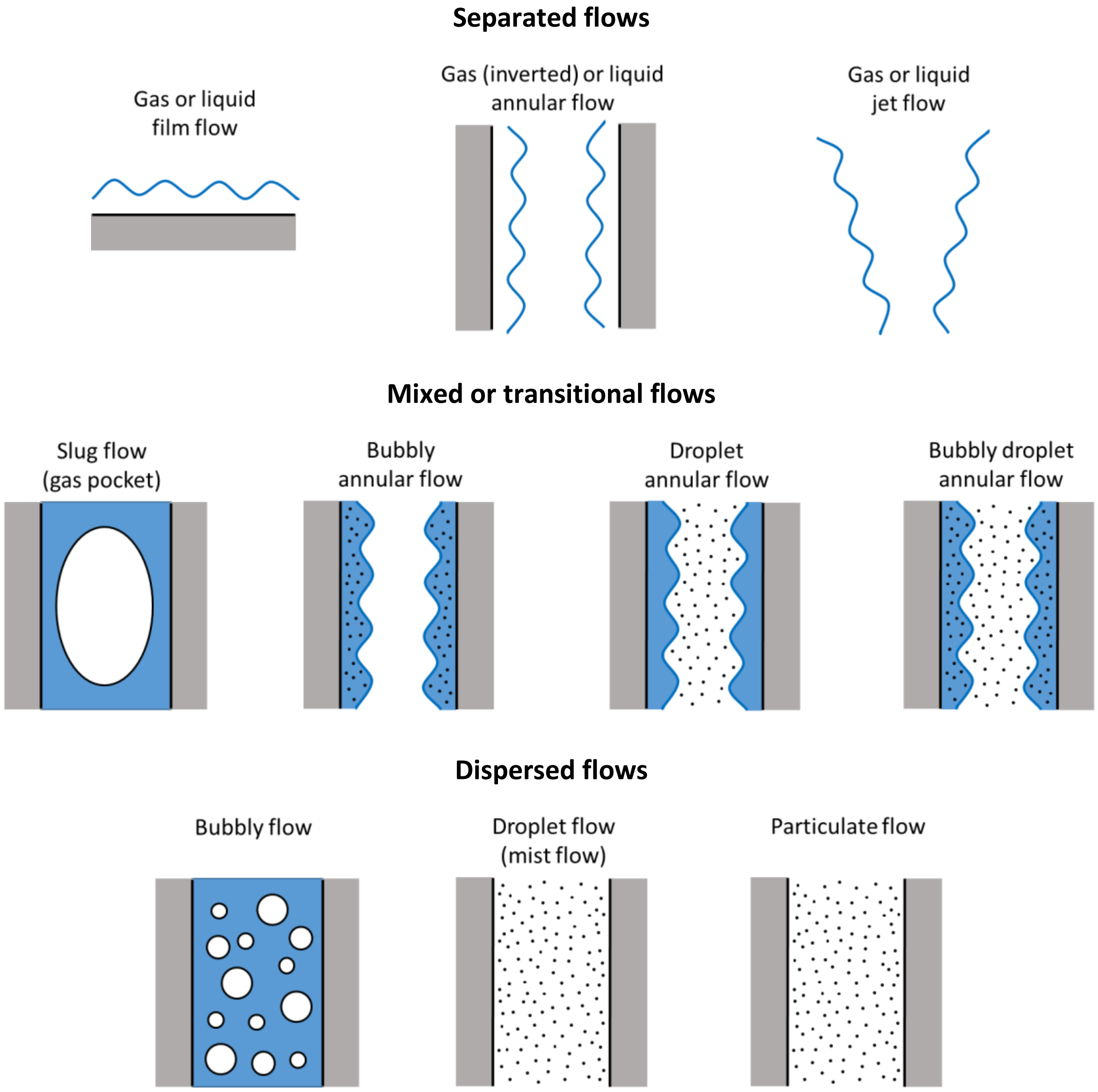


Figure 5: General types of two-phase flow patterns

Transition between these regimes indicates phase change within the flow. Within NPP, this can both be desirable and undesirable, as we can have transition to a number of phenomena, including subcooled and saturated flow boiling, Departure from Nucleate Boiling (DNB), dry-out, flashing, and condensation with and without non-condensables. Two of these which hold critical relevance to NPP safety in LWRs are DNB and dry-out, because they can cause a steep increase in wall temperature, and both of which are directly related to the occurrence of the Critical Heat Flux (CHF). This is the heat flux at which an undesired change in the boiling regime occurs; typically where the rate of vapour being generated from the heated fuel rod surface increases such that it prevents adequate liquid contact with the surface.

The term DNB is usually reserved for the occurrence of CHF in PWRs, where the fluid typically undergoes subcooled nucleate boiling during normal operations. At the CHF, vapour bubbles coalesce on the surface and form a stable vapour layer resulting in a type of annular inverted flow. Dry-out refers to the occurrence of CHF caused by the evaporation of the wall liquid film in the annular flow regime. The reliable prediction of the transition to such phenomena without the need to use empirical models, is probably the greatest challenge here.

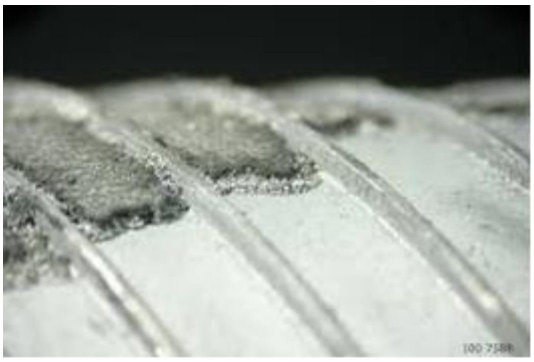
Thermal and fluid phenomena in two-phase flows are strongly linked to the flow pattern, so that mechanistic prediction methods should clearly be flow-pattern based to incorporate the fundamental physics and unique characteristics of each single flow pattern (Thome and Cioncolini, 2015). The “geometric structures” of two-phase flows thus become the mechanistic “building blocks” of mechanistic and theoretically based models, which can then be used to build flow regime specific models for flow boiling heat transfer coefficients, two-phase pressure drops, void fractions, entrainment, dry-out, critical heat flux and so forth.

In fact, the best and most reliable mechanistically based prediction methods currently available attempt to capture the two-phase flow structure of the particular flow pattern to account for its dominant flow phenomena: bubbles, liquid slugs, shear-driven liquid films, entrained droplets, etc. To simulate flow boiling along channels in which the flow pattern goes from one flow regime to another from inlet to outlet, accurate flow pattern maps are thus imperative to reliably identify what type of flow pattern exists at the local flow conditions along the channel whilst mechanistic models try to capture the influence of the two-phase flow structure on the heat transfer and momentum processes.

This vision is quite different to the wholly empirical approach often used in this field, in which ad-hoc non-dimensionless groups or sometimes *dimension* correlations are used to predict local heat transfer coefficients. Notwithstanding this, the empirical approach will continue to play a major role in two-phase convective heat transfer analysis, just like it does in turbulent single-phase flows. One, however, should aim for mechanistic and theoretically based models that are “finished off” by the fitting of a few empirical constants rather than proposing ever more new correlations with 10-30 empirical constants and exponents in which the physical picture of the process is completely lost, as unfortunately is frequently done.

2.6 Rough Wall Friction and Heat Transfer

Many modelling approaches (and experimental investigations) consider solid walls as predominantly ‘smooth’. However, in real NPP, walls are neither smooth nor is their roughness necesasrily a constant through life due to manufacturing processes, ageing, deposition and corrosion. An extreme case being carbon deposition on AGR fuel pins (Figure 6).



(Courtesy of EDF Energy)

Figure 6: Carbon crud on AGR fuel pin (Mowforth et al., 2015)

However, progress in modelling and validation data for wall roughness is very scarce and intermittent. The modelling proposal of Suga et al. (2006) is a notable exception, although detailed validation data is again very sparse, and practically non-existent concerning heat transfer. Rough-wall-effects provide an ideal case for local DNS with bespoke meshing or the immersed boundary technique. However, actual surface topology will need to be experimentally characterised for many types of materials and manufacturing processes with modern tomography methods. In any case, engineering calculations, e.g. rod bundles, require ‘wall function’ type of rough-surface modelling, which need careful validation.

Even on a clean, new AGR fuel pin heat transfer is poorly predicted by classic RANS models so crud effects are best left to experimentalists. Figure 7 shows the huge effect (+/- 100%) of erroneous separation bubble size prediction on wall heat transfer increase (Nusselt number) over smooth pipe value.

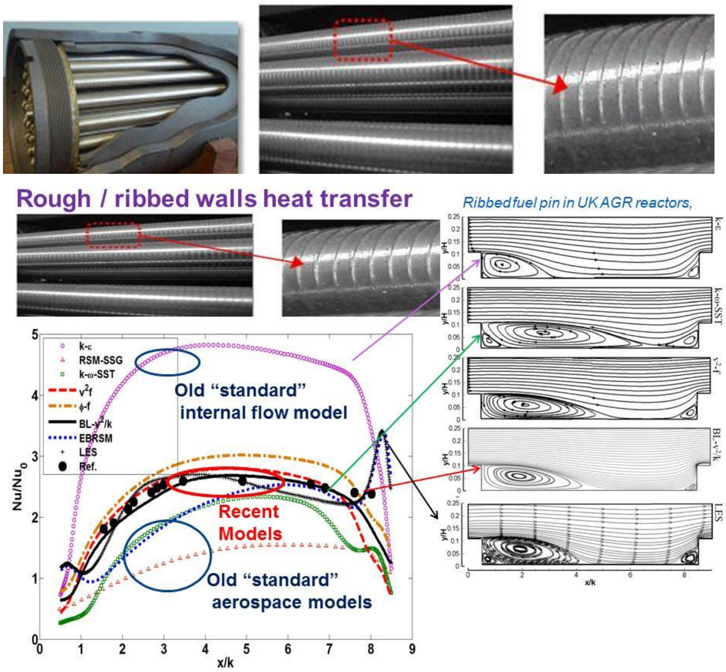


Figure 7: AGR ribbed fuel pin. Separation bubble size effect on wall heat transfer

It is only when detailed mean flow features are reliably predicted that we may see improvements of turbulent heat flux modelling on rough surfaces. There are many more examples where accurate small scale or secondary flow prediction could have large design benefits, such as flow-induced corrosion (see Section 2.7).

Turbulence models for refined CFD, detailed later in Section 5.3, were developed in many different application sectors which perhaps have different “safety margin” focus. For instance “k-omega” rather than “k-epsilon” type models are preferred in the Aerospace sector. They tend to predict weaker turbulent mixing and hence earlier and longer boundary layer separation (with dramatic loss of lift forces). However, but of no concern to Aerospace, they can under-estimate heat transfer or miss re-laminarisation effects (damping of turbulence) in the presence of buoyancy. These features are better reproduced by “k-epsilon” models which are thus more frequently used in the NPP TH sector. Advanced turbulence models providing improved predictions for detailed flow features, such as shown in Figure 7, are now available in major commercial and industrial software for a the wide range of applications.

However, they are only frequently used by R&D CFD specialists while applied CFD NPP engineers are more comfortable with the standard models in their sector, which have been validated on more global values of many established test cases. As finer benchmarking data became available obvious flaws of standard models were proven to be corrected by the more recent ones, but through compensating (opposite) errors global values predicted by older and advanced models are often similar.

The benefits of an advanced model are in the details and reliability over a wider range of applications. It will allow a finer breakdown of safety margins (uncertainty quantification) and exploration of novel designs. For run of the mill CFD studies, over a well-known and validated application range, the extra cost and effort in applying these advanced models was perhaps not perceived worthwhile. This could change with advances in computing: easier to use human-machine interfaces, intelligent “default values of model constants” and cheaper, enhanced computing power.

2.7 Particulates, Corrosion and Ageing

In addition to the more obvious thermal and mechanical cyclic loading over years of operation, there are steady flow phenomena with the potential to limit the lifespan of NPP components by:

- Pure hydrodynamics; erosion, cavitation, droplet impingement;
- Physio-chemical effects; flow accelerated corrosion, particle deposition, altering coolant chemistry.

Because wall thinning often occurs on the inside of tubes it is not detected without very specific and localised inspection devices. Ageing of steel pipes, vessels and heat exchangers are crucial factors to sustain safety but also economic viability of long term NPP operation that have plagued utilities. These could be better addressed at the design stage with artificially accelerated ageing, thanks to better numerical models and experimental methods.

For Flow Accelerated Corrosion (FAC), the chemical process in the surface boundary layer depends on mass transfer and precise flow patterns, which can be modelled by 3D CFD codes. The mass transfer by turbulent diffusion of ions generated at the piping wall to the bulk flow determines the rate of FAC *w*hich increases in regions of high turbulence, such as the flow downstream of orifices, valves and in bend geometries. Corrosive conditions can be further evaluated from concentrations and electrochemical corrosion potential and finally wall thinning rates (Uchida et al., 2012, 2010).

Predictions are harder when the ageing agent is particulate rather than dilute; the complex water droplet/vapour bubble phenomena are discussed in the two-phase flow section (Section 2.5). Solid particle transport and deposition phenomena are perhaps equally daunting. Lagrangian transport research has barely started for non-spherical particles such as carbon flakes growing and blown off AGR fuel pins.

Steam Generators age faster than the reactor core components and replacement is extremely costly. Complex models aim to predict the localisation and the growth rate of deposits in order to simulate tube fouling, as well as tube-support-plate flow blockage leading to Flow-Induced Vibrations (FIV) and tube cracks in some cases, see Prusek et al. (2013).

A PWR steam generator contains thousands of thin tubes separating primary and secondary flow, which can leak after years of use. Several tube support-plates are placed along the tube bundle. Holes allow secondary flow to go through these tube plates, around which deposits are created, by both particle deposition and soluble species precipitation into the pores of the deposits. Corrosion and degradation products such as metallic oxide particles and soluble species produce deposits in low-velocity recirculation zones (Corredera et al., 2008). As the deposit grows, the flow contraction and associated boundary-layer separation will become more severe and the *vena contracta* mechanism tends to become progressively worse.

Highly detailed flow features and multiphysics numerical simulations can now drastically accelerate time. For instance, evolution of the Seine estuary sediment evolution over the past century has been successfully reconstructed in a few hours. Millennium-long TH simulations are ongoing for deep geological waste storage. Moreover, clever dimensional analysis substitution experiments can also mimic ageing or provide validation data. For bends, Mazhar et al. (2013) measured mass transfer using a dissolvable wall in test sections cast from gypsum, to obtain wall wear patterns in a reasonable test time. A probabilistic yet more complete example in terms of multiphysics phenomena can be found in Yuan et al. (2008). Therefore, ageing of reactors should be an integral part of new NPP design and detailed data collection during deconstruction of decommissioned plants would provide a wealth of validation data for TH and materials degradation modelling, alongside imaginative experiments.

2.8 Fluid-Structure Interaction

Fluid-Structure Interaction (FSI), whereby displacement of an elastic structure by hydrodynamic lift or drag modifies the flow pattern which in turn amplifies the displacement, is well known. This feedback effect leading to fretting, and possibly catastrophic rupture, is considered in the design of many engineering systems, e.g. aircraft wings, turbine blades, bridges, piping systems. The very long and slender tubes in heat exchangers and fuel pins are quite susceptible to FSI. Oscillating lift or vortex shedding coupled to structural elasticity for cylinders in crossflow is a text-book example, but flow parallel to tubes is also prone to FSI (Baratto et al., 2006).

Among hundreds of NPP Flow-Induced Vibration (FIV) papers, particularly on tube failures due to fretting-wear and vibration-related damage of reactor internals, a still relevant review by Pettigrew et al. (1998) concludes that “most flow-induced vibration problems can now be avoided by proper analysis at the design stage” but “while much progress has been accomplished to understand flow-induced vibration mechanisms, the effect of two-phase flow requires further attention”.

Today many codes, including commercial solvers permit a monolithic approach (flow and the displacement of the structure solved simultaneously, with a single solver) and should allow more systematic evaluation of FSI risks thanks to High performance Computing (HPC) resources, but when re-meshing is needed for large displacements, or a large number of tubes must be accounted for, this can be costly. Longatte et al. (2013) suggest a hybrid strategy using both numerical local solutions and empirical global solutions.

Pins and tube bundles are reviewed in Section 2.12.3. As a dissimilar, but historical example, a less obvious effect (*a priori)* was the large fluid-elastic vibration of the thermal shield in the French fast breeder reactor SuperPhenix. The top of the cylindrical thermal shield holding cooler liquid sodium against the vessel wall behaved as a flexible weir as fluid was cascading over it into the plenum which had a lower free surface. As the new plant was first tested a loud drumbeat was heard due to shield vibrations and sloshing fluid. After ad-hoc coupling fluid and solid simulations and a reduced scale model using water and a bronze weir (chosen from dimensional analysis, Cauchy number for elasticity and Froude number for gravity) fully explained the phenomenon, this very worrying phenomenon was resolved by simply adjusting free surface levels. The design of a Fast Breeder Reactor, still under construction in India, has led to more recent experiments (Thirumalai et al., 2010).

In areas of complex flow, where accurate prediction of the flow field alone is challenging, FSI adds an extra layer of modelling complexity. Even designers with considerable modelling expertise currently rely heavily on testing to determine if FSI will cause a problem, sometimes resulting in costly rework.

2.9 Transient and Unsteady Flows

Transients occur where a significant change of conditions occurs over time and are a concern in NPP design and operation. Examples are reactor startup or power changes or Loss-of-Coolant Accident (LOCA) depressurisation and coolant injection. Unsteady flows occur where the macroscopic component or reactor conditions are constant, but the flow contains inherent instabilities, that result in either periodic or chaotically changing flow patterns.

Most empirical heat transfer correlations are derived for fully developed steady state conditions while rapid transient and non-established flows exist in most accident conditions. Transient flows make up most of the CSNI 63 SET collection and the effect of downscaled ITF on time similarity is much discussed in the recent Scaling report (Bestion et al., 2016a). Even when vertical scale and velocities are conserved, the inevitable volume and power reductions raise the issue of time-dependency transposition.

Turbulence modelling via RANS is based on steady state mean flow conditions. When the transient timescale is much larger than the turbulent timescale, RANS is generally assumed acceptable but the limit is not clearly defined. For example, in vortex shedding behind a bluff body the issue is still unresolved and there is a wide range of intermediate approaches between RANS and LES where the ranges of applicability are still less clear (Detached Eddy Simulation, Partially Integrated RANS, Stress-Strain Lag model). Transients are very costly to tackle via LES or DNS because of the scale difference between the long timescale transient event and the small, rapid flow instabilities. This is made further challenging if using ensemble averaging (running the same transient many times) instead of time-averaged statistics.

For similar reasons, conjugate heat transfer studies are costly due to the long transient timescales resulting from the thermal mass of structures. This leads to much longer solution timescales than those encountered in steady state heat transfer. Long transients are also found in normal plant operations such as evacuating cold water plugs in lower U-bend piping systems and horizontal stratifications.

Natural convection is another case where transient or unstable events lead to long solution timescales. Even small 50cm cavity experimental rigs are often left running for hours to allow the flow to be fully established, whereas the data acquisition phase might only occur over a matter of minutes. In natural convection simulations, bifurcating or periodic solutions have been observed.

2.10 Liquid Metals

Two of the Generation IV reactors use liquid metal as the primary-circuit coolant, i.e. the Sodium-cooled Fast Reactor (SFR) and the Lead-cooled Fast Reactor (LFR). The convective heat transfer in liquid metals is inherently different from that in water or air due to its very low value of Prandtl number (Pr), normally between 0.01 and 0.001 depending on the temperature under reactor conditions. These values are significantly lower than those of air (~0.7) and water (~7 at room temperature). As a consequence, in contrast to that in air or water, the thermal boundary layer is often much thicker than that of momentum boundary layer, and hence the thermal conduction plays an important role.

For liquid metal, the turbulent thermal diffusivity is only greater than the molecular thermal diffusivity at high Reynolds number: when $Re > 60{,}000$ for $Pr = 0.025$, or $Re > 214{,}000$ for $Pr = 0.007$, where $Re = U_b D_h/\nu$, where U_b is the bulk velocity, D_h the hydraulic diameter and ν the kinematic viscosity (Grötzbach, 2013). The implication of this is that the Reynolds analogy between the thermal and momentum transfer based on $Pr{\sim}O(1)$ implied in conventional turbulence modelling as a basic assumption is no longer valid. The solutions of the energy and momentum equations are normally related through the use of the so-called turbulent Prandtl number, which is commonly taken to be a constant ~0.85. An equivalent Pr_t for sodium would be much smaller than the above value and would be varying in the flow field. Advanced turbulent heat flux models have been developed and used for ‘normal’ fluids, but they will need to be validated/recalibrated for liquid metal flow.

The second challenge associated with Liquid Metal Fast Reactors (LMFR) is related to their particular design which nearly always adopts a pool-type style (except the Japanese SFR design which adopts a loop type). The main components of the reactor including the core, the circulators and intermediate heat exchangers are submerged in a large pool of liquid metal. This inevitably results in the existence of ‘dead’ areas where stratification may occur. Such stratifications are always associated with a high temperature gradient and tend to be unstable/unsteady, which may lead to thermal fatigue of adjacent structures.

Buoyancy force and natural circulation play a more important role in LMFRs than in many other reactor designs in both normal operation and decay heat removal. For the latter, passive cooling decay heat removal with/without the assistance of circulators is an advantage of such reactors. Even though extensive efforts have been directed at the modelling of natural circulation (and mixed convection) in CFD in general and nuclear thermal hydraulics in particular, it still remains as one of the greatest challenges. The main reason is that the thermal and momentum fields are strongly and nonlinearly connected – the buoyancy force resulting from the solution of the energy equation (which depends on the flow field) serves as the source term that drives the flow. In forced convection however, the momentum equation can be solved without considering the thermal field, which can be solved later as a passive scaler. Additionally, natural circulation tends to involve various flow regimes (laminar, transitional and turbulent) and there is a lack of a main flow direction, which all increase the difficulty in modelling.

Another feature of SFRs is the use of an argon cover gas layer above the sodium pool to prevent any leakage air into the vessel from coming into contact with sodium, which creates a free surface above the sodium pool. The heat transfer from the surface to the roof of the core is of significant interest in understanding the behaviour of the reactor. Here the heat transfer is largely by radiation through the argon cover gas with mists of sodium aerosols which may deposit onto the roof. Conversely, the free surface is a major source of argon gas entrainment to sodium. This effect increases as the cover gas space is reduced under the pressure of the reduction in the overall size of the reactor, which leads to greater free surface velocity/disturbances and more/stronger vortices generated around structures protruding the free surfaces, all of which lead to stronger gas entrainment. The principal concern of gas entrainment is the possible positive reactivity, followed by adverse impacts on the circulator pumps.

Other challenges include thermal striping and gapping instability. The former is due to the potential differences in temperature between the outgoing fluid streams from the core - these ‘jets’ are rather unstable and take time to mix, which are potential sources of thermal fatigue of the above core structures. The latter is a phenomenon that occurs in closely-packed tube bundles when Kelvin Helmholtz instability may induce vibration. These are also complicated by the use of spiral spacer wires used in-between the fuel rods which create additional disturbances to the flow and challenges for prediction of flow and temperature.

Molten Salt Reactors (MSRs) can be included here in passing as they are more similar to liquid metal than water cooled reactors. Advantages (in addition to the strong negative temperature coefficient of reactivity) are that core pressure can be low and the temperature much higher (lower leak risk yet higher efficiency). Risks of corrosion and alloy embrittlement under high neutron flux are perhaps more severe, but not new. The additional TH modelling challenges are mostly related to varying and composition dependent fluid properties, but otherwise the same turbulent flow and heat transfer models used for water are expected to be applicable to MSRs

2.11 Multiscale

A Light Water Reactor holds a fluid volume of 100's of m^3 at 16.0 MPa pressure and 315 °C. A PWR steam generator is approximately 20 m high, with the core diameter approximately 3m. On the other hand, the gaps between the fuel pins are typically several millimetres, while the dimensions of the vortex generator and the fluid gaps behind the springs of PWR mixer grids are sub-millimetres. These must be represented to study mechanical loading, vibrations and thermal hydraulic homogenisation across fuel bundles (Chabard and Laurence, 2009). Consequently, inside the reactor bounding volume, flow paths have hydraulic diameters spanning 3-4 decades from mm/cm to 10 m. This poses a huge challenge to modelling as well as physical testing. On the modelling side, multi-level fidelity prediction tools are necessary, including, for example, system codes or sub-channel approaches based on 0 or 1 dimensional modelling for the system/multi-channel modelling and conventional CFD for local flow phenomena.

Integral experiments must also drastically reduce scales, especially volumes to reduce cost and power to a manageable level while trying to still represent buoyancy, and hence with a smaller reduction in height. This huge variation in scale represents a significant challenge in both thermal hydraulic modelling and testing best illustrated by the examples below.

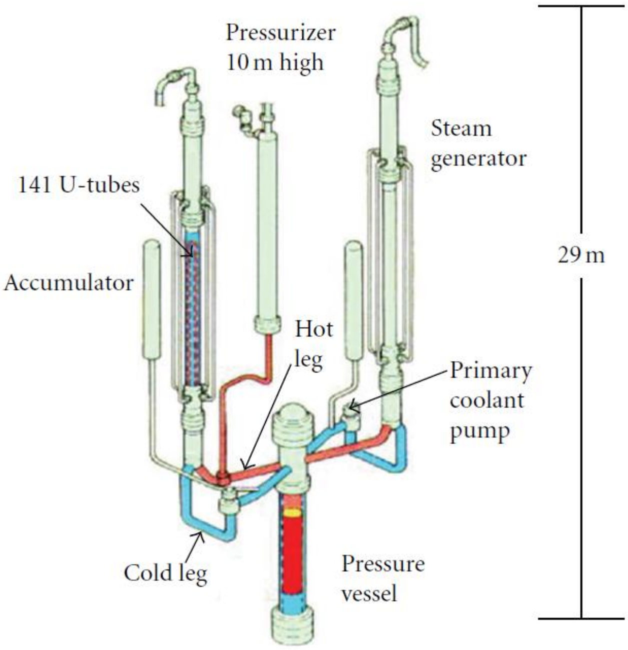


Figure 8: ROSA/LSTF rig example (Takeda et al, 2012)

The Japan Atomic Energy Agency's Rig of Safety / Large Scale Test facility (ROSA/LSTF) is a very large integral test facility (Figure 8) designed to investigate multi-dimensional thermal-hydraulic responses during PWR transients and accidents.

The total height is 29 m such that major components are exceptionally kept at full-scale to correctly capture gravity effects. The volume is scaled down to 1/48 and the power represents

14% of the Westinghouse 3,400 MW reactor thermal power because of an obvious limitation in the capacity of power supply for 1,008 electrically heated rods. Such large experiments, whilst carefully designed to avoid distorting buoyancy and turbulence effects, are obviously very expensive.

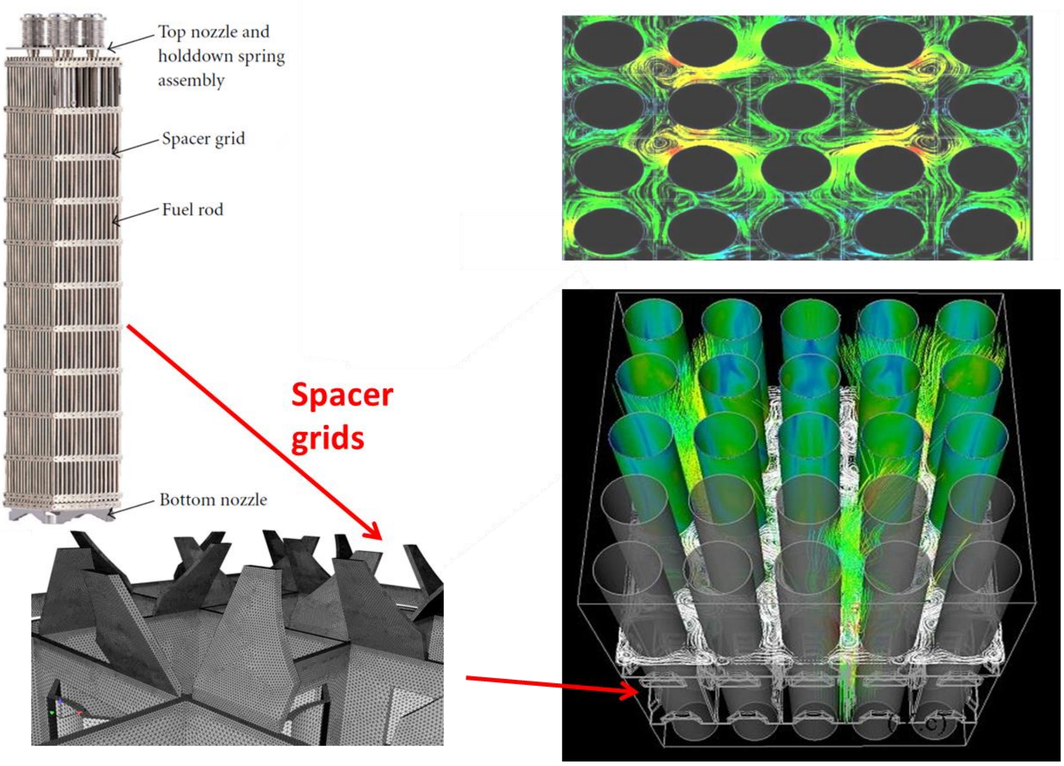


Figure 9: Multiscale challenge of representing 1.2 mm thick springs and swirl generators of spacer grids in long PWR fuel bundles (Code_Saturne CFD and Song et al. 2012)

At the other extreme mm scale details of vortex generators and fluid gaps behind springs of PWR mixer grids (Figure 9) must be represented to study mechanical loading, vibrations and thermal hydraulic homogenisation across fuel bundles.

Needless to say the tiny fluid passages in this tight arrangement are inaccessible to measurements. The quasi-random orientation of the vortex generators prevents use of periodicity to reduce the number of tubes in the model. Moreover, when conjugate heat transfer is required, experiments are simply impossible. Kraus et al. 2020 are running a 4.3 billion points DNS on this reduced 5x5 only rod bundle and Re number of 19,000 to provide RANS or LES validation data.

The geometry of SFR wire wrapped fuel pins is even more inaccessible and pose severe meshing challenges because the contact point rotates, as shown in Figure 10. Bundle casing side effects have been noted (Rolfo et al., 2012) and the actual design contains not 7 but 217 pins. Argonne National Laboratory (ANL) is computing the latter with the first principles code NEK 5000 and offering it as benchmark to the international community (Merzari et al. 2016). Modelling of the small details and small scale flow features are needed to enable the prediction of important reactor parameters. However, studies of this level of detail over entire bundles, let alone entire reactors are not generally practicable.

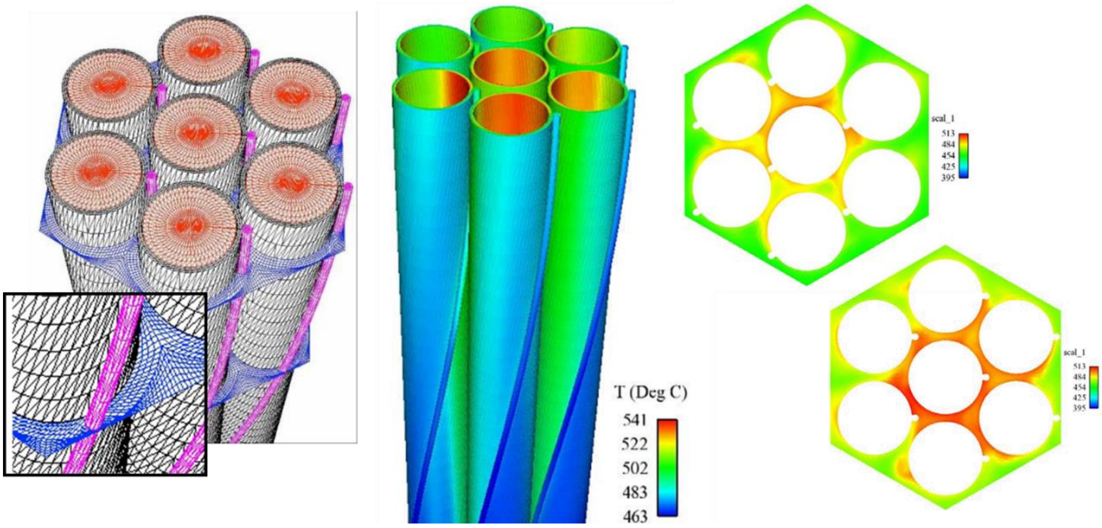


Figure 10: Conjugate heat transfer of wire-wrapped SFR fuel bundles (solid Code_Syrthes, Fluid Code_Saturne). Wires instead of spacer grids prevent vibrations and induce temperature homogenisation by swirling flow, but forbid experimental investigations in the very narrow fluid gap (blue mesh in zoom bottom left).

2.12 Examples of the Impact of Thermal-Hydraulic Phenomena

2.12.1 Pressurised Thermal Shock (PTS)

Thermal loads on the Reactor Pressure Vessel (RPV) may lead to very large stresses and growth of possible flaws present inside the RPV in a PWR. Fan et al. (2009) shows temperature in a laminar transient simulation of a Small-Break Loss Of Coolant Accidents (SBLOCA) PWR. laminar for a tiny cold water release in the surge line that connects to the hot leg. This laminar simulation solving the original Navier-Stokes equations is exact, free of modelling assumptions, but is only valid for small velocities, small geometries or very viscous fluids as mixing occurs only at molecular level.

In the case of real, intentional Emergency Core Cooling (ECC) during a LOCA with larger velocities turbulence appears and its effects need to be accounted for. These effects can be modelled either entirely from the computed flow fields based on the RANS equations or partially in the LES case when computer resources are sufficient to capture the large scale fluctuations while modelling only small scale motions (using an adequately increased viscosity related to the computational mesh that filters out smaller eddies).

It is theoretically possible to capture all scales of fluctuations by solving only the Navier-Stokes equations as in the laminar case, but even the most gigantic computer resources are still insufficient for this purpose in 2017.

In all cases, cold water injection remains mostly stratified in the inlet pipe then only partly mixes in the downcomer where it “cascades” along the RPV wall with large scale quasi 2D unsteadiness in the form of meandering wall jets, and eventually merging jets (Coanda effect), and mushroom-like coherent structures due to density differences (Rayleigh-Taylor instability) appear.

Pressurised thermal shock is a key reactor safety issue that also determines the lifespan (and subsequently economics) of the plant due to radiation embrittlement of materials over time (Lucas, 2009), so EU and international programs invested extensively in experiments and extreme simulations addressing this issue. Therefore, it is worth explaining, as a generic example, why neither “downscaled” experiments nor simulations are sufficiently reliable to determine the key parameter for the design of safety margins and lifespan of the vessel: what are the real thermal stresses experienced by the embrittled sections of the vessel? The coherent quasi 2D structures in the annular downcomer shown above “look like” the flow visualisations from the Plexiglas adiabatic experimental rigs, but this does not mean that the simulations, extrapolating from scaled experiment validations to actual reactor scale give an accurate prediction of the heat flux *into* the RPV wall, for many reasons:

- The Reynolds number in the RPV PTS is Re ~10^6, but experiments are at Re ~ 20,000. Experiments also use sugar or salted water to reproduce density variations, but the Prandtl number is then distorted (acceptable for large scale mixing but not down to the wall effects). Besides, the full scale RPV may be in a different wall-roughness regime to the plexiglass.
- Non-adiabatic steel rigs provide some solid temperature data, but no velocity, they are for simplified geometries and measurements inside the steel are not available or strongly attenuated.
- Can the Nusselt number (dimensionless wall heat transfer), really be assumed to scale as $\mathrm{Nu} \propto \mathrm{Re}^{0.8}$ because this correlation is for steady state mean pipe flow?
- The wall heat transfer is highly sensitive to the 3D Turbulent Boundary Layer (TBL) which scales down to much smaller scales at Re 10^6. The TBL is distorted in downscaled experiments, absent in the laminar simulation and modelled by wall-functions (mean velocity/wall-friction and temperature/wall-heat-flux steady state correlations) in the RANS and LES simulations.
- RANS or LES wall-functions are based on correlations derived from steady-state mean-flow, very far from the meandering cascade and coherent structures seen here (a Log-law velocity profile in a pipe flow is only established hundreds of diameters downstream of the inlet). Simulations conducted for different Re, do not prove that Re number is high enough to be unimportant, as standard wall functions are precisely based on equilibrium / Re number invariance assumptions.

The approximations and uncertainties listed for the above pressurised thermal shock case may or may not err on the conservative side. Heat transfer coefficients designed for mean thermal fields (RANS) then applied to fluctuating temperatures lead to overvaluing. Even the more advanced methods used in industry (Moriya et al., 2003) for evaluating the fluctuating heat transfer from the ratio of power spectrum of a probe in the fluid and another in the solid is erroneous. This is because it ignores the real 4D nature of the fluctuating thermal field in the solid and assumes a planar wave: $T(y = 0, t)$, i.e. homogeneous in the wall parallel x, z directions. The real higher frequency fluctuations, on the other hand, will be damped increasingly with depth ($y < 0$) by the wall thermal mass (a typical RPV is made of 70 mm alloy plus 200mm steel). If the temperature map on the solid surface is non-uniform, $T(x, y = 0, z, t)$ peaks and troughs will penetrate as cones or wedges and diffuse in the x, z directions, attenuated by inertia and diffusive cancellation. It is therefore not known if the design safety margins and plant life assessment are conservative.

2.12.2 T-Junction Thermal Mixing

Besides radiation decreasing the vessel resistance to emergency thermal shocks, thermal cycle ageing of the piping materials over years is a key turbulence issue overlooked in earlier designs. Welds are less resistant and located in areas where differential dilatation of pipes is constrained by the geometry. Thermal stratifications also lead to stress accumulation but these are more predictable than purely turbulence induced thermal stresses.

In May 1998, a through-wall crack was discovered on the Residual Heat Removal system (RHR) of the French Civaux 1 PWR only five months after finishing construction, resulting in early pipe rupture and release of radioactive steam into the reactor building. It resulted in a hot shutdown. Other non-through cracks were then detected in other piping systems. This accident was classified as Level 2 on the INES scale. Later research found the cracks were due to thermal striping (Stephan et al., 2002).

The crack happened downstream of a T-junction where two streams of fluid at different temperatures encounter each other. The turbulent mixing of hot and cold fluid introduced temperature fluctuations. Such temperature fluctuations penetrated into the wall of the pipe and caused high-cycle thermal stresses which induced the subsequent fatigue cracking of the wall material. The Japanese Tsuruga-2 and Tomari-2 PWR plants in 1999 and 2003 (Le Duff et al., 2007) are two other accident examples among this type of safety incidents.

T-junction test cases were in collaborative projects set up to assess the predictive capabilities of CFD techniques, for example the test rig by Vattenfall in Sweden. Data from this test have been used specifically for an OECD CFD benchmark exercise (Smith et al., 2013a). The computational results of 29 participants show that RANS models fail to predict a realistic mixing between the fluids. The results were significantly better with scale-resolving methods such as LES, showing fairly good predictions of the velocity field and mean temperatures. The calculation predicts also similar fluctuations and frequencies observed in the model test.

Unfortunately such rigs focus on long straight inlet pipes to facilitate boundary conditions whereas Tunstall et al. (2016a, 2016b) showed that most large scale fluctuations are generated by the instability of a pair of Dean vortices generated in an upstream bend. This pair tends to be asymmetric, one vortex larger than the other generating persistent swirl in the downstream pipe and over the T-junction, which then switch over time, a phenomenon called “switch-swirling.

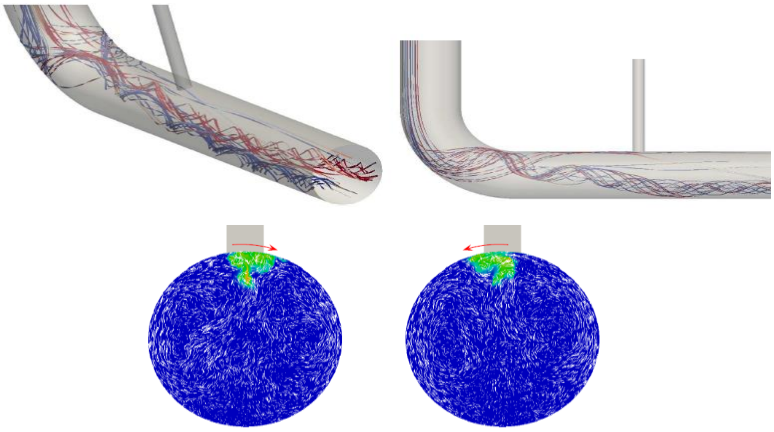


Figure 11: Swirl effects of upstream bend on TEE Junction flow Tunstall et al. (2016a, 2016b)

Test rigs are also limited by the fact that they have isothermal or adiabatic walls so temperatures inside the walls cannot be validated. Extending a CFD simulation to include temperatures inside solid walls is easy; it suffices to solve the same equation as in the fluid while setting the convective velocity and turbulence generation to zero. Alternatively, the CFD code can be coupled to a finite element structures code. Applied studies have so far only considered mean temperatures, with some extensions to fluctuating temperatures inside the solid by LES, and only recently by first principles DNS (Flageul et al., 2015; Wu et al., 2017).

Material scientists can use this information to assess whether a component will fail through high-cycle fatigue crack growth.

2.12.3 Tube Bundles

Flow around fuel pins are mostly guided and parallel so can be related to pipe flow correlations. Tube banks in crossflow are more complex and mostly a concern for utilities regarding the life-span of heat exchangers. In PWR steam generators the primary fluid flows inside thousands of thin U-shaped tubes. Vibrations coupled with crossflow on the secondary side may induce wear against support grids, and a few primary circuit tubes may be blocked without much effect on efficiency but temperature heterogeneity needs to be studied. Secondary flow comes at all angles of attack, crossflow in the lower inlet and outlet regions and the top 180° bends.

Despite a dozen PhD projects over the last 30 years at EDF R&D, downsizing of the whole domain simply cannot be trusted to be predictive, even for the simplest square arrangement exactly aligned with pressure gradient. The mean flow often exhibits non-symmetric solutions as in Figure 12.

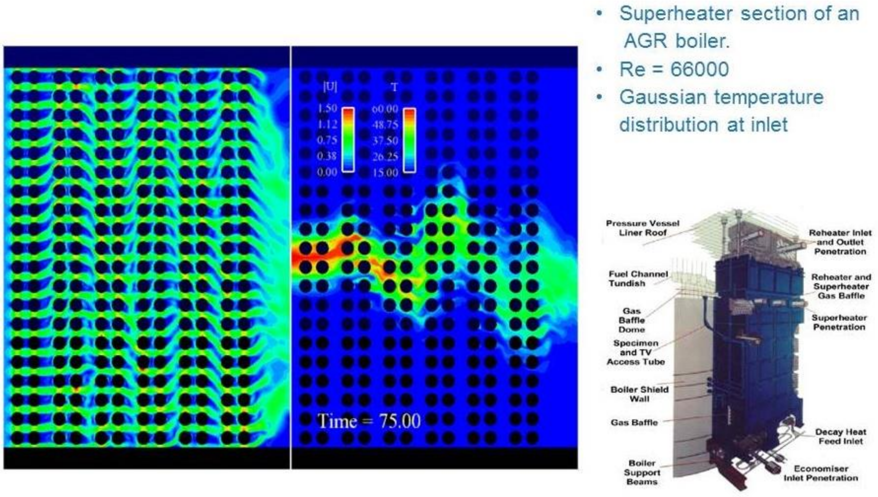

- Superheater section of an AGR boiler.
- Re = 66000
- Gaussian temperature distribution at inlet

Figure 12: Flow across tube bundles are rarely symmetrical and steady (West, 2013)

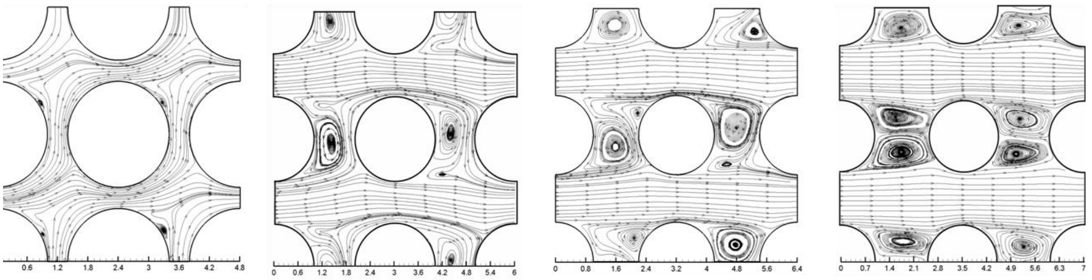


Figure 13: Time averaged streamlines in tube array, Gap/Diameter = 0.2, 0.5, 0.6 and 0.75 All cases “inline” (horizontal) mean pressure gradient (Afgan, 2007)

For a Gap/Diameter (G/D) of 0.2, the flow is globally deflected to one side, and obviously to conserve mass, pressure will build up on lateral end walls which will force the flow to be deflected to the other side in another cross-section. It seems that a gap of 0.75 G/D is the minimum for 2 symmetric vortices to be installed (although some vortex shedding is still apparent on instantaneous snapshots). The actual design value is about 0.5 G/D, which is the most unstable case with room for only one vortex, but this one flips clockwise or anti-clockwise in both tube-row and time.

To make LES feasible, a smaller computational domain is usually generated by assuming periodic patterns (values at top open boundary equal to ones at bottom), but then the results are sensitive to the number and parity of tubes 2x2, 3x3, 4x4, 5x5, etc. included between periodic boundary conditions, which are presumed able to represent an infinite number of tubes. The depth of the domain, where again periodicity is assumed, is also influential. A deeper domain will allow more deflections. The patterns in Figure 13 should not be considered general.

LES has been useful in understanding the complexity and versatility of this type of flow, because there was, for decades, an expectation to study a range of attack and inclination angles, flow induced vibration, heat transfer, two-phase flows. A tube bank simulation, however, needs to represent a very large section to be relevant to actual steam generator geometry, perhaps up to 100’s of long tubes. Current HPC resources are insufficient for this, so unsteady RANS models (URANS) seemed an alternative, but (with the qualification that this should not be re-quoted out of context): “*it is impossible to conclude other than that the quality level of the URANS predictions is poor*” (Iacovides et al., 2014). Concerningly, a large variation in flow pattern and local heat transfer coefficient was exhibited by changing only the turbulence model.

3 Current Practice and Procedures

The body of work available covers several decades of world-wide government, academic and industry collaborations, covering thousands of documents and hundreds of concepts. Because of this scale, the coverage in this section is intended to highlight current trends and their application to future tools for NPP design. In particular, the challenges of scaling and uncertainty evaluation are discussed and a number of important references to NRC publications covering additional areas are included.

3.1 Scaling

Scaling is key to the whole area of NPP design and safety assessment since a full-size reactor experiment is not achievable and must be replaced by a clever combination of integral and separate effects test facilities, ITF and SETF respectively, and simulation, tied together by scaling principles. Dimensional analysis and the reduced number of significant parameters enabled by the Buckingham π theorem is, therefore one of the most important tools in thermal hydraulics.

System codes or 3D CFD can be used at full-size reactor scale because there is no limit to the value of the dimensionless parameters (Reynolds, Froude, Euler, Weber, etc.) whereas they are always distorted in the Integral Tests and more or less in SETF; e.g. in a simple friction and buoyancy balance test a factor of 4 length scale reduction requires a 4-fold increase in reference velocity to conserve the Reynolds number, but a factor of 2 reduction of the same velocity to conserve the Froude number[4].

Credibility of the simulations is established through a code-validation process by comparing the results of the code's prediction for separate-effect and integral-effect tests data. The codes are then used to extrapolate from ITF values up to dimensionless parameter values of the actual NPP.

ITFs are necessarily downscaled in some dimensions, size, volume, flow rate and power otherwise they would cost as much as a full scale prototype and need a second real plant to provide the heat or electricity replacing the nuclear energy in the instrumented vessel. ITFs are intended to encompass multiple phenomena in transients and accident scenario, but cannot conserve all dimensionless parameters. Moreover, fluid properties vary with pressure and temperature during TH transients.

The SET data is essential in ensuring that codes are able to extrapolate from the downscaled ITF to the actual scale of the phenomenon expected in the plant. This is possible since when the SETs are focussed on a single phenomenon, the reduced number of dimensionless parameters alleviates most of the down-scaling conflicts.

Scaling compromises in NPP TH are much more elaborate than the above simplistic introduction and have been discussed by hundreds of experts over decades. The state of the art CSNI report on scaling (Bestion et al., 2016b) is very timely and comprehensive, indeed "The need for this document testifies the importance of scaling in nuclear technology, but also the controversial evaluations of scaling-related findings by the scientific community".

The CSNI "scaling" report covers in much detail the scaling distortion: technological limitations in constructing and operating test facilities, and computer code scalability, uncertainty methods across all aspects, and relationship of scaling and uncertainty, in measurements and in

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[4] at EDF R&D cooling tower plumes were studied in a water channel to gain a factor 10 on Re thanks to water/air viscosity ratio

simulations. CSNI also usefully revisits the SET and IET matrices of 1996, adding more recent data and acknowledges the much larger contribution of codes today and noted that even “failed agreement” between different scaled experiments can be useful for code validation: if the code can explain the discrepancy it adds credibility.

It is impossible to summarise further this 400-page review work and selection of 300 references, but the 8 classes of scaling methods identified in Chapter 2 give an idea of its breadth (quoting):

1. **Linear scaling:** “The same aspect ratio and the same velocity in the model as in the prototype. This approach can excessively distort gravity effects.”
2. **Power-to-volume scaling:** “This method conserves time and heat flux in the prototype and can reproduce phenomena in which the gravity effect is significant. It is suitable to simulate an accident in which flashing occurs during depressurisation. It was successfully used to design most of the integral-effect test facilities.... However, when it is applied to a smaller facility with the full height, due to the smaller area ratio, some important phenomena can be distorted, for example, the excessive stored heat in structures...”
3. **Three-level scaling:** “The first step is an integral - or a global-scaling analysis to conserve a single and/or a two-phase natural circulation flow, using a 1-D non-dimensional governing equation of natural circulation. The second step is a boundary flow and inventory scaling. ... In the last step, a local phenomenon scaling is performed to conserve the important thermal-hydraulic phenomena occurring in each system… The three-level scaling method is characterised by relaxing restriction on the length scale…”
4. **Hierarchical 2-Tiered Scaling (H2TS):** “The procedure consists of four stages, i.e. system decomposition, scale identification, top-down analysis, and bottom-up analysis. At the first stage, the system conceptually is decomposed into subsystems, modules, constituents, phases, geometric configurations, fields, and processes. The scale identification … provides the hierarchy for the characteristic volume fraction, spatial scale, and temporal scale. …by dividing by the system’s response time based on a volumetric flow-rate. The top-down scaling as in the 3rd stage offers a scaling hierarchy, using the conservation equations of the mass, momentum, and energy in a control volume. ... All the processes can be compared, and ranked for importance on the system to establish priority in the scaled models. The bottom-up scaling, as the 4th stage of the method, offers a detailed scaling analysis for key local phenomena, such as the CCFL and choking…”
5. **Power to Mass Scaling:** “This method determines scaled core-power according to the initial coolant’s mass inventory in the reactor’s coolant system... The mass flow rate of the core is scaled down according to the power and heat capacity relationship…”
6. **Modified Linear Scaling:** “The multi-dimensional behaviours of the Emergency Core Cooling (ECC) water in the downcomer (e.g. the ECC bypass) are observed during the LBLOCA refill phase. … Twelve dimensionless parameters were obtained from the two-fluid momentum equations in the downcomer.”
7. **Fractional Scaling Analysis (FSA):** “FSA is a hierarchic approach similar to H2TS. In the first step, the regions of interest and the durations of the transients are specified. The rate of change of the state variables over the region are connected to the transfer functions defined at the boundary, and inside the volume. The relative effect of components is based on their relative impact on state variables in the transfer function connected to that component. ... FSA offers a systematic method of ranking components and their phenomena in terms of their effect on the Figure Of Merit (FOM), or the safety parameter. It can also estimate scale distortions, and synthesise data from different facilities for the same class of transients. …”
8. **Dynamical System Scaling (DSS):** “To address the time dependency of scaling distortion, [it converts] the transport equations into a process space through a coordinate

> transformation, and exploits the principle of covariance to derive similarity relationships between the prototype and model. After the transformation, the target process can be expressed in the process-time space as a three-dimensional phase curve, called geodesics. .. Any deviation of the process curves represents the deviation of scaling as a function of time… this generalised approach offers the benefit of identifying the distortion objectively and quantitatively at any moment of the transient.”

3.2 Uncertainty Management

Thanks to wider usage of advanced mathematical/probabilistic theory and computer power this science is rapidly progressing, breaking down and quantifying sources of uncertainty, improving reliability of model predictions, planning of experiments, ultimately speeding up, reducing costs and broadening the scope of engineering designs. Progress in Uncertainty Management will radically change engineering and decision making in the future, particularly for NPP design and licensing.

Rather than another catalogue of past practices, a brief overview is given of current trends in Uncertainty Quantification (UQ) while concepts and maturity of this combined mathematics, statistics and engineering science for predictive assessments of risk for design actions is assessed in a recently published 2,000 page book by top international experts (Ghanem et al., 2017b) with contributions from the NPP sector (Sandia National Labs, EDF R&D, CEA etc.) (Baudin et al., 2017; Beck and Zuev, 2017; Mousseau and Williams, 2017; Rider et al., 2015).

3.2.1 Uncertainty Quantification and Conservative Safety Limits

In a nutshell, a safety analysis element or result that is within limits specified by regulators is “conservative” when at each stage the most pessimistic choices have been made for baseline models, codes, initial plant conditions, readiness of equipment and accident sequences.

“Best estimate” models and codes provide the most realistic estimate (based on current knowledge) of individual phenomena and overall response of the plant during an accident, assuming the plant is as built and operations as designed. Obviously error bands around the best estimate need to be carefully calculated for the predicted result to be of any usefulness.

Safety regulations of the 70s were based on large global safety margins to compensate “lack of knowledge or confidence”, and so model predictions in each worst case scenario were expected to demonstrate that the design and operation procedures were “conservative”. This mostly involved checking that a single value predicted by the licensing applicant was below a severe threshold set by regulators. Therefore, all the protection against “lack of knowledge or confidence” (used here instead of “uncertainty” which has a clearer probabilistic sense) in the acceptable threshold determination and design value prediction methods was lumped into the conservative limit. “Sensitivity” to input parameters and different models was recommended, but this was down to rather ad-hoc user choices.

Uncertainty Quantification is in a way the reverse approach to raising the final thresholds. It ensures that predicted values are framed by realistic error bands, confidence intervals or probability distributions. In complex systems the uncertainty can be propagated from input parameter probabilities throughout all components of the modelling process. It is then easier to assign an uncertainty measure to each stage and mathematical tools enable this is to be transferred to a total uncertainty around the final result. Forward uncertainty propagation can be by brute force Monte Carlo simulation or mathematical manipulation of equations such as polynomial chaos expansions.

In Monte Carlo, sensitivity analysis input values are simply randomly sampled. The number of required simulations rapidly increases with degrees of freedom. Latin Hypecube Sampling more efficiently maps the field of input values with each one representing an equi-probable section of the fields. This brute force empirical method still requires large statistical samples and thus is potentially very costly. Alternatively, models can be enhanced with multiple regression on input variables (least squares fit plus confidence interval).

In thermal hydraulics, UQ developed rapidly and naturally around System codes and CFD in the 2000's (RANS model, after all, based on predicting mean behaviour plus variance). Inserting probability density functions into the NS equations is common in e.g. reacting flows or two-phase flow bubble size distribution (population balance) models. A Best Estimate Plus Uncertainty (BEPU) approach is more realistic than "Conservative" assumptions. The latter might drive safety margins on the basis of impossible events, but neglect other combinations, for example, the co-incidence of two "less serious" and more frequent events with a more severe combined outcome.

3.2.2 Best Estimate Plus Uncertainty (BEPU) Development and Acceptance

Quantification of Margins and Uncertainty (QMU) originated in the 1990's mainly from HPC equipped Lawrence Livermore, Sandia and Los Alamos National Labs. Along with HPC it is now developing in all complex engineering where experimentation and modelling have limitations.

Around 2000, HPC became more widespread and system codes had been sufficiently validated to allow a statistical approach. Complexity and multiple unknowns in LBLOCA accident studies was an obvious application area for the researchers and NPP designers, but authorities needed to be convinced before these could be included in Safety Analysis Reports (SAR) submitted to licensing. Transients such as LOCA mitigating measures must lead to "conservative" parameter values defined by regulators, e.g. Peak Cladding Temperature (PCT) or a maximum overall oxidation value to limit hydrogen release. The safety margins were added to values determined by simple empirical models to account for limited confidence in peak value predictions and unknown effects. Other "conservative" measures were more qualitative than numerical but erred on the pessimistic side e.g. degraded cooling effects (high steam/water ratio), geometrical deformation (ballooning blocking of coolant passages), required duration of cooling, etc. These are described in the vast safety regulations documents of the U.S. (NRC) or IAEA, which are publically available e.g. for emergency cooling:

- Code of Federal Regulations, Title 10, "Energy," Part 50, "Domestic Licensing of Production and Utilization Facilities," Appendix K, "ECCS Evaluation Models," U.S. Nuclear Regulatory Commission (1996).
- "Accident Analysis for Nuclear Power Plants," IAEA Safety Reports Series, No. 23, International Atomic Energy Agency (2002).

In the US, Code Scaling Applicability and Uncertainty (CSAU), and Phenomena Identification and Ranking Table (PIRT) marked the kick-off of a variety of code simulation and statistical uncertainty quantification methods developed around the world, with an associated flurry of acronyms now designated under the common name BEPU. Wilson (2013) gives a historical perspective of the original CSAU and PIRT processes and subsequent improvements through to 2010 in BEPU methodologies.

Initially the methods acceptable in safety analysis reports were combined: BEPU was acceptable only in the computer code part while availability of systems as well as initial and boundary conditions remained conservative. Gradually, the latter 2 physical inputs are being replaced by BEPU, i.e. realistic thermomechanical values, whereas for readiness of equipment, harder to mathematically quantify, is still based on conservative assumptions.

The previously described extensive work on cataloguing, quality and completeness assessment of SET and ITF data by OECD/CSNI enabled a better evaluation of the degree of confidence in system codes predictions. CSNI then promoted a number of international conferences around uncertainty methodologies leading to a flurry of publications from academics and industrial stakeholders.

A summary and independent view of these international efforts to use BEPU for licensing can be found by Prošek and Mavko (2003). An overview of the theories and application examples to LOCA is given by Prošek and Mavko (2007). Bucalossi et al. (2010) show the benefits of BEPU over the conservative approach in terms of increased margins to acceptance criteria. D'Auria et al. (2006) detail the process, qualification issues and sources of uncertainty for operating system codes under BEPU and licensing issues are discussed in e.g. D'Auria et al. (2012), Glaeser (2006), and Hrehor et al. (2007).

Beyond system codes applied to LOCA, Unal et al. (2011) make a case to stakeholders and US NRC for extending BEPU to multiphysics modelling and simulation and extending applications even beyond the code's validation and calibration range thanks to data assimilation.

To conclude, there is now a wealth of theory and demonstration papers clearly addressed to Licensing Authorities who monitor and interact on this research progress and will probably decide when BEPU is mature enough to advantageously replace conservative margins. A selection of BEPU papers with quite explicit titles is simply listed below.

Theory

- "The State-of-the-Art Theory and Applications of Best-Estimate Plus Uncertainty Methods" (Prošek and Mavko, 2007).
- "Review of best estimate plus uncertainty methods of thermal-hydraulic safety analysis" (Prošek and Mavko, 2003).
- "Historical insights in the development of Best Estimate Plus Uncertainty safety analysis" (Wilson, 2013).
- "Comparison between Best-Estimate Plus Uncertainty Methods and Conservative Tools for Nuclear Power Plant Licensing" (Bucalossi et al., 2010).
- "Perspectives on the application of order-statistics in best-estimate plus uncertainty nuclear safety analysis " (Martin and Nutt, 2011).
- "State of the art in using best estimate calculation tools in nuclear technology" (D'Auria et al., 2006).

Licensing

- "The Best Estimate Plus Uncertainty (BEPU) approach in licensing of current nuclear reactors" (D'Auria et al., 2012).
- "Task Group on Safety Margins Action Plan (SMAP) Safety Margins Action Plan - Final Report " (Hrehor et al., 2007).
- "Evaluation of Licensing Margins of Operating Reactors Using 'Best Estimate' Methods Including Uncertainty Analysis " (Glaeser, 2006).
- "Improved best estimate plus uncertainty methodology, including advanced validation concepts, to license evolving nuclear reactors " (Unal et al., 2011).

BEPU Application examples

- "Analysis of LBLOCA using best estimate plus uncertainties for three-loop nuclear power plant power uprate " (Kang, 2016).

- "Best estimate plus uncertainty analysis of departure from nucleate boiling limiting case with CASL core simulator VERA-CS in response to PWR main steam line break event" (Brown et al., 2016).
- "RELAP5 Code Analysis of LSTF Small Break LOCA Tests With Steam Generator Intentional Depressurization as an Accident Management Procedure: Investigation on Base Case Result Appropriate for the Best Estimate Plus Uncertainty (BEPU) Application" (Kinoshita et al., 2014).
- "Application of the best-estimate plus uncertainty approach on a BWR ATWS transient using the NURESIM European code platform" (Perin and Escalante, 2017).
- "Application of the best estimate plus uncertainty method to the small break LOCA with high pressure injection failure: Effect evaluation of the model uncertainty on the safety evaluation parameter" (Torige et al., 2015).
- "Application of the Best Estimate Plus Uncertainty method to the small break LOCA with high pressure injection failure: Uncertainty quantification of the RELAP5 model related to fuel clad oxidation, decay heat, fuel clad deformation and SG U-tube condensation" (Torige et al., 2014).

3.3 US NRC (Nuclear Regulatory Commission)

The NRC oversees reactor safety and security, administering reactor licensing and renewal, licensing radioactive materials, radionuclide safety, and managing the storage, security, recycling, and disposal of spent fuel.

The NRC documents complete collections online[5], including ADAMS, the Agency wide Documents Access and Management System[6], which contains ¾ million full text online publically available documents and 2 million pre-1980 document bibliographic citations.

Progress in risk management and modelling techniques is carefully monitored by NRC and eventually accredited, backed by massive record keeping for public inspection, but also for guidance and training to stakeholders. Using keywords from the present literature review, the database can be consulted to check currently acceptable practices.

3.4 OECD/NEA

The NEA offers technical knowledge bases to assess the safety of nuclear reactors and fuel cycle facilities and promotes research or the sharing of data on a cost-sharing basis:

- Ongoing experimental projects[7]
- Ongoing event records database projects[7]
- Completed projects
- CSNI Code Validation Matrix Integral Test Data[8]
- CSNI Code Validation Matrix Separate Effects Test Data[9]

Quite relevant herein are the CFD for Nuclear Reactor Safety Applications (CFD4NRS) workshops and reports providing guidance on CFD application to NRS. The Committee is made up of senior scientists and engineers, with broad responsibilities for safety technology and research programmes, and representatives from regulatory authorities:

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[5] https://www.nrc.gov/reading-rm/doc-collections/
[6] https://www.nrc.gov/reading-rm/adams.html
[7] http://www.oecd-nea.org/jointproj/
[8] https://www.oecd-nea.org/dbprog/ccvm/
[9] https://www.oecd-nea.org/dbprog/ccvm/indexset.html

- “Best Practice Guidelines for the use of CFD in Nuclear Reactor Safety Applications”, NEA/CSNI/2(2014)11[10] (Mahaffy et al., 2014).
- “Assessment of CFD Codes for Nuclear Reactor Safety Problems - Revision 2”, NEA/CSNI/R(2014)12[11] (Smith et al., 2015).
- “Extension of CFD Codes Application to Two-Phase Flow Safety Problems - Phase 3”, NEA/CSNI/R(2014)13[12] (Bestion et al., 2014).
- “Review of Uncertainty Methods for Computational Fluid Dynamics Application to Nuclear Reactor Thermal Hydraulics”, NEA/CSNI/R(2016)4[13] (Bestion et al., 2016c).
- “Uncertainty and sensitivity analysis of QUENCH experiments using ASTEC and RELAP/SCDAPSIM codes”, (Vileiniškis et al., 2014).

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[10] https://www.oecd-nea.org/nsd/docs/2014/csni-r2014-11.pdf
[11] https://www.oecd-nea.org/nsd/docs/2014/csni-r2014-12.pdf
[12] https://www.oecd-nea.org/nsd/docs/2014/csni-r2014-13.pdf
[13] https://www.oecd-nea.org/nsd/docs/2016/csni-r2016-4.pdf

4 System and Subchannel Codes

A large number of computer codes have been developed to design, analyse and operate nuclear reactor systems. Modern nuclear reactor systems operate at a level of sophistication whereby human reasoning and theoretical models alone are not capable of bringing to light full understanding of a system's response to some proposed perturbation. There is, however an inherent need to acquire such understanding, notably for safety analyses. Over the last few decades there has been a concerted effort on the part of the power utilities, regulatory bodies, research organisations and academia to develop advanced computational tools for simulating reactor system thermal hydraulic behaviour during real and hypothetical transient scenarios.

The presence of two-phase flows poses additional complications not encountered with single-phase flows:

- The thermo-physical properties (notably the density, viscosity, and thermal conductivity) of two-phase flows are not readily available as is the case with single-phase flows, and cannot be simply calculated by averaging the liquid and vapour values as the two phases normally flow at different velocities and the apparent density, viscosity and thermal conductivity of the mixture changes dynamically with the flow pattern.
- The two phases can arrange themselves in a variety of flow patterns, and the flow pattern largely controls the physics of the two-phase flow.
- Mass, linear momentum and energy are exchanged through the interface that separates the two phases, which changes dynamically in time.
- Two-phase flows are intrinsically intermittent with local time constants that may differ by orders of magnitude, implying that two-phase flow simulations should be time varying and capable of handling phenomena that vary very fast as well as slowly varying ones.
- The presence of evaporation, condensation and mass transfer between the phases, and their dependence on complicated phenomena such as surface morphology for flow boiling and the presence of non-condensable gases for condensation.
- Thermodynamic non-equilibrium phenomena that appear in sub-cooled flow boiling and in evaporation beyond the boiling crisis.

There are broadly two categories of non-CFD thermal hydraulic analysis tools applied in nuclear power plant design; system codes (Section 4.1) and subchannel codes (Section 4.2).

4.1 System Codes

System codes are conceived to deal with the entire nuclear power system and predict its overall behaviour during numerous scenarios that span both normal and off-normal operating conditions, including the extreme transients encountered during severe accidents. System codes must thus be able to simulate every sub-system and component present in the system, together with their respective couplings and all relevant physical phenomena and processes that characterise their behaviour.

System codes contain many more empirical correlations than 3D CFD codes (Section 5), but System Codes have been extensively validated on a much wider range of NPP-specific test cases than CFD and will remain a major modelling tool in this sector. However, as they are custom-made for PWRs mostly and a few gas or liquid metal cooled reactors, novel design exploration might rely increasingly on CFD codes, where the modelling is less geometry specific and empirical and they are validated on a much wider range of flows and fluids across many industrial sectors. An example of the level of detail represented by a typical system code model is shown in Figure 14.

The principal system codes currently in use in the nuclear industry worldwide are RELAP, TRACE, CATHARE and ATHLET: these codes are briefly described in the following subsections.

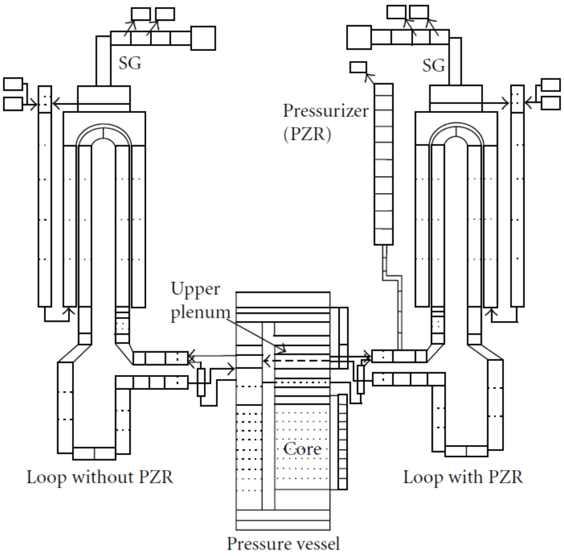

Figure 14: Representative example of RELAP5 nodalisation (Takeda et al., 2012)

4.1.1 ATHLET

The thermal hydraulic computer code ATHLET (Analysis of Thermal-Hydraulics of LEaks and Transients)[14] is being developed by the Gesellschaft für Anlagen und Reaktorsicherheit (GRS) for the analysis of operational conditions, abnormal transients and all kinds of leaks and breaks in nuclear power plants (Di Marcello et al., 2016, 2015; Glaeser, 1995; Hainoun and Schaffrath, 2001; Kirmse et al., 1995; Zhou et al., 2012). The code covers the whole spectrum of design basis and beyond design basis accidents (without core degradation) for PWRs, BWRs, SMRs and future Gen IV reactors with one single code.

ATHLET-CD (Core Degradation) has been developed for accidents with core damage to extend the simulation to include mechanical fuel behaviour, core melting and relocation, debris bed formation as well as fission product release and transport. The range of working fluids covers light and heavy water enabling the transition between sub-critical and supercritical fluid states, and uses the same input deck as ATHLET.

In addition, ATHLET can simulate advanced reactor coolants (helium, liquid metal and molten salt), although these extensions are subject to further development and validation. Numerous institutions in Germany and abroad are applying ATHLET, and the German Federal Ministry for Economic Affairs and Energy (BMWi) sponsors its development and validation.

4.1.2 CATHARE

The CATHARE code (Code for Analysis of THermalhydraulics during an Accident of Reactor and safety Evaluation) is a two-phase thermal hydraulic simulator. Code development began in 1979 at CEA-Grenoble as part of an agreement between the CEA, EDF, AREVA and the IRSN (Bandini et al., 2011; Barre and Bernard, 1990; Bestion, 1990; Emonot et al., 2011; Geffraye et al., 2012, 2011; Valette et al., 2011). The software is currently in its third major revision and is

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[14] https://www.grs.de/en/computer-code-athlet

used, in particular, for PWR safety analyses, verification of post-accidental operating procedures, and research and development.

CATHARE has a modular structure capable of operating in 0D, 1D or 3D. It is capable of modelling any type of water-cooled reactor (PWR, RBMK, VVER, etc.), several types of system loop and also contains a module capable of simulating the behaviour of a nuclear reactor containment vessel in the event of a break in either the primary or secondary circuit. It is capable of simulating the physical phenomena that occur during small and large-break loss-of-coolant accidents, steam generator tube ruptures, feed water line breaks, residual heat removal failures and steam line breaks.

For the investigation of transients leading to severe reactor core degradation (severe accident), CATHARE has been linked to the ICARE software. CATHARE has also been integrated into the IRSN SOFIA (Simulateur d'Observation du Fonctionnement Incidentel et Accidentel) accidental simulator for the EDF reactors. This simulator is used to train specialists, prepare crisis management exercises and to carry out studies in support of reactor assessments.

4.1.3 RELAP

The RELAP5-3D (Reactor Excursion and Leak Analysis Program - Three-Dimensional) code is part of a series of computer programs developed at Idaho National Laboratory (INL) for modelling nuclear power plants (Berar et al., 2013; Guillen et al., 2006; Hoffer et al., 2011; Hou et al., 2017; Mangal et al., 2012; Mesina, 2016, 2010; Mesina et al., 2014). The first RELAP code release was funded by the US Atomic Energy Commission, which is now the US NRC, to model small-break loss-of-coolant accidents specifically for PWRs.

In the early 1980s, the United States Department of Energy (US DOE) began sponsoring additional RELAP5 development, which continued until 1995 up to the release of RELAP5/MOD3.2. At this point, the code was split into a US NRC version (TRACE) and a US DOE version (RELAP5-3D).

The RELAP5-3D code maintains the proven performance and validation history of RELAP5/MOD3.2 with additional enhancements, including a fully integrated, multi-dimensional thermal hydraulic and kinetic modelling capability, a new matrix solver for 3D problems, new water properties and improved time advancement.

RELAP5-3D's modelling capability has expanded to include large-break loss-of-coolant accidents and operational transients for PWRs, BWRs, MSRs, LMFRs, HTGRs, supercritical fluid and advanced reactor designs. Most recently, RELAP5-3D is being applied to model advanced reactor designs such as small modular reactors and a traveling wave reactor.

The RELAP code is also installed in nuclear plant operator training simulators at many sites around the world and in universities and research centres to train operators on basic reactor dynamics. Notably, the RELAP code is used in industry, research centres and academia for pre-test and post-test simulations to support the design of nuclear thermal hydraulics test facilities, and interpret the experimental data that these provide.

4.1.4 TRACE

The code TRACE (TRAC-RELAP Advanced Computational Engine) is the thermal hydraulics analysis tool used by the US NRC for nuclear reactor design licensing in the USA (Berar et al., 2013; Freixa and Manera, 2011; Jaeger et al., 2013; Lin et al., 2014; Mascari et al., 2011; Wulff, 2011). The code consolidates and extends the capabilities of NRC's 3 legacy safety codes: TRAC-P (system code originally designed to model large-break loss-of-coolant accidents and system transients for PWR reactors), TRAC-B (system code originally designed to model small and large-break loss-of-coolant accidents and system transients for BWR reactors) and RELAP (see above).

TRACE is able to analyse small and large-break loss-of-coolant accidents and system transients in both PWRs and BWRs. The capability exists to model thermal hydraulic phenomena in both one-dimensional and three-dimensional space.

4.2 Subchannel Codes

The whole plant behaviour, as predicted by system codes, is only part of the process of determining the thermal hydraulic operating limits and safety margins of a reactor because the representation of a reactor core is coarse grained to the point where the behaviour in individual channels is not captured (Figure 14). The thermal hydraulic safety margins of most reactors are currently assessed using subchannel analysis codes, where the governing equations of mass, momentum and energy are solved in control volumes that are resolved at a level of the gaps between individual fuel rods.

The flow distributions in the rod bundle geometries are predicted by empirical correlations for heat and momentum transfer at surfaces and interfaces, as well as inter-channel mixing models to account for the transport between adjacent sub-channels. These subchannel codes require empirical correlations to be implemented and are a representation of intermediate level of detail: they are coarser than a CFD model, but resolved sufficiently to provide estimations of the local conditions of the sub-channels in the limiting fuel assembly of the core. Subchannel codes involve more complex representations of the physics of thermal hydraulic phenomena than system codes, and are required to predict local fuel temperature, void fraction, and the margin to CHF.

Increased computing power has allowed subchannel codes to represent entire reactor cores, rather than just a single channel, and have progressively added 3D solution features, resulting in a gradual overlap with lower-resolution forms of CFD. Another technique that has approached this functionality, but from the opposite direction is Coarse-Grid-CFD where flow between fuel pins and large and medium scale flow features are simulated, but at a lower fidelity than ‘true’ CFD.

Examples of subchannel codes in current use and under further development are CTF, FLICA, SUBCHANFLOW and VIPRE.

4.2.1 CTF

The COBRA (COolant Boiling in Rod Arrays) software was developed to solve the flow and enthalpy distribution in nuclear fuel rod bundles and cores by Pacific Northwest National Laboratory (PNNL) in the 1960s. This was expanded by PNNL in 1980 under sponsorship of the US NRC to form the original COBRA-TF (Two-Fluid) code. Since then, various organisations have adapted and further developed the code, resulting in many other COBRA variants, such as F-COBRA-TF, COBRA-FLX, COBRA-IE, MATRA and ASSERT-PV (Galimov et al., 2015).

CTF is the name given to the version of COBRA-TF developed and maintained by Oak Ridge National Laboratory (ORNL) and the Reactor Dynamics and Fuel Modelling Group (RDFMG), initially at Pennsylvania State University, and currently at North Carolina State University (NCSU). CTF is based on a separated flow representation of two-phase flow into three fields: liquid film, liquid droplets and vapour. It is capable of modelling solid structure and fluid regions within the core under normal operation and accident scenarios. Improvements in CTF include turbulent mixing, void drift and grid-spacer heat transfer enhancement.

CTF has recently been included in two large projects: US DOE CASL and European Commission (EC) NUclear REactor SAFEty simulation platform (NURESAFE). This has led to a number of developments within the code and resulted in a significant amount of verification and validation testing. CTF has also been integrated into the Virtual Environment for Reactor Applications (VERA) Core Simulator environment, and work is underway to modify and validate CTF for MSR and SFR reactor technologies.

4.2.2 FLICA

FLICA-4 is a 3D two-phase flow code for reactor core analysis that began development in the 1970s at CEA (Fillion et al., 2011). It uses a four-equation mixture model (mass, momentum and energy of mixture and mass of vapour) with a drift-flux model to simulate the relative velocity between phases.

CEA began developing FLICA-OVAP in 2005, which builds on FLICA-4 and includes both a two-fluid two-phase flow model and a multi-field model that accounts for both liquid and vapour phases. The FLICA-OVAP platform incorporates both subchannel and CFD scale applications and can be coupled to multi-physics and multi-scale applications.

FLICA was used as part of the EC NURESAFE project, and can be applied to two-phase flow in PWRs and BWRs.

4.2.3 SUBCHANFLOW

SUBCHANFLOW is based on COBRA and was developed by the Institute for Neutron Physics and Reactor Technology (INR) at the Karlsruhe Institute of Technology (KIT).

SUBCHANFLOW is a single- and two-phase (three-equation mixture model) subchannel code that is used to simulate core geometries built from rectangular and hexagonal fuel bundles. Empirical correlations are then used for pressure drop, heat transfer coefficient and void generation with mixture equations for wall friction, wall heat flux and slip velocity. The solution progresses axially up the core, which limits the code to cases with positive flow up the core.

SUBCHANFLOW was used as part of the EC NURESAFE project, and can be coupled to a number of multi-physics codes. It includes properties for liquid metal, water, helium, and air, and so can be applied to PWRs, SFRs, LFRs and HTGRs.

4.2.4 VIPRE

VIPRE-01 (Versatile Internals and component Program for REactors) was originally developed from COBRA by Battelle Pacific Northwest Laboratories under sponsorship of the Electric Power Research Institute (EPRI). The VIPRE User Group is run by Zachry Nuclear Engineering Inc., who manage the maintenance and development of the code for member organisations and EPRI.

VIPRE-01 predicts the three-dimensional flow field and fuel rod temperatures for single- and two-phase flow in PWR and BWR cores for an interconnected array of channels. It solves the finite-difference equations assuming homogeneous equilibrium (empirical models are included for vapour/liquid slip and subcooled boiling) incompressible flow with no time-step or channel size restrictions for stability.

4.3 Summary

System and subchannel codes have been developed since the start of the application of computer analysis to nuclear thermal hydraulics. They have gradually been developed and can deal with many of the complexities of nuclear power systems. System codes are the only tool presently available that are capable of predicting the overall performance of a nuclear power system and its evolution during transients and accidents.

The system and subchannel codes are all based on best-estimate methodologies: this approach aims at providing a detailed realistic description of postulated accident scenarios based on best-available modelling methodologies and numerical solution strategies sufficiently verified against experimental data from differently scaled separate effect test and integral effect test facilities.

Nearly all current two-phase flow models used in present best-estimate thermal hydraulic system codes are based on the so called two-fluid model (Bestion, 2008; Levy, 1999; Todreas and Kazimi, 1990). Phases are treated as interpenetrating continua and macroscopic separate balance equations for each phase are obtained by a space and/or time or ensemble averaging of the local instantaneous basic flow equations, with source terms representing the interfacial transfers for mass, momentum and energy. The presence of different flow patterns in two-phase flow is recognised by implementing different closure laws for mass, momentum and energy exchange that are tailored to each specific flow pattern.

Physical models are required in system and subchannel codes to close the system of equations. Closure relationships concern mass, momentum, and energy exchanges between phases and between each phase and the wall. Specific separate effect tests are performed and analysed to investigate two-phase flows in conditions representative of the reactor transients to be simulated. Based on these data new correlations are developed when existing models were not satisfactory. The degree of empiricism depends on the comprehension of the physical mechanisms involved. Modern system and subchannel codes implement so many empirical correlations that it would be impractical to provide a complete review here.

5 Computational Fluid Dynamics (CFD)

CFD simulations provide predictions of 3D and time dependent velocity, pressure, temperature fields, by numerical solution of fundamental partial differential equations, on meshes which divide the domain of interest into cells. When turbulent eddies, droplets or bubbles are small compared to the cell size, their effects still need to be modelled. CFD often includes multipurpose empirical models for small scale features which cannot be captured on meshes comprising millions of cells (as are often employed by industry).

Currently the use of CFD in the design of NPP is often limited by both the timescales/cost associated with performing the modelling and uncertainty in the final predictions. As computing power grows and the costs of finer meshes are reduced, there is the potential for CFD to employ fewer modelling assumptions and inevitably CFD will be used for a wider range of applications. As System codes integrate more 3D modules and commercial CFD codes provide easy-to-implement 1D links between components the frontier between the two becomes blurred. With this flexibility one can envisage a gradual and automatic evolution of the simulation from a coarse quick prototyping idea to a fully refined geometry as the idea matures.

CFD is another chapter that would need to be blown up to encyclopaedic proportions to give an impartial and comprehensive picture of its inception, 50 years evolution, current practises and progress due to exponential growth of affordable computer power. This section is shaped by the excellent and timely contribution (by the Chief Editor of the journal of Nuclear Engineering and Design) to the TH of nuclear reactors handbook:

- Hassan, Y., (2017). “An overview of computational fluid dynamics and nuclear applications”, in: D’Auria, F. (Ed.), Thermal-Hydraulics of Water Cooled Nuclear Reactors. Woodhead Publishing, pp. 729–829.

Hassan’s presentation (which at 100 pages is still brief) is highly relevant because it concentrates on the heart of NPP TH modelling by avoiding the easy route of bland technical overview, it explains why “*Some think that the CFD is promising and can play a key role in nuclear thermal fluid problems now and in the near future, while others think that CFD is not reliable compared to the experiment and it will take a very long time*”. In short, CFD is now a very mature self-standing technology, developed and applied in all areas of Engineering, but due to the complexity of its practice, the reliability of CFD results is reliant on user expertise and validation for a given range of applications.

Best Practice Guidelines and thorough validation has been the aim of numerous international efforts, particularly in the NPP sector which Hassan was also able to reasonably summarise, notably the large efforts by OECD/ NEA/CSNI, and CFD4NRS series of Workshops, with both praise and criticisms (which we share).

To summarise Hassan’s synopsis of *a “work-in-progress building site”* the list below reproduces some of the NPP TH CFD modelling insights he provided:

- Motivation for CFD in NPP: is the right representation of CFD available to decision makers and end users?
- Emphasising differences between CFD and System TH codes: what System TH codes cannot do.
- The ideal and real in nuclear thermal fluid CFD:
  - Ideal: 3D computed data is accurate, reliable and trustworthy.
  - Real: the need to calibrate, verify and validate models against the results of experiments.
- Emphasising the issues with System TH codes that CFD codes cannot address.

- Detailing the variety of NPP TH problems which can be addressed by CFD analysis.
- Addressing the difficulties in applying CFD analysis to nuclear thermal hydraulic problems.

As a complement we will explain why the same approach of extending mathematically sound finite element approach to continuum mechanics to fluid flow simulation has failed. Instead the exotic and disparate range of 'recipes' developed separately by hundreds of fluid-dynamists finally converged toward unstructured-grid finite volumes in 3 world-leading commercial codes, Fluent, CFX, STAR-CCM+, and in the open source OpenFOAM and *Code_Saturne*.

5.1 Finite Volume Codes

What can be notable to numerical engineers outside of the discipline is the large variety of different CFD methods that have been developed. Conversely, the structures and solid mechanics communities settled on Finite Elements with a clear breakdown of the problem solving steps into:

- Meshing; easily automated when using tetrahedrons;
- Discretisation; mathematical transformation of partial differential equations (p.d.e.) into a system of algebraic linear equations, e.g. integrating by parts the beam p.d.e. pre-multiplied by known shape functions several times;
- Linear systems solvers; vector-matrix product inversion, which can be efficiently executed by computers; and
- Post-processing.

Each of these steps was highly optimised by specialists from different disciplines, especially applied mathematics, while physicists could focus on the phenomena with little FE expertise.

In fluid dynamics, the variety of phenomena originating from the non-linearity of the p.d.e. is so broad that for each one, a different CFD method has emerged: panel methods for potential flow, vorticity-stream function for vortex shedding, marker and cell for free-surface flows, spectral methods for DNS, Approximate Riemann solvers for shock waves and finite volume methods for RANS models. Each method is highly efficient for its particular application area because the physicists have intervened at each stage to choose an appropriate trade-off, for example:

- Choice of original form of flow p.d.e., either Lagrangian or Eulerian; quasi-linear or conservative forms, e.g. $u\,du/dx + \rho^{-1}dP/dx$ or $d(1/2u^2 + \rho^{-1}P)/dx$ respectively; choice of velocity, vorticity or momentum as primitive variables etc;
- Structured grid meshing for thin boundary layers (initially hand-made rather than Voronoi-tetra);
- Conservation of mass and momentum rather than local accuracy in sharp gradient regions for time-dependent flows; and
- Iterative rather than exact linear systems solver (since the matrices containing convection, density, turbulent or temperature dependent viscosity… change at every time-step or global iteration it is extremely wasteful to use a direct matrix inversion).

5.1.1 Origins and Originality of CFD

CFD for time-dependent flows such as a drop hitting a fluid surface, a dam break, a vortex street really took off at Los Alamos National Labs (Harlow and Welch, 1965) where instead of direct finite differences applied to the Navier-Stokes equations Harlow's fluid dynamics group combined a range of physicist's ideas: tracking particles moved by forces, writing balance equations on 3 overlapping staggered grids for velocities and pressure etc.

As Harlow (2004) recalls: *“Early 1960s there was a lot of suspicion about numerical techniques. Computers and the solutions you could calculate were said to be the playthings of rich laboratories. You couldn’t learn very much unless you did studies analytically. The truth, of course, has turned out to lie in the complementary interaction between calculations and analysis and in the validation of both, through comparisons with experiments. .. improvement came with the capability to record our flow calculations on 35-mm film …we found that many universities, industries, and governmental agencies began to solve problems of interest using numerical techniques…”*

CFD in the US was also developing along similar principles in weather prediction. The co-inventor of the Smagorinsky-Lilly model for LES noted (Lilly, 1965) “*finite differences may be appropriate for problems involving a single energetic event …[but] are severely inadequate for highly non-linear atmospheric and oceanographic equations which require that momentum, energy, circulation, heat and other be created, transformed, dissipated through several cycles [be computed] with minimum consistency i.e. non-random computational error… A numerical calculation in which 10% of the mass of the atmosphere is lost through computation error may be highly suspicious*”.

5.1.2 UK’s “Practical CFD” Developments

Simultaneously in the UK, Brian Spalding and his Imperial College group in the mid-60s and mid-70s developed general purpose CFD software tools for “engineering” flows of interest to the industry, i.e. able to deal with turbulence, chemical reactions and combustion, incorporating the k-ε model with Brian Launder, upwind differencing for convection etc.

PHOENICS was the first commercially available code (through CHAM Ltd[15]) in 1978, gradually incorporating multiphase flows, combustion, and radiation. Like the Los Alamos group Spalding also promoted a physical rather than a mathematical approach where the focus of interest should not be variables but their “fluxes” and “control volumes” viewing each node of a grid as an independent tank which exchanges fluxes with other tanks/nodes, a precursor of the “Finite Volume” method (Runchal, 2009).

The FV method stems from the basic physics principal that rate of change of a quantity inside a control volume or mesh cell is equal to the sum of the fluxes across the bounding (flat) surfaces. Heat, mass or momentum flowing out of one cell is exactly equal to what goes into the neighbouring cell, such that these quantities are globally conserved even on coarse meshes. The convection and pressure terms lend themselves to this integration by Gauss theorem directly while some approximations are needed to compute the second order viscous or diffusion terms, interpreted as divergence of a gradient times a diffusivity, but in turbulent flows the latter is only an approximate rheology model anyhow while divergence-to-fluxes integration by Gauss formula ensures conservation. The p.d.e. of a scalar variable submitted to convection, diffusion + source term is first written in conservative form:

$$\frac{\partial \rho\varphi}{\partial t} + \nabla \cdot (\mathbf{U}\rho\varphi) = \nabla \cdot \big(\rho\gamma\nabla(\varphi)\big) + q_\varphi$$

Integrating on a (here fixed) control volume Ω of surface *S* with normal n pointing outside and using Gauss’ formula gives the finite volume (FV) conservation equation:

$$\frac{\partial}{\partial t}\int_\Omega \rho\varphi \,\mathrm{d}\Omega + \int_S \rho\varphi\mathbf{U}\cdot\mathbf{n}\,\mathrm{d}S = \int_S \rho\gamma(\nabla(\varphi)\cdot\mathbf{n})\,\mathrm{d}S + \int_\Omega q_\varphi\,\mathrm{d}\Omega$$

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[15] http://www.cham.co.uk

Also at Imperial College, David Gosman and his group later developed the STAR-CD code which was particularly successful in the automotive, heat transfer and combustion sectors, but was also used for NPP TH e.g. by AREVA. Joining a US partner to form CD-Adapco, the software was completely re-written in object-oriented C++ language in 2004 with new code name STAR-CCM+, the "CCM" standing for "Computational Continuum Mechanics". C++ facilitates modular developments, friendly interfaces and integration with CAD. STAR-CCM+ included the world's first commercially available polyhedral meshing algorithm, i.e. control volumes with any number of faces based on agglomeration of tetrahedra and hexahedra thus enabling easy automatic meshing or mesh refinement with e.g. both wall-normal boundary layer refinement of structured CFD codes and flexibility of finite elements in complex geometries. In 2016, Siemens acquired CD-Adapco.

5.1.3 Finite Volumes Versus Finite Elements

Fully unstructured finite volumes had been a target for STAR-CD early on (Muzaferija and Gosman, 1997) but also at Fluent Inc. in the US (Mathur and Murthy, 1997). Both papers describe how the Taylor series expansion of the finite difference method may be combined with FV to interpolate or extrapolate the value from the cell centre to the surfaces or even to neighbouring cells.

A pragmatic presentation of the FV method common to current major commercial and in house engineering CFD codes can be found in the book by Ferziger and Perić (2002). As with Harlow and Spalding the book takes the fluid dynamist’s point of view rather than mathematicians as there a number of approximations, e.g. the FV balance gives the average value in the cell which is later interpreted as the local value at the cell centre in interpolations; as the Gauss theorem can only be used once, second order derivatives (diffusion, pressure equations) are problematic; the extrapolation from 2 neighbour cell centres sharing a common surface may lead to over-determination resolved by a least square method; the interpolations assume that the line connecting 2 cell centres cut the surface orthogonally at its centre, then corrected using older values (“deferred correction”).

As a result of approximations in distorted cells the method may converge even more slowly than first order. However, the flexibility of polyhedral cells allows high quality grids to be automatically generated, even for LES (Moulinec et al., 2005) or DNS (Addad et al., 2015) where fine tuning the grid to the local turbulent length-scale is the key factor.

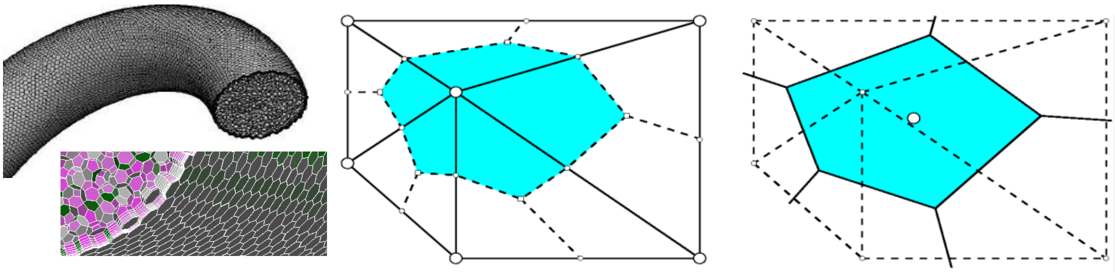

Figure 15: Polyhedral cell mesh for pipe bend LES with boundary layer insertion, initial tetra grid and dual mesh to polyhedral transformation

Also UK based and similar to STAR-CCM+ (FV and unstructured grids in C++) is OpenFOAM which origin is traced back to Henry Weller and others from Gosman’s Imperial College group. It is general-purpose open-source, i.e. with free access to the source-code. It has spread rapidly around the international CFD research community, but also into large companies particularly in the automotive and naval sectors. This large research community interacts via forums and wikis, while support, training and code development can be commissioned from OpenCFD Ltd and CFD Direct.

ESI based in Paris developed FE software with large deformations PAM-CRASH from 1985 and in 1997 acquired the Framatome (now AREVA) software branch Framasoft. In 2012, it bought OpenCFD Ltd and the OpenFOAM trademark, but the OpenFOAM code itself continues to be freely accessible under an open source license.

FLOW3D was the UK's Atomic Energy Authority (AEA) CFD code. Its privatised business, AEA Technology bought the Canadian unstructured solver TASCflow in 1997 which later became CFX. It was used in by NPP stakeholders in the UK and Europe.

ANSYS, a leading commercial supplier of Computer Aided Design Engineering, purchased ICEM CFD, specialised in meshing for CFD and FE analysis. As a sign that FE was not suitable for TH, ANSYS also bought the CFX division of AEA Technology in 2003, then in 2006 ANSYS acquired Fluent Inc. developers of the most widely used CFD code.

EDF R&D’s open source *Code_Saturne* is similar to the major CFD codes star (CCM+, Fluent, OpenFOAM). It is based on a co-located Finite Volume approach that can handle meshes built with any type of cell (tetrahedral, hexahedral, prismatic, pyramidal and polyhedral) combined with any type of grid structure (unstructured, block structured or mismatching grid-blocks). It is able to simulate either incompressible or variable density flows, with a large variety of models to account for turbulence. *Code_Saturne* is particularly optimised for massive TH simulations and hence often benchmarked on the world’s largest computers such as Julich, DOE Argonne, Barcelona SPC and UKRI-STFC Hartree Centre, in addition to EDF’s own. For instance Moulinec et al. (2016) report a 1 billion cell simulation of flow inside the AGR fuel assembly, including the tiny spiral ribs, and mixing with cold gas leakage through the graphite sleeve (Figure 16).

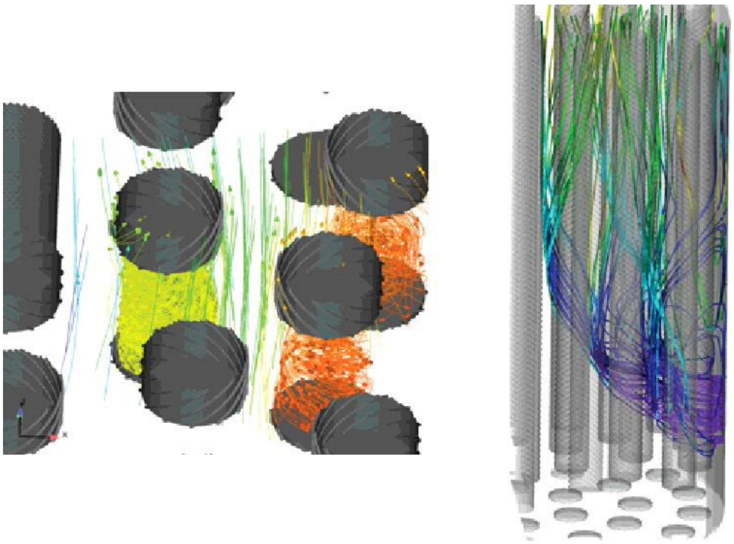

Figure 16: One Billion cells *Code_Saturne* simulation of flow in AGR fuel assembly (Moulinec et al., 2016)

In 1982-2000, EDF R&D had the largest HPC computers in France (CRAY-1, YMP, and later BlueGene) and “practical” fluid dynamists were following UK and US original developments. While theoreticians in the “Informatics and Applied Mathematics” department were given decades and large budgets to extend finite element approaches to fluid-dynamics (and struggling to compute the simplest laminar flows), engineers were developing ad-hoc FV type codes to provide quick responses to industrial fluid mechanics problems. Collaborations with Stanford, Imperial College, UMIST Manchester and the CEGB greatly helped this “pragmatic” technology transfer.

Whereas it is quite easy for physicists to directly update their constantly evolving models in the FV framework (“tanks and pipes”), FE requires a number of mathematical manipulations (integration by parts to weak formulation, assembly sub-matrices), it is limited to few cell shapes (tetrahedron, hexahedron, square pyramids and triangular prisms), struggles with concepts such as upwinding and does not lend itself to massive parallelisation as easily as FV. Iterative solvers such as GMRES (Generalised Minimal RESidual) don’t even need a vector-matrix structure; a direct measure of the physical imbalance i.e. “residual = rate of change in volume minus sum of fluxes” is sufficient to improve the next iteration. As fully unstructured finite volumes became possible, the last advantage of FE disappeared. Physicists and applied mathematicians joined efforts to create a “common solver” with all of the physical models and HPC performance gains. This later became *Code_Saturne*.

In 2007, in order to establish a large community of users and to extend, by this means, the confidence it can have in its software, EDF made *Code_Saturne* open-source. It is provided under the GNU General Public Licence. Associated libraries for “Base Functions and Types” and “Finite Volume Mesh” are provided under the GNU Lesser General Public Licence (LGPL).

5.1.4 Merging of CFD codes

20 years ago fluids groups were either developing their own codes or adapting one from early inventors such as ICL’s group, recruiting their students or experimenting yet more exotic techniques. There was no documentation other than PhD dissertations or proximity of the code author. A number of industry and academic groups further developed their specific “in-house” codes or rather versions so these diverged except where centralised funding encouraged collaborations (such as in EU Aerospace programmes). The EU Science Foundation interviewed many of the authors of this review to ask “why the CFD community is so fragmented” (and requesting funding for several dozens of codes).

The diversity of flow regimes and optimisation to specific HPC hardware led to this fragmentation. However, as the number of users grew, the imperative for documentation and validation (which programmers found tedious) became obvious, but only affordable in large projects.

After a series of acquisitions and mergers a large number of “in-house” CFD codes (notably originating from the UK), the world-wide commercial CFD market is dominated by 2 companies and 3 unstructured FV codes with very similar models and numerical solvers. Enormous efforts could then be devoted to ease of use but also documentation (theory manual, user manuals, examples, Best Practice Guidelines (BPG) specific to numerous fluid-flow types and complex thermodynamics). This html documentation spanning tens of thousands of pages is outstanding even from an academic view, explaining not only the physical phenomena models but also the way they are discretised and solved. Training of Engineers in fluid mechanics is now based on experimenting with these virtual wind tunnels and power plants, even in academic birthplaces of CFD, then pitfalls and BPG are taught later. How CFD works in detail is mostly delayed to Master level. This new generation will be more open to accepting, perhaps too accepting, NPP design by CFD than the retiring System Code and ITF facilities experts.

Alongside commercial software models, CFD techniques are still progressing through “open-source” codes and consolidating through natural selection (if it’s free, choose the best and most widely accepted). Less user-friendly interfaces, documentation and validation are compensated by large and serious Wiki and open forum communities.

Far from competing, collaboration between commercial and open-source developers and academia benefit each other, ending the era of a fragmented CFD community. Experts train and move between the 2 poles and, with the now common FV framework, prototypes of improved models in the later are more rapidly integrated in the former benefiting the whole industry.

Similar open-source communities are preparing the longer term evolution beyond FV with more exotic discretisation methods, some starting upstream of the Navier-Stokes equations, e.g. with simpler particle collision type algorithms, the crudeness of which is compensated by more efficient use of the simple, but raw power step change of swarms of graphic processing units

In his CFD chapter contribution to the book on NPP TH, Hassan, Y., (2017) lists Lattice Boltzmann methods (LBM)[16] and Immersed boundary methods (IBM)[17] as most relevant. Entry points for similar emerging simple and brute force methods may be found on Wikipedia. For example, Smoothed-Particle Hydrodynamics (SPH)[18], mesh-free methods[19], moving particle semi-implicit method[20], multi-particle collision dynamics[21] and stochastic Eulerian Lagrangian method[22].

5.2 Mesh Generation and Optimisation

Independent of the physics being tackled (single-phase flow, multi-phase flow, multi-physics including Fluid-Structure Interaction (FSI), Conjugate Heat Transfer (CHT), or multi-scale involving CFD and neutronics, for instance) thermal hydraulic simulations are of two kinds, either high-fidelity simulations targeting petascale and now exascale machines, potentially requiring meshes of up to 10s or 100s billions of cells or elements, or much smaller scale simulations involving more modelling, but on optimised meshes designed to capture a given physics. Since the latter are most commonly used in industry, the design and build of a suitable mesh is both vital for success and a significant proportion of the cost of building a model for use in a CFD code.

This section presents both aspects separately, even if optimised meshes should eventually be used for some high-fidelity simulations. ‘High-fidelity’ CFD simulations refer to Direct Numerical Simulation (DNS) or Large-Eddy Simulation (LES).

5.2.1 Mesh Generation

Generation of structured meshes, Cartesian or body-fitted for finite difference-based codes for DNS is usually handled by the codes themselves using on-the-fly meshing. This also has the huge advantage of not having to deal with Inputs/Outputs because no mesh is read. However, for other types of software, such as the ones based on the Finite Volume Method (FVM), Finite Element Method (FEM) or HP-spectral method, for instance, the size of the mesh used in high-fidelity simulations (multibillion cells) makes serial mesh generation unrealistic, because of both memory and time required for the operation. There is therefore an obvious need for parallel mesh generators. An example of a parallel, open source mesh generator is snappyHexMesh,

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[16] https://en.wikipedia.org/wiki/Lattice_Boltzmann_methods
[17] https://en.wikipedia.org/wiki/Immersed_boundary_method
[18] https://en.wikipedia.org/wiki/Smoothed-particle_hydrodynamics
[19] https://en.wikipedia.org/wiki/Meshfree_methods
[20] https://en.wikipedia.org/wiki/Moving_particle_semi-implicit_method
[21] https://en.wikipedia.org/wiki/Multi-particle_collision_dynamics
[22] https://en.wikipedia.org/wiki/Stochastic_Eulerian_Lagrangian_method

which is part of OpenFOAM. Good overviews of mesh generation are given by Chrisochoides (2005) and Hassan et al. (2007).

Alternative ways to full mesh generation do exist, though, such as mesh joining of already very detailed parts of the final configuration as well as mesh multiplication. There principles are briefly presented here.

5.2.1.1 Mesh Joining

Current serial mesh generators are limited to a few hundred million cells/elements because of the memory they require. Moreover, generating meshes is a task that requires great expertise, especially for complex geometries, where cells/elements of a high quality should be generated at walls and around obstacles. Memory requirements of 1 to 3 GB per million cells can be used as a rule of thumb to estimate the largest size of mesh that can be generated on a single computer.

Mesh joining is then a very attractive option to circumvent the problem of generating huge meshes, as the original geometry is split into several parts that can be meshed independently. Faces at the interfaces between the different parts might be non-conforming. These are detected by an octree algorithm, before conforming sub-faces, and then new cells are built. A detailed explanation of how this technique works is available in Fournier et al. (2011).

5.2.1.2 Parallel Mesh and Surface Multiplication

Mesh multiplication or global refinement or homogeneous mesh refinement consists of homogeneously splitting all the cells of an original mesh to end up with a much finer mesh. This method is increasingly popular to work on meshes using hexa-, tetrahedral and prismatic cells (Houzeaux et al., 2013; Moureau et al., 2011; Yilmaz et al., 2012) but the generalisation to arbitrary polyhedral cells is difficult. The principle of the method is to start with parent hexahedral, tetrahedral and prismatic cells all split into sub-cells, which are of the same type as the original cell. This allows the conservation of the aspect ratio of the initial mesh.

This process is run in parallel, but using the partitioning of the original mesh. The quality of this partitioning for the finest mesh might not be sufficient enough for the solver to exhibit good performance with the finest mesh, as any load-unbalance is magnified by the multiplication process. A new partition of the refined mesh should be computed to ensure a better load balance.

Curved solid surface features are lost from one level of refinement to the next one because linear interpolation is carried out. To improve wall description, Yilmaz et al. (2012) suggest starting from a very fine original surface mesh, which would be suitable for the finest mesh, and after each subdivision to linearly map the subdivided surface mesh onto the fine original surface mesh. A similar technique is available in Gargallo-Peiró et al. (2017).

5.2.2 Mesh Optimisation

This section is split in two, focusing first on static mesh optimisation, where prior simulations are performed in order to optimise mesh density as for a given turbulence model, for instance, and dynamic mesh optimisation, relying on Adaptive Mesh Refinement (AMR).

5.2.2.1 Static Approach

This approach requires prior simulations on lesser quality meshes. It is used to optimise wall treatment, as for instance by computing an estimation of the turbulence and thermal boundary layer thicknesses. This helps determine the height of the prismatic layers generated at the wall and the number of layers, adapting both to the turbulence model used (low or high Reynolds modelling). A new mesh is then generated, either by the mesh generator itself, or by the CFD solver, if this feature exists, as in *Code_Saturne*.

Prior simulations using RANS modelling might also be used to prepare meshes for LES, by computing the Taylor turbulent micro-scale. This estimation is then used to refine some parts of the original mesh Addad et al. (2008).

5.2.2.2 Dynamic Approach

Adaptive mesh refinement (see Berger and Colella (1989) and Plewa et al. (2003) for instance) consists of dynamically refining or de-refining some parts of the mesh, in the course of a simulation. Triggering refinement/de-refinement is usually automated. It might be performed by computing the gradient or the second derivative of a quantity of concern and then analysing its steepness. If the gradient/second derivative is beyond a given threshold, refinement/de-refinement is activated.

Another possibility is to compute an error representative of the quality of the solution. If this estimation is too large, mesh refinement is carried out. The key issue when performing AMR and HPC (several 1,000s of processors) is to preserve the good load-balance of the original mesh. This is possible either by re-partitioning and re-distributing the new mesh over all the processors, or by identifying the processors which are over-loaded and re-distributing some of the new cells/elements to the other processors.

5.2.3 Concluding Remarks

The way forward to generate meshes to run for high fidelity simulations targeting peta- and exa-scale would combine both techniques, mesh joining of detailed parts of a complex configuration and mesh multiplication. Smoothing the final mesh might be required for the cells located at the interfaces between the various parts of the original mesh to be less skewed. Highly optimised meshes could be generated by static of dynamic approaches.

5.3 Turbulence Modelling

The subject of turbulence modelling for CFD, even purely restricted to thermal hydraulics applications, is a vast one, and a comprehensive coverage is beyond the scope of the present document. However, the sections below serve to outline the main approaches currently employed in industrial and research applications.

Section 2 has introduced a number of modelling challenges in nuclear thermal hydraulics, most of which, for example conjugate heat transfer, fluid-structure interaction, surface roughness, transience, and low values of the molecular Prandtl number, have significant turbulence modelling challenges to be addressed. In addition, Section 2 specifically identified phenomena such as those of natural and mixed convection which increase the anisotropy of turbulence, the modelling of near-wall turbulence and representation of the turbulent heat fluxes as major turbulence modelling challenges in nuclear thermal hydraulics.

This section provides an overview of the most widely used models of turbulence employed within the framework of Reynolds-Averaged Navier-Stokes (RANS) equations, which provide the most cost-effective approach to the representation of turbulent motion, and presents predictive comparisons for cases relevant to nuclear TH. Higher fidelity, and more costly, turbulence modelling methodologies (LES and DNS) are also introduced and their role in TH hydraulics simulations is briefly discussed. Subsequent sections also touch upon turbulence modelling issues related to specific challenges.

The starting point for all approaches is the Navier-Stokes (NS) equations which remain valid in turbulent flows, but to reduce the cost of tracking all turbulent eddies as in Direct Numerical Simulation (DNS) some averaging is generally introduced. This leads to “average of velocity products”, which differ from “products of averaged velocities”. The difference between the two are the Reynolds Stresses or more generally “second moments”, while “first moments” are mean velocity, temperature or concentration obtained by numerically solving the Averaged Navier-Stokes equations.

Exact equations for second moments can be derived but will contain 3rd moments etc. A model or “closure” must be introduced. This closure is semi-empirical, based on experimental correlations for some dimensionless coefficients valid for a range of baseline flow regimes and the general shape of equations (inevitably there will be many in this section) derived from the original NS and subsequent higher moments equations. The original RANS approach is based on a very wide spatial, or very long-time, averaging for homogenous or steady state cases respectively. In Large Eddy Simulation (LES) the averaging (called “filtering”) is more limited such that turbulent structures large enough to be captured on the mesh are computed while only the smaller “sub-grid scale” ones need to be modelled.

Hassan’s (2017) chapter in the TH book covers the whole range of models from RANS to LES and in-between hybrids with virtually no equations but a focus on benchmarking, NPP applications and authoritative opinions, as chief editor of Nuclear Engineering and Design and a CFD expert. Complementarily, and as model developers, we present below some of the more popular types of models while applications to NPP are presented throughout this report.

5.3.1 Reynolds-Averaged Navier-Stokes (RANS) Approaches

In these approaches none of the turbulent structures within the flow are resolved by the simulation. Instead, the “averaged” flow field is solved for, and the governing equations for momentum and temperature then contain additional terms (the Reynolds stresses and turbulent heat fluxes respectively) that have to be modelled.

5.3.1.1 Linear Eddy-Viscosity Models

Linear Eddy-Viscosity Models (EVMs) use a simple linear algebraic relationship to model the Reynolds stresses in terms of the mean strains and a turbulent viscosity:

$$\overline{u_i u_j} = -\nu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) + 2/3\, k\delta_{ij}$$

Models within this class are typically categorised into zero-equation (or mixing length), one-equation, or two-equation models, depending on how many additional transport equations are introduced to model the turbulent viscosity. Of these, the two-equation models are generally seen as the most realistic prospect for general flow modelling, as the others usually require significant case-to-case and ad-hoc input (for example, in prescribing the variation of turbulence length scale across the flow).

The k-ε model (Launder and Spalding, 1974) is one of the most well-known and widely-used two-equation linear EVMs. In its original form this did not account for viscous effects found in the very near-wall flow layers, but a number of so-called low-Reynolds-number variants have also been proposed which do include terms to allow the model to be applied in such regions (e.g. Launder and Sharma (1974), Chien (1982), Yang & Shih (1993), among many). These examples of low-Reynolds-number models, and a multitude of others, introduce near-wall “damping” and other terms into the modelled turbulence equations, typically based on the local turbulence Reynolds number, or non-dimensional wall-distance. For general applications the former is usually seen as preferable, because of the difficulty in uniquely defining wall-distance in complex or intricate geometries.

Other approaches to developing near-wall models have also been proposed, including a number based on the v^2-f model of Durbin (1991), in which further transport equations are solved to approximate the wall-normal Reynolds stress, and this then used to provide the near-wall turbulence damping effects. Variants of this have been put forward by Billard & Laurence (2012), amongst others.

In addition to ε-based schemes such as those above, other two-equation modelling frameworks have been proposed, including a number of k-ω schemes such as that of Wilcox (1988). A variant on this proposed by Menter (1994) , which has enjoyed a certain amount of popularity, is the so-called k-ω Shear Stress Transport (SST) model designed to behave like the k-ω model near the wall, but switch to what is essentially the k-ε model away from it. Although this has proved reasonably successful in a number of external aerodynamic flows, both it and other ω-based schemes have often not proved to be so reliable in buoyancy influenced applications.

As an example, Figure 17 shows a number of predictions of heat transfer in buoyancy-aided pipe flow. One of the best models in capturing the decrease and subsequent increase in heat transfer as the buoyancy force is increased is the Launder-Sharma k-ε scheme, which interestingly has also often proved to give reasonable results in many similar related flows. In this case its success is largely due to the modelled ε equation responding correctly to the accelerated near-wall mean flow (as a result of the buoyancy forces), leading to reduced turbulence levels. This is, in fact, linked to the model's known success in predicting the reduction in turbulence levels (and eventual laminarisation) in an accelerated boundary layer.

Whilst models such as the Launder-Sharma k-ε (Figure 17) can achieve a certain level of accuracy in some buoyancy-influenced flows, it often does so largely by responding correctly to changes brought about in the mean velocity field by the buoyancy. The direct effects of the buoyancy on the turbulence itself are typically not so well captured. One of the reasons for this is that the buoyancy effects on the turbulent kinetic energy depend on the turbulent heat fluxes, and at this level of modelling these are usually approximated via a simple gradient diffusion model, which takes no direct account of the buoyancy influences on the heat fluxes.

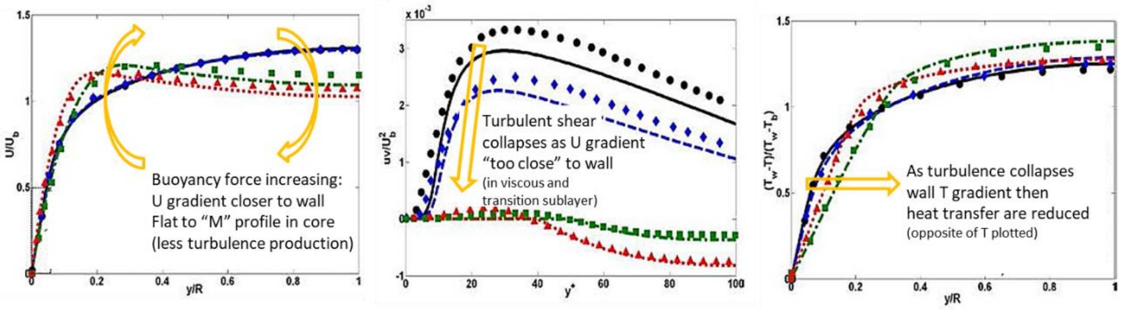


Figure 17: Vertical heated pipe heat transfer collapse: Velocity, turbulent shear stress and temperature profiles for 4 increasing buoyancy numbers 0 < Bo < 1. Symbols = DNS, lines = Low Re k-ε (Launder Sharma). Corresponding Nusselt numbers in Figure 1

As an example of such a failure, salinity profiles across a stably-stratified mixing layer were studied experimentally by Uittenbogaard (1998) and computed by Kidger (1999). In this case the stable stratification should strongly decrease the turbulence levels, leading to very little mixing between the two streams. However, the k-ε scheme does not capture the buoyant damping of the turbulence levels and therefore predicts an almost completely mixed stream by the downstream profile station.

Some proposals have been made for improved turbulent heat flux models within the EVM framework, including the four-equation model of Hanjalić et al. (1996). In this, additional transport equations were solved for the temperature variance and its dissipation rate, with the former being used to approximate the effects of buoyancy within an extended algebraic expression for the turbulent heat fluxes.

Linear EVMs have often been described as largely being the workhorse for industrial CFD, and from the above it can be seen that some such schemes can be used with a certain amount of success in a number of thermal hydraulics applications. However, since they all employ the algebraic linear stress-strain relationship, they cannot represent the highly anisotropic nature of buoyancy forces on the Reynolds stresses and may, therefore, often fail in situations where the direct influences of buoyancy on the stress levels are a dominant feature. Such models do also, of course, suffer the same well-known problems that any linear EVMs exhibit in complex flows (e.g. impinging flow, streamline curvature, rotation, strong unsteadiness), where the linear stress-strain is simply unable to represent the interactions between the mean strain field and the Reynolds stress anisotropy in an accurate manner.

5.3.1.2 Non-linear EVMs

As a result of the weaknesses of linear eddy-viscosity models in complex flow fields, noted above, non-linear EVM’s were largely developed as an attempt to provide a more reliable linkage between mean strain and Reynolds stresses, whilst still retaining a relatively cheap computational modelling framework. Most such schemes therefore fall within the two-equation class of models, but extend the linear stress-strain relation to include suitable non-linear product combinations of mean strain terms.

Some of the original ideas for these non-linear schemes goes back to the work of Pope (1975), although most practical schemes were developed somewhat later. A number of models including quadratic products of mean strain have appeared in the literature, including those by Speziale (1987), Myong and Kasagi (1990) and Shih et al. (1993), whilst the proposals of Craft et al (1996) and Apsley and Leschziner (1998) have gone further, by including cubic products in their stress-strain relationships. One of the advantages of going to the added complexity of cubic terms is that features such as the effects from flow curvature and rotation on the Reynolds stresses can then be accounted for, at least qualitatively.

Whilst non-linear EVM’s have gained some popularity as a relatively cheap method to improve the Reynolds stress representation in complex strain fields, they have not been so widely employed in studying thermal hydraulics related buoyancy influenced flows. Part of the reason for this would appear to be that although one might expect the non-linear formulation to be able to capture the response of the Reynolds stresses to changes in the mean velocity field somewhat better than with a linear scheme, none of the forms proposed have included any direct buoyancy-related influence on the Reynolds stresses themselves (and it is not obvious how one might develop such interactions within the algebraic stress-strain formulation). As a consequence, they have often not performed particularly better than linear schemes when applied to thermal hydraulics problems with strong buoyancy influences.

5.3.1.3 Stress Transport Models

At the stress transport modelling level, instead of employing an algebraic stress-strain relationship, a separate transport equation is solved for each of the Reynolds stress components, of the general form

$$\frac{D\overline{u_i u_j}}{Dt} = P_{ij} + G_{ij} + \phi_{ij} - \varepsilon_{ij} + d_{ij}$$

Although some terms (ϕ_{ij}, ε_{ij}, d) in these equations do have to be modelled, one of the strengths of stress transport models is that the generation terms P_{ij} (dependent on mean strains) and G_{ij} (due to buoyancy, and dependent on the turbulent heat fluxes) can be represented exactly, and thus do not require any direct modelling input. This means that such schemes can, in principle, fairly naturally account for the highly anisotropic effects of buoyancy (or other force fields) on the Reynolds stress tensor. This was illustrated by Figure 4.

Of the terms that require modelling, the pressure strain, ϕ_{ij}, is usually the most influential, and a number of different closure schemes have been proposed. Two well-known linear formulations that are often available in software are those of Launder et al. (1975) and Gibson and Launder (1978). Both of these are high-Reynolds-number models, so cannot be applied directly across the near-wall viscous layer, although there have been proposals that extend them to low-Reynolds-number regions, including those of Shima (1998), Hanjalić and Jakirlić (1998), Manceau and Hanjalić (2002).

Speziale et al. (1991) introduced some non-linear elements into their proposed pressure-strain model, whilst Craft et al. (1996) reported a non-linear form that was designed to also satisfy the two-component turbulence limit (meaning the Reynolds stress field will remain realisable, even when one component vanishes). Although such a limiting case might seem a little academic, it is worth noting that the very near-wall flow does approach such a limit, as can a strongly stable buoyancy-affected flow.

Stress transport models have not been as widely employed as linear EVM’s in most industrial CFD. This is probably for a variety of reasons, including the fact that the larger set of coupled equations may make solution algorithms slight less stable, and increase computational cost. A number of early studies also reported relatively small predictive improvements in complex flows when using stress transport models, although in at least some cases this conclusion was partly clouded by the lack of numerical grid resolution, meaning that purely modelling errors could not be entirely distinguished from numerical discretisation ones.

With greater computing resources now available, a number of more recent studies have demonstrated that such schemes can often return more accurate and reliable predictions than many of the simpler EVM’s in complex flows, particularly those involving highly anisotropic forcing, such as strong buoyancy.

One such example in a simple geometry is from the work of Omranian (2011), who modelled natural convection in a tall rectangular cavity at different angles of inclination (the flow being driven by differential heating/cooling from opposite side walls of the cavity). When the cavity was inclined in an unstable configuration (with the lower wall being heated), many models could return reasonable results, since the flow is dominated by large-scale unsteady roll cells. However, when inclined in a stable configuration, stress transport models, together with advanced near-wall modelling treatments, were able to capture the subtle secondary flows present in the measured flow field (Figure 18).

A much more complex application example is the simulation of heterogeneities at the exit of a PWR upper plenum by Défossez et al (2012). The secondary motions seen in Figure 19 arise from the conditions in the upper vessel, and are well-captured by a stress transport scheme once a fine enough grid is employed to adequately represent the intricate geometry details that generate these motions. At such a grid resolution the improvement from a simpler k-ε scheme was much clearer than on an earlier, and much coarser, 1M cell mesh.

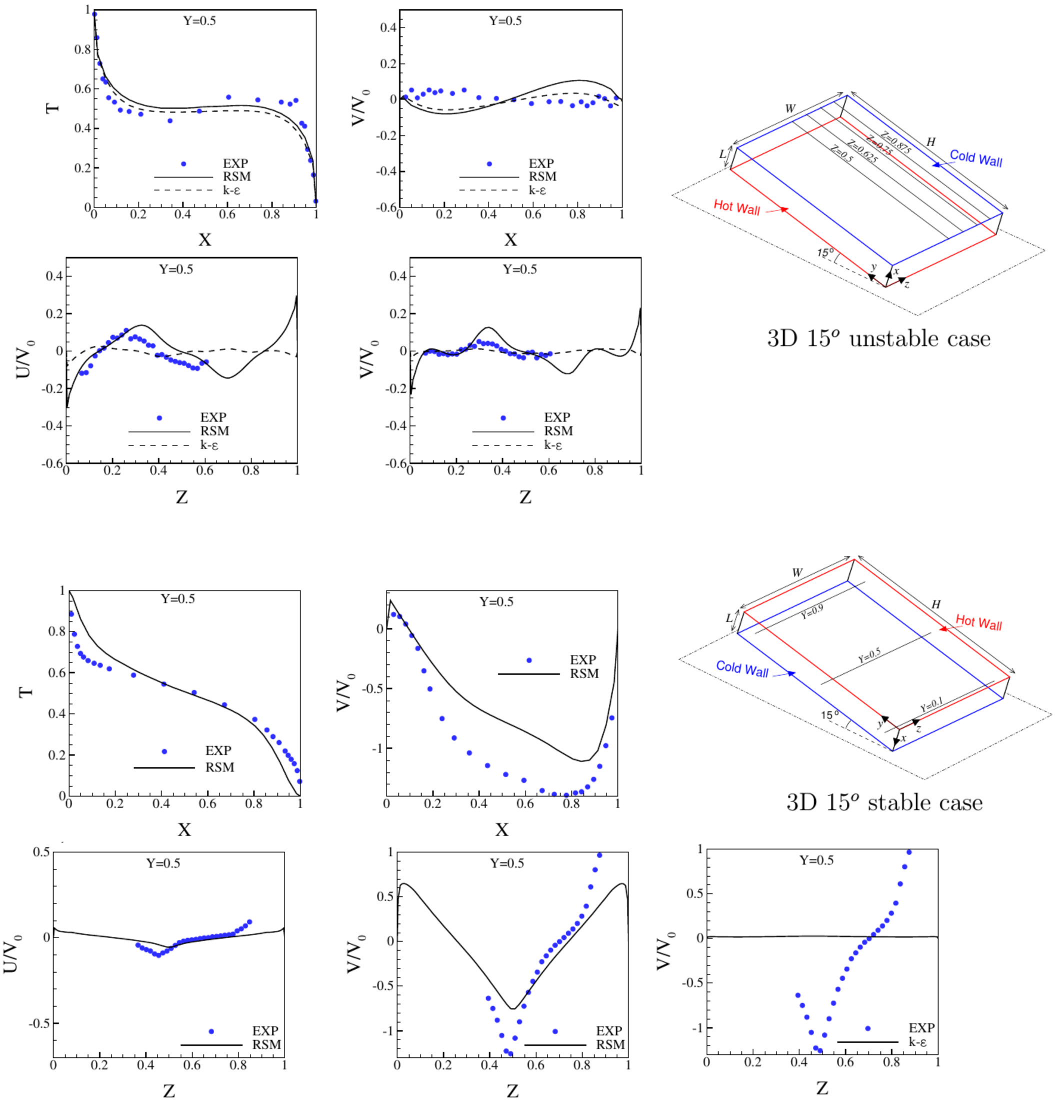


Figure 18: RSM and k-ε model predictions of the time-averaged velocity field across midplanes in highly inclined tall cavity natural convection flows
Upper: Unstable heating arrangement; Lower: stable arrangement. From Omranian (2011)

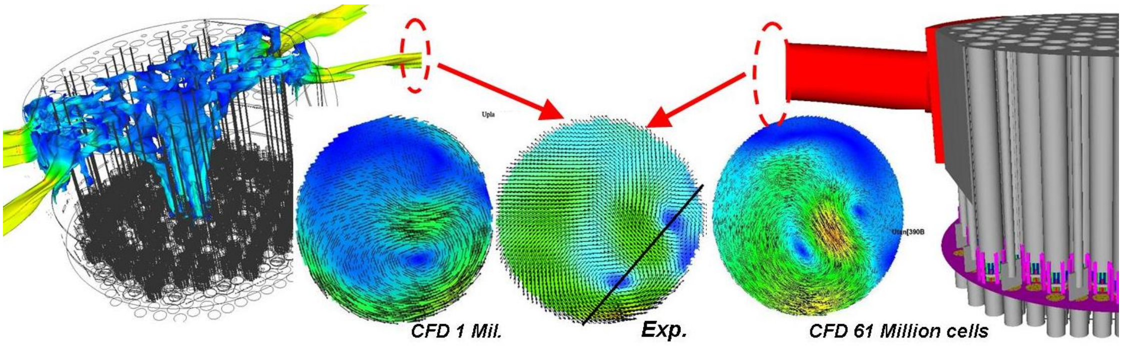


Figure 19: RSM simulation of heterogeneities at the exit of a PWR upper plenum Scalar tracers through plenum to 4 hot leg exits (left); geometrical details as seen from actual mesh surface (right); secondary motion in hot leg cross-section (centre). From Martinez and Alvarez (2009)

5.3.2 Near-Wall Modelling Treatments

One of the challenges in modelling large and complex industrial applications is how to handle the very thin near-wall viscosity-affected regions of the flow in both an accurate and computationally efficient manner. Because of the steep flow field and thermal gradients that occur across these regions, properly resolving them requires a very fine grid (together with a turbulence model designed to account for viscous and other near-wall effects). In thermal hydraulics applications this region is often of crucial importance, since wall heat transfer is strongly affected by the near-wall flow and turbulence behaviour. In large high-Reynolds-number cases, even with relatively simple wall geometries, this can result in a substantial proportion of the computing time being associated with a very fine grid covering only a few percent of the overall flow domain volume.

The traditional alternative to fully resolving the near-wall viscous layers has been to use wall-functions, which provide estimates for the wall shear stress, wall heat flux and other quantities that may be needed from approximations regarding the shape of velocity and temperature profiles across the near-wall computational cell. Most of the forms readily available in commercial CFD software are based on assumed logarithmic near-wall profiles for mean velocity and temperature, broadly following the practices of, for example Launder and Spalding (1974) and Chieng and Launder (1980).

Whilst logarithmic-based wall functions can perform reasonably well in certain flows, the assumptions behind them are essentially local equilibrium boundary layer conditions. In practice, such conditions are rarely found in complex flows, and particularly not in thermal hydraulics problems where there can be strong near-wall buoyancy, pressure gradient and other forces. There have been a number of modified forms proposed, although most are based on what are essentially still log-law type of near-wall profiles (e.g. Ciofalo & Collins, (1989)).

A more radical departure was developed by Craft et al. (2002), in the Analytical Wall Function (AWF). This was obtained from a simplified analytical integration of the near-wall mean velocity and temperature transport equations, which includes terms to represent the near-wall convection, pressure gradient and buoyancy forces.

5.3.3 Large Eddy Simulation

LES has been used as a valuable tool to study fundamental thermal hydraulic flows, and produce detailed data for RANS model validation. This is a significant computational cost, which increases rapidly with Re if the near-wall regions are to be adequately resolved.

In a Large Eddy Simulation, instead of solving for the Reynolds-averaged flow field, one solves transport equations for the spatially filtered flow field, essentially meaning that “large” turbulent eddies should be resolved, but the smaller ones will not be. A sub-grid-scale model therefore has to be introduced into the equations to account for the effect of the unresolved structures. However, these models tend to be quite simple, often following the proposals of Smagorinsky (1963), on the basis that the smallest eddies tend to be significantly more isotropic than the more complex large turbulent structures.

Despite not resolving all of the turbulent structures, a good quality LES for complex flows still requires very significant computational resources, since it should resolve a large fraction of the turbulence spectrum, meaning that the approach is still not generally a feasible option for everyday design applications. It can, however, be used to study particular problems in detail, and well-resolved LES has been employed to provide valuable data for some fundamental thermal hydraulics problems. As an example, Ammour (2013) performed well-resolved simulations of natural convection flows in inclined rectangular cavities, as well as horizontal cylindrical penetration cavities, with the data being used in that and the study of Omranian (2011) to assess the performance of a range of turbulence models and near-wall treatments in such flow situations.

One significant challenge with LES for thermal hydraulics flows is that the near-wall regions can often be quite important, because of the influence of the near-wall turbulence on heat transfer rates. In a near-wall region the range of turbulent eddy sizes is diminished (since larger ones are broken down), and so if the LES is to resolve a significant percentage of the turbulence energy it does have to resolve down to smaller scales (in some cases approaching a Direct Numerical Simulation) in these areas. This can lead to large increases in cost as the Rayleigh number increases. Although there have been some attempts at developing wall-function approximations for LES, they are typically even more restrictive than the RANS counterparts (since they are making assumptions about fluctuating velocity profiles, which are even less likely to fit any particular shape).

5.3.4 Hybrid Models

Because of the cost associated with applying LES over the whole flow domain, there has been some considerable interest in developing hybrid RANS/LES methods. The idea behind such approaches is that parts of the flow field should be resolved by LES, whilst in other regions, where the details of the turbulent structures are deemed to be less important, a cheaper RANS model could be applied. A number of such approaches have been proposed in the literature, ranging from some in which the location where one switches between modelling schemes is user-prescribed, to ones in which the two treatments are blended to give a smooth transition (such as the Detached Eddy Simulation (DES) and variants of Spalart et al. (2006, 1997) and Shur et al. (2008), through to some approaches in which both models are solved in overlapping regions of the flow domain (such as that of Uribe et al. (2010)).

Whilst some success has been reported, most such hybrid approaches still generally appear to require quite significant case-by-case modifications or adjustments, and a good pre-knowledge of the flow in question, to avoid problems arising from the interface and matching conditions between the two conceptually different modelling strategies.

5.3.5 Summary

This section has presented different approaches to the modelling of turbulence, with special emphasis on RANS modelling. It has introduced different approaches to the modelling of the turbulent stresses and also different strategies to the modelling of the effects of near wall turbulence.

Comparisons with data from experiments relevant to nuclear TH applications demonstrate the importance of adopting models which reproduce the anisotropy of turbulence, such as stress transport models and also the critical significance of strategies for the modelling of near-wall turbulence.

5.4 Two-Phase Flow and Phase Change Modelling

As detailed in Section 2.5, two-phase flows can be present in a variety of flow configurations ranging from bubbly, where gas 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 an arbitrary shape, and the interphase transfers of mass, momentum and energy. Naturally, this increased physical diversity within the flow means that there is now a much broader range of modelling methodologies which can be used to construct viable numerical models.

When compared with their single-phase counter-parts two-phase flows present a number of characteristics which complicate their modelling:

- For a dispersed phase within a continuous phase, there are various types of interphase and intraphase interactions which can be taken into account. For example, in a two-phase bubbly flow the vapour bubbles can be observed to coalesce, collapse and elastically collide. Thus, the dispersed phase can affect the flow of the continuous phase, changes in the continuous phase can affect the dispersed phase and the dispersed phase can interact with other instances of itself. Each of these represents a different level of coupling between the two phases and will require a suitable mathematical treatment.
- A defining feature of two-phase flows is the deformable interface region which separates the two phases. Once this is coupled with the naturally occurring turbulence in either phase, the picture becomes quite complex. Approaches for single-phase flows generally assume that the fluid forms one continuous region which spans the domain of interest. With two-phase flow, a means of tracking or determining the position, shape and size of the interface is required.

These complexities mean that a truly ‘one size fits all’ approach to modelling two-phase flow does not, and might likely never, exist. Whilst models are developed to be as widely applicable as possible, different modelling approaches are generally suited only to particular flow regimes or patterns. Thus the successful application of two-phase CFD models generally requires prior assessment by other means to determine the dominating flow regime or the regime of interest. Models are then chosen based on their applicability to that regime of interest. This makes ‘blind flow’ calculations currently difficult, if not impossible, and restricts the range of effects which might be captured with any particular model.

5.4.1 Overview of Two-phase Modelling Approaches

In a two-phase flow, the phases interact at the interfacial areas which separate them. Thus, a locally complete and correct description of the flow would require separate governing equations to be composed for each and every contiguous volume that each phase occupies. The interface areas then form the boundary conditions for each of the equation sets, of which there could be many. Such an approach remains practically impossible due to both the excessive computational cost required, especially for highly dispersed flows, and the sheer difficulty in actually numerically implementing such a multi-boundary approach (Crowe, 2006).

Current two-phase CFD modelling approaches can be broadly split according to way in which the flow field of each phase can be described. For dispersed flows, the dispersed phase (particles, bubbles or droplets, for instance) is usually thought of as being immersed within a continuous carrier phase. The latter typically invites an Eulerian description of the flow. For the dispersed phase itself, both Eulerian and Lagrangian approaches have been employed. In the Lagrangian description a number of individual fluid/solid ‘particles’ are identified and their positions, velocities and other properties are tracked and computed throughout time. The particles can exchange momentum, mass and energy with the continuous phase by the presence of suitable terms in the governing equations. Since trajectories have to be computed for each particle included, the approach can quickly become computationally expensive for highly dispersed phases, which thus require a large number of particles.

If an Eulerian description is applied to the dispersed phase, then the approach is usually termed Eulerian-Eulerian and a number of different modelling strategies arise depending on how the governing equations are formulated. These include the *two-fluid* approach, where the phases are treated as interpenetrating with separate sets of governing equations for each phase, the *one-fluid* 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 *one-fluid* 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.

5.4.2 Eulerian-Eulerian framework

From a numerical perspective, applying an Eulerian description to both phases is particularly attractive since the governing equations can then be discretised and solved using existing, and naturally efficient, numerical solution methods. It also provides a common framework in which to utilise the more mature modelling strategies and techniques developed for single-phase CFD.

5.4.2.1 Two-fluid

In the two-fluid approach, both phases are treated as continuous and interpenetrating. That is, the fields that represent the phases mathematically exist at all points within the solution domain. Since, however, only one phase can occupy any given volume at a time, separate sets of governing equations can be derived for each phase by introducing the concept of a volume fraction, or void fraction, to the Navier-Stokes equations and applying an averaging procedure. The volume fraction determines the fraction of volume that each phase occupies within each control volume in the domain. Interfacial interactions between the phases can then be incorporated through prescribing source terms in the momentum and energy equations, which couple the phases together. The phases are often also assumed to share a single pressure field (Ishii and Hibiki, 2011).

The two-fluid approach (sometimes termed the six-equation model) is considered to be the most general of the two-phase models since, in principle, it can be used to model any number of phases which may interact. Its success, however, hinges on accurate formulation of the constitutive equations for the interfacial exchange terms (Ishii and Kocamustafaogullari, 1983). This is complicated by the fact that interfacial transport mechanisms differ according to the flow regime present and most terms still rely on empirical correlations. Unless these interaction terms are accurately modelled, the advantage of the two-fluid model over simpler models disappears (Ishii and Mishima, 1984).

Early approaches to modelling the interfacial forces in one-dimensional system codes typically expressed them in terms of a generalised drag force; a linear combination of terms which model the effects of momentum transport due to mass transfer, interfacial shear stress, interfacial pressure and the various forces (drag, lift, etc.) which may affect the secondary phase. These are also used in three-dimensional CFD calculations and Table 1 provides a sample of those currently found within the literature. Their applicability varies depending on the validation process used and most are formulated using experimental data or with phenomenological arguments which may only be valid for the regimes in which they have been calibrated. They can also seldom reflect the true dynamic nature of changes in the interfacial structure, nor any gradual regime transition. For example, nearly all drag force models only provide a drag coefficient based on the Reynolds number and the particle/bubble diameter, with the latter generally being user specified prior to computation.

Interfacial force	Model reference
Drag force	Schiller and Naumann (1935)
	Morsi and Alexander (1972)
	Clift et al. (1978)
	Ishii and Zuber (1979)
	Tomiyama (1998)
	Universal Drag Laws (Kolev, 2007)
Lift force	Moraga et al. (1999)
	Saffman (1968, 1965)
	Legendre and Magnaudet (1998)
	Tomiyama (1998), later modified by Frank et al. (2004)
	Hibiki and Ishii (2007)
Wall lubrication	Antal et al. (1991)
	Tomiyama et al. (1995)
	Nguyen et al. (2013a)
	Lubchenko et al. (2018)
Bubble-wall collision	Chuang and Hibiki (2017)
Turbulent dispersion	Lahey et al. (1993)
	Burns et al. (2004)
	Lopez de Bertodano et al. (2006)
	Balachandar and Eaton (2010)
	Laviéville et al. (2017)
Bubble collision	Alajbegovic et al. (1999)
	Sharma et al. (2017)
	Chuang and Hibiki (2017)
Interfacial pressure force	Vaidheeswaran and de Bertodano (2016)
Interfacial shear force	Antal et al. (1991)
	Ishii and Hibiki (2011)
Virtual mass force	Ishii and Mishima (1980)
Basset force	Ishii and Hibiki (2011)

Table 1: Models for Interfacial forces available in the literature, partly drawn from Chuang and Hibiki (2017)

Most current research focuses on the calibration of the coefficients which appear in those models (Chuang and Hibiki, 2017). Frank et al. (2004) applied the two-fluid model with the commercial ANSYS CFX-5 package in order to predict the development of upward directed gas-liquid flows in a vertical pipe. Models were used for drag (Clift et al., 1978), lift (Tomiyama, 1998), wall lubrication (Antal et al., 1991) and turbulent dispersion (Burns et al., 2004) with correlations providing the interfacial area concentration. Turbulence in the liquid phase was modelled with a k-ω SST model (Menter, 1994) and in the bubble phase with a zero-equation model. Results demonstrated good agreement with benchmark experimental data from the MT-Loop test facility (Zschau et al., 2003).

5.4.2.2 Interfacial Area Transport

Improvements to the above approach can be sought by recognising that the forcing models can generally be represented as the product of a driving force and the interfacial area concentration (the interfacial area per unit volume). Whilst the constitutive relations above provide a measure of the forcing mechanism, they rely on empirical correlations or user-input to specify a representative interfacial area (which is, of course, regime dependent). To tackle this, Kocamustafaogullari and Ishii (1995) developed an Interfacial Area Transport Equation (IATE) for the interfacial area concentration. This provides a mechanistic way to predict the evolution of the flow structure and particle/bubble interaction phenomena, such as coalescence and breakup. It can be incorporated through modelled source and sink terms. To take account of differences in bubble shape, two-group (Takashi Hibiki and Ishii, 2000; Sun et al., 2003) implementations of the IATE have been proposed in addition to one-group (T. Hibiki and Ishii, 2000; Wu et al., 1998) formulations.

The IATE has been used to produce improved results in 1D two-fluid modelling of subcooled boiling flow (Lee et al., 2009), various two-phase flows in microgravity (Takamasa et al., 2003; Vasavada et al., 2007) and with rod bundle geometry (Paranjape et al., 2010). Wang and Sun (2010) modelled air-water bubbly flow using ANSYS Fluent, extending and calibrating the IATE 1D model coefficients against experimental data to make them suitable for 3D use. Nguyen et al. (2013b) looked at bubble coalescence and breakup, taking into account turbulent suppression phenomena found in the bubbly flow regime (Serizawa and Kataoka, 1990). Comparisons against the experiments of Hibiki et al. (2001) showed improvement over the earlier model of Yao and Morel (2004). Lee et al. (2013) used the two-group formulation of (Sun et al., 2004) in ANSYS CFX to compute non-bubbly adiabatic air-water upward flows and showed promising results against the benchmark experimental data of (Sun, 2001). They noticed some discrepancies, however, which were attributed to underestimated source terms in the IATE and momentum equations.

5.4.2.3 Population Balance Models

The IATE approach can be viewed as a simplification of the more general Population Balance Model (PBM) approach. These are concerned with maintaining a record for the number of entities (bubbles, droplets etc.), whose creation, destruction and presence may dictate the behaviour of the system (Ramkrishna and Mahoney, 2002). PBM's have significant history (Hulburt and Katz, 1964; Ramkrishna and Borwanker, 1973; Randolph, 1964) but their potential for solving multiphase engineering problems was not fully realised until early 2000 (Ramkrishna, 2000).

The general aim is to provide a means to predict the number density of particles within the primary phase and several approaches within the PBM framework have been developed to achieve this, including Class Methods, which directly solve for a set of discrete size classes, and Moment Methods, which solve equations representing the moments of the number density. The latter is particularly attractive from a computational point of view as it only tracks a small number of moments rather than a potentially large number of discrete size classes (Yeoh et al., 2014). Despite this, for the MUltiple-SIze-Group (MUSIG) model (Lo, 1996), a type of Class Method, a significant number of studies adopting it have been reported in the scientific literature. The MUSIG model approximates the continuous particle size distribution by a specific number of size fractions and balances mass conservation within each size fraction with the inter-fraction mass transfer which results from particle-particle phenomena. Two formulations of the MUSIG exist; the homogeneous, which assumes the size fractions all move with the same velocity, and the inhomogeneous, which allows groups of size fractions to have different velocities.

Frank et al. (2008) applied the inhomogeneous MUSIG approach in ANSYS CFX to experimental mono and poly-disperse air-water flows at the MT-Loop (Lucas et al., 2005) and TOPFLOW (Prasser et al., 2006) test facilities. Good agreement was presented but improvements to the bubble break-up and coalescence models were suggested; conclusions which were echoed in a similar study by Krepper et al. (2008).

Bannari et al. (2008) implemented a Class Method into OpenFOAM to model dispersed bubble columns, where turbulence was modelled using a modified k-ε equation with additional source terms to incorporate the effects of the dispersed phase on the turbulence. Good agreement is obtained against experimental data (Buwa et al., 2006; Pfleger et al., 1999) whilst results obtained using a fixed bubble size were inferior.

Peña-Monferrer et al. (2016) applied the Quadrature Method of Moments model in OpenFOAM to upward bubbly flow, showing satisfactory agreement with experimental data. Cheung et al. (2013) compared the capability of the Direct Quadrature Method of Moments (DQMOM), the homogenous MUSIG model and an Average Bubble Number Density (ABND) model in capturing bubble coalescence and break-up in bubble columns. Comparisons with experimental results from the TOPFLOW and MT-Loop facilities were satisfactory, with the ABND providing substantial computational economy but losing information on bubble size distribution. The DQMOM and MUSIG models demonstrated similar performance, with the DQMOM offering greater potential for computational savings.

5.4.2.4 One-fluid: Mixture/Homogenous

Many of the early approaches to modelling multiphase flow in one-dimensional nuclear thermal hydraulic system codes were developed by noting that, generally, only information on the dynamics and response of the phases as a whole (i.e. the mixture) was required, rather than on the responses and interactions between the individual phases in the system. Thus the basic concept was to consider the mixture as a whole rather than as separate intertwined phases. This first gave rise to the Homogenous model, which considered the phases to be moving uniformly with one another, and then separated-flow models, where the two phases were allowed to have different averaged velocities. A notable separated-flow model is the frequently used drift-flux model (Zuber and Findlay, 1965), which uses constitutive relations to take account of the relative motion and interfacial transport between the phases (Hibiki and Ishii, 2003).

The application of the above concepts within the context of CFD results in the homogeneous and mixture one-fluid models. The governing equations are written for the balance of mixture mass, momentum and energy in terms of the mixture properties by summing together the equations for individual phases. The resulting set of equations bear resemblance to those of single-phase flow except for the presence of two additional source terms in the momentum equations; one representing the effects of interfacial surface tension and the other the momentum diffusion due to the relative motion between the two phases. The latter term requires a kinematic constitutive relationship to link the relative, or slip, velocity between the phases to the mixture velocity. This is usually called an algebraic slip or drift-flux model and most are based on a simple force balance over a dispersed fluid particle. Further constitutive relationships are required for the viscous stresses and turbulent stresses, since those usually employed for single-phase flows may no longer be applicable to the mixture (Hibiki and Ishii, 2003). A continuity equation is also solved for one of the phases, in terms of the mixture velocity, in order to provide a volume fraction, which is used to evaluate the properties of the mixture (Ishii and Hibiki, 2011; Manninen et al., 1996).

If the relative motion between phases can be considered negligible (i.e. the phases are very tightly coupled), then the slip velocity is zero and the mixture model reduces to the homogenous model. This allows the constitutive relations be reduced to much simpler forms, but does reduce the overall applicability of the model. Conversely, there are cases, such as when the two phases flow in opposite directions, driven by different forces, when it is not possible to determine the slip velocity from the local mixture flow conditions. The phases can no longer be considered coupled together and the approach then breaks down.

Whilst one-dimensional drift-flux, and to a lesser extent homogenous, models feature frequently in the scientific literature, and are still undergoing development in the context of system codes (Chen et al., 2012; Gao et al., 2008; Hashemi-Tilehnoee and Rahgoshay, 2013; Hurisse, 2017; Talebi et al., 2012; Talebi and Kazeminejad, 2013), the majority of the work on the use of mixture models in the context of CFD is in the field of nanofluids. Examples include Akbari et al. (2012), Chen et al. (2014) and Ghaffari et al. (2010). Hadad et al. (2013) investigated the thermal hydraulic behaviour of a water/Al_2O_3 nanofluid in a single fuel assembly of the VVER-1000 nuclear reactor and found the mixture model offered improved results over a single-phase approach. Other recent applications of the mixture model include sediment flows (Liang et al., 2017) and liquid atomisation (Jayanthi and Peddieson, 2014).

5.4.2.5 One-fluid: Interface Capturing

Interface capturing methods focus on providing a means to infer the interface area between the two-phases. Generally, the specific numerical approach must provide a spatial resolution fine enough to be able to capture some form of discernible interface, and thus they cannot be readily applied to heavily dispersed phases. They are, however, particularly suited to stratified flows, free-surface flows and slug flows, where a large interface is the most dominant characterising feature.

One set of governing equations is solved throughout the domain and the fluid velocity, pressure and energy fields are shared amongst the phases. The material properties appearing in the transport equations are determined by the properties of the phase present locally within a particular control volume which, in turn, is dependent on the value of a phase-indicating scalar. Thus, the two-phase system is treated as one continuous fluid whose properties vary sharply across the interface region. A number of different formulations exists; those most frequently employed are the Volume Of Fluid (VOF) method and the Level-Set (LS) method.

The VOF method (Hirt and Nichols, 1981; Rider and Kothe, 1998) is perhaps the most widely used interface capturing model and relies on providing a definition for the volume fraction occupied by one of the phases as the phase-indicating scalar. This is obtained through solution of a transport equation:

$$\frac{\partial}{\partial t}(\chi^k \rho^k) + \frac{\partial}{\partial x_j}(\chi^k \rho^k U_i^k) = 0$$

where χ^k is the phase-indicating scalar, ρ^k is the density and U_i^k the velocity for phase k. The phase-indicating function is constructed to take a value of 1 if the phase is present and zero otherwise.

Following solution of the above equation, regions purely occupied by one particular phase can be identified by the value of χ^k, with cells containing the interfacial regions being identified such that $0 < \chi^k < 1$. Central to the VOF method is the use of the resulting χ^k field to provide the interface geometry. Once this has been established, the interface curvature and surface normal are computed and used to determine the surface tension force, which is added as a source term in the momentum equations. Typically the Continuous Surface Force model of Brackbill et al.

(1992) is used, but other, more elaborate, models exist (Francois et al., 2006; Renardy and Renardy, 2002; Scardovelli and Zaleski, 1999).

Although the form of the equation for the phase indicating scalar lends itself readily to solution by conventional finite-difference and finite-volume schemes, the computation of the numerical fluxes of χ^kat the cells containing the interface is not straightforward. The numerical diffusion generated by some discretisation schemes can lead to numerical smearing of the interface and issues with preserving the boundedness of the volume fraction (Gopala and van Wachem, 2008). A significant number of schemes have been proposed in the literature to correctly account for this that fall into two main approaches; geometric reconstruction of the interface or the use of non-linear higher-order discretisation schemes to directly advect the sharp interface.

Early geometric reconstruction schemes such as the Simple Line Interface Construction (SLIC) of Noh and Woodward (1976) used only lines parallel to the cell faces to define the interfaces. A frequently used refinement is to fit oblique lines or piecewise linear segments through the interface in each cell by estimating the interface normal; a technique called Piecewise Linear Interface Construction (PLIC) introduced by Youngs (1982). Further improvements were made by Ashgriz and Poo (1991) with their Flux Line-segment model for Advection and Interface Reconstruction (FLAIR) algorithm, which required the piecewise segments to be joined at the interface.

More recent advancements include second order algorithms by Pilliod and Puckett (2004), which can reproduce linear interfaces exactly, algorithms which fit quadratic (Diwakar et al., 2009) and cubic (López et al., 2004) splines to the interface given by the PLIC method, which allow a direct estimate of the interface curvature, and methods which attempt to resolve subgrid sized particles (Sun, 2011), which can provide a direct measure of the interface normal by directly integrating equations for it. Unfortunately, many of the PLIC based methods focus on two-dimensional structured implementations, since most of the algorithms become cumbersome and difficult to implement in 3D. Some extensions to arbitrary unstructured and three-dimensional meshes have been presented however (Ito et al., 2013).

Due to the above mentioned difficultly of implementing geometric reconstruction methods in 3D, another approach is to instead solve the phase-indicating scalar equation in a way which keeps the interface sharp. Early 1D schemes, such as the Donor-Acceptor algorithm of Hirt and Nichols (1981), were based on a variation of the Flux-Corrected Transport (FCT) algorithm (Boris and Book, 1973) which combined first-order upwind and downwind fluxes in such a way as to maximise stability whilst minimizing diffusion. A 2D implementation by Rudman (1997) showed superior results over earlier multi-dimensional work by Zalesak (1979). H

High resolution schemes based on the TVD (Total Variation Diminishing) and NVD (Normalised Variable Diagram) can maintain a sharp interface, but have been shown to distort or wrinkle the interface when the free surface is not aligned with the control volume faces (Lafaurie et al., 1994). Thus various blending schemes have been proposed in the literature, which switch between high-resolution schemes and compressive schemes. These include CICSAM (Ubbink and Issa, 1999), HiRAC (Heyns et al., 2013), SURFER (Lafaurie et al., 1994), STACS (Darwish and Moukalled, 2006), HRIC (Muzaferija et al., 1998), FBCIS (Tsui et al., 2009) and THOR (Hogg et al., 2006). An altogether different approach is the so-called Tangent of Hyperbola INterface Capturing (THINC) method (Xiao et al., 2011, 2005) which approximates the interface jump with a hyperbolic tangent function and avoids the need for any interface reconstruction.

VOF methods are inherently conservative, which is a major advantage, and have seen continuous development in the past two decades, as evidenced by the plethora of different formulations available within the overall approach. The VOF formulation also can account for interface interactions (merging/collapse) in a natural fashion, but requires sufficient grid resolution to capture interfaces. Meier et al. (2000) used a 2D PLIC based VOF method to numerically model the downward injection of air bubbles into water and verified the results against small-scale experimental data (Meier, 1999). Liovic et al. (2004) and Liovic and Lakehal (2007) used a 3D LES PLIC based VOF approach to model the same experimental data (Meier, 1999). Results from Liovic and Lakehal (2007) demonstrated the potential of LES VOF to capture the chaotic fully 3D effects seen in bubble growth. Yamashita et al. (2017) first validated the VOF-THINC scheme against the single rising bubble problem of Hnat and Buckmaster (1976) and then applied it to the severe-accident corium spreading benchmark experiment VULCANO (Journeau et al., 2006). Results showed reasonable agreement but problems in reproducing detailed phenomena were highlighted.

Simulations of unstable stratified two-phase flows that are potentially present during a Pressurised Thermal Shock (PTS) scenario were presented by Bartosiewicz et al. (2008) as part of the European NURESIM program. They compared a geometric reconstruction VOF method implemented in Fluent and a two-fluid approach modified for surface tension in NEPTUNE_CFD against experimental data from the Thorpe experiment (1969). Results demonstrated both approaches produced results in agreement with the experimental data and showed the potential of the two-fluid approach in modelling complex stratified flows; something that it is not inherently suited to. Comparisons between the two-fluid, in ANSYS-CFX and NETPTUNE_CFD with an added interface detection algorithm, and VOF, in Fluent, were also presented by Apanasevich et al. (2014) for a PTS scenario as part of the European NURISP program. Whilst all codes produced reasonable results there were considerable differences between them and further modelling work on key PTS relevant phenomena, like interfacial momentum transfer and turbulence, was suggested.

As an alternative to the VOF formulation, originally introduced by Osher and Sethian (1988), Level-Set (LS) methods are a family of surface tracking methods that define the interface as the zero-contour, or zero level-set, of a higher dimensional function termed the level-set function ϕ. Typically this function is initialised as a signed function from the interface, where negative values correspond to one of the phases, positive to the other and the zero value corresponds exactly to the interface. The interface evolves with the local fluid velocity through the solution of a transport equation for ϕ, which resembles a simple scalar advection equation.

First applied to model two-phase flow by Sussman (1994), LS methods make use of a unit-step (Heaviside) function to compute the respective fluid properties for each phase, which is typically smoothed to aid numerical stability. Whilst the transport equation for ϕ appears straightforward, an important distinction is that here it does not arise from a conservation law and thus its solution can lead to difficulties in conserving mass and preserving interface sharpness. To alleviate this, ϕ can be regularly reinitialised so that it again satisfies the properties of the signed function (Russo and Smereka, 2000; Sussman et al., 1994) but mass conservations errors can be compounded over relatively long time durations. This has led to some authors finding more conservative LS approaches using alternative LS functions (Olsson et al., 2007; Olsson and Kreiss, 2005) or applying explicit mass corrections schemes (Chang et al., 1996; Zhang et al., 2010) with some success.

Major strengths of LS methods include the fact that ϕ varies smoothly across the interface, which allows the interface curvature and surface normal to be represented using convenient formulae, and the simplicity of the method, which eases multidimensional implementation. They have seen considerable use and development within the literature over the past few decades (Gibou et al., 2018; Osher and Fedkiw, 2001; Sethian and Smereka, 2003). Recently, Bilger et al. (2017) implemented an advanced compressive VOF approach and a conservative LS approach (Olsson and Kreiss, 2005) in the open source OpenFOAM code and applied it to a series of test cases, including Rayleigh-Taylor instability and static droplets. They showed that both methods compared favourably with the standard VOF solver (interFOAM) within OpenFOAM but required some tuning specific to each case.

The difficulties with mass conservation in LS methods together with inaccurate interface capturing methods of the VOF method has led some authors to propose coupling the two methods together. In one approach, the LS distance function is advected and the interface reconstructed using the LS method, which corrects interface inaccuracies in the VOF method. Then the VOF method is used to re-initialise the distance function, which tackles the issues with mass conservation. Results have shown improvements over pure LS or VOF methods for rising air bubbles (Sussman and Puckett, 2000; Yokoi, 2013), wave breaking problems (Wang et al., 2009), impacting droplets (Dianat et al., 2017). Another approach reverses the order of coupling, solving only for the volume fraction in the VOF method but using an iterative LS based method to then compute the distance function and the interface position. This also offered improvement over LS or VOF methods for dam-breaks and rising gas bubbles (Sun and Tao, 2010).

5.4.2.6 Two-Phase Turbulence Modelling

Accurately accounting for turbulence still poses a significant challenge in single-phase flows, where it is tackled with a variety of different closure approaches (eddy-viscosity, stress-transport, etc.) within a number of distinct numerical frameworks (Reynolds-averaged Navier-Stokes, Large Eddy Simulation etc.). Multiphase flows are, like their single-phase counterparts, invariably turbulent and this adds further complexity to an already significantly challenging modelling task. Within the Eulerian framework, this is largely tackled by generalising the well-known single-phase turbulence modelling approaches and introducing further closure models for any additional terms. For two-fluid multiphase models, however, concepts like Reynolds averaging are not trivial since phasic-averaging (be that volume or ensemble) has already been applied to the instantaneous equations in order to numerically represent multiple phases. Performing a Reynolds-decomposition directly on the phase-averaged quantities does not yield the fluctuating component as one might expect. This is something which, unfortunately, does frequent the literature (Crowe, 2000).

Early approaches to modelling turbulence in the two-fluid approach consisted of ad-hoc phenomenological modifications to the turbulence in the carrier phase (Drew and Lahey, 1981; Sato et al., 1981) but their application was limited by their dependence on experimental data. Following this, later efforts focused on direct derivation of the equations for the various turbulence modelling approaches guided by their single-phase counterparts. RANS multiphase equivalents of algebraic closure approaches (Michiyoshi and Serizawa, 1986; Sato and Sekoguchi, 1975), two-equation eddy-viscosity models, including k-ε (Besnard and Harlow, 1988; Elghobashi and Abou-Arab, 1983; Kataoka and Serizawa, 1989; Lopez de Bertodano et al., 1994) and k-ω (Bellakhal et al., 2004) variants, and Reynolds stress models (Chahed et al., 2003; Kumar, 1995; Lance et al., 1991; Lopez de Bertodano et al., 1990) have been presented in the literature. A recent review by Vaidheeswaran and Hibiki (2017) provides a comprehensive overview. The resulting two-phase models most closely resemble their single-phase counterparts, with a key common difference being the appearance of additional modelled terms representing inter-phase turbulent interactions.

One of the most widely studied contributions to inter-phase turbulent interactions is that seen in bubbly flows. The presence of bubbles is known to modify the structure of the liquid turbulence and turbulent production through shear, which can then affect bubble distribution, break-up and coalescence (Lance et al., 1991). The bubbles act as a source of bubble-induced turbulence, which generally leads to an increase in turbulent intensity (Shawkat et al., 2008) and can cause turbulence generation in flows that would otherwise be laminar (Hosokawa and Tomiyama, 2013). Thus accurate modelling of this is essential. Rzehak and Krepper (2013) performed a comparison numerical benchmark against a comprehensive set of experimental data for vertical bubbly flow using a two-fluid approach with modified k-ε and k-ω SST two-equation models. Turbulent kinetic energy plots along the pipe radius showed that it was largely underestimated by nearly all models with significant differences seen between them.

Multiphase turbulence model implementations in the major commercial CFD codes (CFX, Fluent) provide options to apply the models to each phase, to the continuous phase with additional terms representing the dispersed phase interactions, and to the overall mixture. The latter utilises mixture properties and mixture velocities much like in the one-fluid mixture approach considered in Section 5.4.2.4. Zhang et al. (2015a) compared these approaches by modelling subcooled nucleate boiling in a vertical heated pipe. Results showed that the per-phase and continuous only treatments provided no major advantage over the mixture treatment, despite being computationally more expensive.

A further complication is the approach taken in the near wall region for coarse meshes. A number of studies simply use the well-known single-phase logarithmic law of the wall but this has been shown to over-predict velocity distributions in the near-wall boiling region in subcooled boiling (Lee et al., 2002). Končar and Borut (2010) extended the standard logarithmic law of the wall using the idea that nucleating bubbles disturb the boundary layer in a similar fashion to surface roughness. This was implemented in the NEPTUNE_CFD code and validated against three sets of upward boiling flow experiments. Results showed that the new formulation generally offered improved near-wall predictions.

5.4.3 Eulerian-Lagrangian framework

For two-phase flows in which one of the phases is sufficiently dispersed, i.e. it can be described as a collection of discrete particles, bubbles or droplets, a Lagrangian description can be used to compute and track the trajectories of these particles throughout the computational domain. This can provide detailed information on particle position, velocity, temperature and other scalars and has the potential to handle certain physical phenomena, such as particle-particle collision, heat transfer, mass transfer and turbulent interactions, in a more natural fashion (Yeoh and Tu, 2010).

To determine the particle trajectories, the forces which act on each individual particle need to be computed. There are two main approaches to this. In the point-force (or point-particle) approach, the surface forces acting on the particles (pressure, viscous) are approximated as surface-averaged forces based on analytical or empirical expressions (drag, lift, virtual mass etc.). In the resolved surface approach, the surface forces are fully resolved over the entire surface of the particle and then integrated to obtain the overall hydrodynamic forces (Crowe, 2006). This approach requires a high spatial resolution of the continuous phase in order to properly resolve the surface forces. Once the forces have been computed, the trajectories can be determined by applying a simple force balance over the particle and integrating in time. If particle rotation is of interest, a torque balance can also be applied. Since this has to be done for each particle in the flow, the Lagrangian technique becomes computationally demanding when large numbers of particles are introduced. Particles can be grouped together into representative discrete elements to alleviate this somewhat.

The level of coupling between the discrete and continuous phases depends on the particle size. If the particle size associated with the dispersed phase is small, then its influence on the continuous phase can often be neglected and the coupling between the phases is only one-way. This can greatly simplify the computation, since the trajectories of the dispersed particles can be computed completely independently of the continuous phase. Two-way coupling can be employed, where the behaviour of particles does influence the motion of the continuous phase. Particle-particle collisions can also be included (so-called “four-way coupling”) with additional modelling. The number density of the particles can then be used to compute a volume fraction, which is used in the solution of the continuous phase. The inter-phase exchange of mass, momentum and energy is incorporated through source terms in the continuous phase equations (Crowe, 2006).

Deterministic computation of the particle trajectories within a turbulent flow poses some difficulty in a Lagrangian framework, since it is the *instantaneous* flow velocity which is required to compute the forces on the particle; something which may not be readily available. Thus, in order to include the effects of turbulence on the particles, i.e. turbulent dispersion, a stochastic model can be used with the aim of generating the random velocity fluctuations which will affect the particle during its lifetime. A widely used stochastic model is the Discrete Random Walk Model (Gosman and Ioannides, 1983) which assumes that as a particle is captured by a turbulent eddy, the instantaneous velocity will be equal to the mean fluid velocity plus a random contribution drawn by multiplying the RMS value by a Gaussian distribution. When the lifetime of the eddy is over, or the particle travels a distance greater than the size of the eddy, another interaction occurs with a different eddy and another random value is sampled. The time and length scales associated with the eddy are typically provided by a turbulence model. Other ways of computing this effect include the Continuous Random Walk Model (Iliopoulos et al., 2003) and methods utilising probability density functions (Subramaniam, 2013).

Whilst Eulerian-Lagrangian methods are commonly used to simulate a variety of multiphase flows, including bubble columns (Delnoij et al., 1999, 1997a, 1997b, Laín et al., 2002, 1999; Lapin and Lübbert, 1994), biomass gasification (Ku et al., 2014), coal gasification (Snider et al., 2011; Xie et al., 2013, 2012), particulate flows (Patankar and Joseph, 2001) and sedimentation (Snider et al., 1998), their use in the context of nuclear thermal hydraulics is much more limited. Exploratory work by Badillo and Andreani (2017) as part of the European NURESAFE project looked at modelling the cooling effect of small droplets entrained in the flow of superheated steam during a LOCA in a LWR. They used a Lagrangian model implemented in Code_Saturne and looked at the effect of various simulation parameters, including the lift force model, the number of particles injected and the particle diameter. Results showed that the cross-sectional distribution of the droplets only had a mild effect on the temperature of the stream, in agreement with Andreani, (1992), but the authors use of “soft” two-way coupling, in which only thermal exchanges between the phases are considered (i.e. the presence of the droplets cannot modify the flow structure), is limiting. The results do, however, demonstrate the method has potential should the community carry out further development and modelling.

5.4.4 Modelling Phase Change

Owing to the ability of fluids to store or release large amounts of latent heat upon phase change, vaporisation and condensation phenomena form a significant aspect of many engineering processes. They feature extensively in the context of nuclear thermal hydraulics. On design phenomena such as subcooled boiling are integral to plant operation whilst off-design phenomena, such as pressurised thermal shock, departure from nucleate boiling, core re-flooding, condensation (steam discharge into a pool, for example) and flash boiling following a PV rupture, can present challenges. Accurate predictions of such phase change phenomena are thus essential for the safe design and operation of Nuclear Power Plants.

Away from walls, phase change can be handled by including suitable formulations of the interfacial mass and heat flux terms which appear in the balance equations for mass, momentum and energy. Due to their empirical nature, there is, however, no universally accepted approach to formulating these terms. A number of mass transfer models appears within the literature. These include the Schrage model (Schrage, 1953), which utilises the kinetic theory of gases but requires an identifiable interface, and the Lee model (Lee, 2013), which identifies phase change as driven primarily by a deviation of interface temperature from the saturation temperature. Both of these approaches require empirical coefficients and others (Jeon et al., 2011; Krepper et al., 2007; Zhuan and Wang, 2010) are based largely on heat transfer correlations or experimental data. An alternative is the so-called "two-resistance" model, which is implemented in commercial codes Fluent and CFX. Originally inherited from thermal hydraulics system codes, where it was typically called the "heat conduction limited" model, this computes the mass transfer rate as that required to satisfy a heat balance applied over the interface.

At the walls, additional modelling is required to take account of the heat transfer mechanisms present in nucleate boiling. Vapour generation at nucleation sites leads to the growth of bubbles, which in the presence of convective forces may detach and interact with the bulk liquid. Aside from the strong interfacial transfers, under certain conditions this can cause significant changes in interface topology; even to the point where a change in flow regime is seen.

5.4.4.1 Boiling

Owing to its importance in many engineering processes, a significant amount of literature can be found on efforts to accurately numerically predict boiling (Kharangate and Mudawar, 2017; Liao and Lucas, 2017a). Of the three modes; film, transition and nucleate - subcooled nucleate boiling has received the most attention owing to its significance in LWR sub-channel heat transfer.

Nucleate boiling is characterised by liquid-vapour phase change at nucleation sites along a heated wall. When the wall temperature rises above the saturation temperature of the contacting fluid, vapour bubbles begin to grow at the nucleation sites and eventually detach, transferring heat away from the wall in the process. If the bulk liquid temperature remains below the saturation temperature, then the boiling is said to be subcooled. After the bubbles detach, the temperature difference between the vapour and subcooled liquid drives condensation which will eventually lead to bubble collapse.

The inclusion of nucleate boiling within a CFD package requires accurate modelling of the wall heat flux. Early efforts were primarily aimed at developing empirical correlations (Warrier and Dhir, 2006), but these are generally only valid for the flow configuration in which they were formulated and are limited to the prediction of the total wall heat flux. Physically, the heat transfer at the wall is consumed by different mechanisms over the course of the boiling cycle:

- Vapour generation during bubble nucleation and growth;
- Wall-liquid transient conduction as cooler liquid replaces the departing bubble; and
- Single-phase conduction at locations without bubble growth (Crowe, 2006).

Reflecting this, the predominant methodology within the literature is mechanistic (Yeoh et al., 2008), with a number of different heat flux partitioning schemes being reported (Del Valle and Kenning, 1985; Graham and Hendricks, 1967). The most popular is the so-called Rensselaer Polytechnic Institute (RPI) wall boiling model of Kurul and Podowski (1991), which considers the total wall heat flux as the sum of three parts: evaporation, quenching and single-phase (turbulent) convection.

With the exception of single-phase convection, the sub-models required for each of these components are heavily dependent on the vapour bubble dynamics; coefficients representing bubble detachment diameter, nucleation site density, bubble departure frequency and bubble growth rate all typically factor in some fashion and a large number of formulations for these have been proposed (Mali et al., 2017; Mohanty and Das, 2017). Later extensions to the RPI model for vertical flows also included the effects of bubble-slide (Basu et al., 2005; Gilman and Baglietto, 2013; Thorncroft and Klausner, 2001), which was noted by Thorncroft et al. (1998) as playing an important role in enhancing energy transfer. Some of these sub-models have been shown to produce satisfactory results (Prabhudharwadkar et al., 2014), but a recent numerical assessment by Thakrar et al. (2014) highlighted various deficiencies in others.

Krepper et al. (2007) used a two-fluid Eulerian approach with a modified RPI wall boiling model to model subcooled boiling in vertical heated pipes and PWR coolant channels. Validation against experimental data for the former showed good agreement, but no experimental data was available for the latter. Zhang et al. (2015b) reported similar results. Gu et al. (2017) extended the RPI approach to ultra-high pressure conditions in a vertical heated tube demonstrating good agreement against the experimental data of (Bartolomei, 1982). An extensive comparison by Mali et al. (2017) of a number of recent computational efforts for subcooled boiling in vertical heated tubes or annuli (Braz Filho et al., 2016; Chen et al., 2009; Colombo and Fairweather, 2016; Gao et al., 2016; Končar et al., 2004; Končar and Krepper, 2008; Krepper et al., 2007; Krepper and Rzehak, 2011; Li et al., 2011; Mimouni et al., 2016; Murallidharan et al., 2016; Prabhudharwadkar et al., 2014; Zhang et al., 2015a) noted that there is a lack of consistency in the selection of RPI sub-models due to no readily identifiable (or agreeable) criterion and that models for bubble induced turbulence showed large disagreements.

Interface capturing methods have also seen significant application to nucleate boiling but the inherent requirement to resolve (or infer) the interface currently renders large scale nucleate boiling simulations unfeasible, with most recent efforts focusing on investigating single bubble dynamics at single nucleation sites (Jia et al., 2015; Kunkelmann and Stephan, 2010, 2009; Mukherjee and Dhir, 2005; Son et al., 2001, 1999; Welch and Wilson, 2000). This, however, is quite useful, since accurate descriptions of single bubble dynamics are essential in order to make improvements to the mechanistic wall boiling sub-models which prevail in two-fluid approaches. Most of the modelling efforts within these are directed towards accurate representation of the microlayer, a thin layer, generally too thin to be resolved, of superheated liquid known to exist beneath a large majority of the developing vapour bubble (Moore and Mesler, 1961). The exact contribution of this layer to bubble growth, however, is still debated (Hänsch et al., 2017).

The **film boiling** regime is characterised by the presence of a stable vapour layer that separates the liquid phase from the heated surface. Vaporisation now occurs at the liquid-vapour interface, rather than at the nucleation sites along the now dry heated surface. With a continued increase in wall temperature, this regime emerges from nucleate boiling after a transition period that has the following features:

- Vapour bubbles begin to laterally coalesce and the heat transfer rate relative to the surface temperature then begins to drop as the significant generation of vapour starts to prevent the surface from being continuously wetted.
- A peak in wall heat flux, with increasing wall temperature, is observed, the critical wall heat flux, before it begins to decrease.
- As the wall temperature rises further the vapour bubbles begin to dominate the surface, drastically reducing the heat transfer into the fluid.
- Eventually, beyond a certain wall temperature, the surface becomes completely covered by a thin film of vapour and the vapour bubbles generate at the liquid-vapour interface.

Film boiling has historically received significant attention in the literature (Bui and Dhir, 1985; Ellion, 1953; Kalinin et al., 1975; Nishio and Ohtake, 1993), since it can pose issues for many engineering processes. The poor heat transport properties of the vapour (compared with the liquid) mean that, at constant heat flux, transition to this regime can lead to a sudden jump in heated surface temperatures. Within nuclear thermal hydraulics, film boiling can be present during a boiling crisis (Theofanous, 1980), which can challenge the structural integrity of the fuel rods, or during ECC (Emergency Core Cooling) quenching (Hsu et al., 2015; Kopun et al., 2014; Srinivasan et al., 2010; Yagov et al., 2016). It is also important in cryogenics (Ahammad et al., 2016, 2016).

The modelling of film boiling phenomena requires accurate relationships for the interfacial heat and momentum transfer between the superheated vapour blanket and the subcooled or saturated liquid core. The net interfacial heat transfer determines the rate of vapour generation and, therefore, the film thickness. As with two-phase modelling in general, the main challenge resides in the proper choice of the interfacial heat and momentum exchange correlations. Initially for thin vapour films, the heat transfer from the wall to the liquid is primarily by conduction across a laminar vapour layer. Once the thickness increases, however, turbulent flow occurs in the film and the liquid-vapour interface is agitated and becomes wavy. Wave structure on the interface is determined from experiments to be important (Greitzer and Abernathy, 1972; Vijaykumar and Dhir, 1992) and thus provides a challenge when it comes to numerical models.

Classical laminar film boiling correlations by (Bromley, 1950; Ellion, 1953; Hsu and Westwater, 1960) are still used, but are generally limited to the flow conditions and thermal ranges of the experiments they were constructed from. Most current efforts revolve around interface capturing and tracking methodologies to resolve the thin interface. Two-dimensional horizontal film boiling has been tackled using VOF (Agarwal et al., 2004; Samkhaniani and Ansari, 2017; Sun et al., 2014, 2012; Welch and Wilson, 2000), level-set (Gibou et al., 2007; Son and Dhir, 2007) and FT (Esmaeeli and Tryggvason, 2004; Juric and Tryggvason, 1998) with generally good results. Since these approaches require mesh resolutions fine enough to resolve/reconstruct the interface, computational requirements generally prohibit their application to larger scale problems, but they provide useful insight into localised behaviour. There are very few reported studies using full Eulerian two-fluid approaches. Srinivasan et al. (2010) used the AVL-FIRE commercial code to simulate the quench cooling of a hot solid rod inside subcooled liquid. The Bromley correlation (Bromley, 1950) was used to compute interfacial heat transfer coefficients and numerical simulations showed good agreement with concurrent experiments.

Flash boiling occurs when a sudden reduction in ambient pressure to below that of the fluid saturation pressure causes boiling and uncontrolled vapour growth. It differs from most other kinds of boiling in that the phase change is caused by depressurisation, rather than an external heat source. It is a common phenomenon in many industrial applications, including fuel atomisation (Kawano et al., 2006), paper drying (Woods et al., 2000) and desalination (Kalogirou, 2005), but can have an unwanted, and decisive, presence in nuclear thermal hydraulics applications, including LOCA in PWRs (Imre et al., 2010), pressure release through blow-off valves and two-phase critical flow through constrictions (Liao and Lucas, 2017b).

Flashing is initiated through two primary mechanisms: homogenous nucleation and heterogeneous nucleation. The former occurs homogenously in the bulk of the fluid due to thermal fluctuations and is often neglected, since it typically requires much larger degrees of superheat (Marsh and O’Mahony, 2009). The latter occurs at cavities on the walls or on small impurities in the fluid; these unwettable sites provide the initial interfacial area required for heat transfer and vapour generation (Janet et al., 2015). Accurate modelling of the heterogeneous mechanisms is thus the focus of most modelling efforts, but a major difficulty is how to determine the distribution and density of activated nucleation sites, as well as the nucleation rate and bubble size. A recent survey by Liao and Lucas (2017a) noted that the few models that have been presented are generally inadequate or based entirely on empiricism. Most studies assume that vapour generation occurs solely due to interphase heat transfer, and thus use variations on the wall-nucleation models considered earlier.

Liao et al. (2013) used a two-fluid approach to model the flashing evaporation of water inside a vertical pipe; a test case based on the TOPFLOW pressure release experiment (Schaffrath et al., 2001). Citing a lack of nucleation models, a small non-zero (10^{-9}) steam volume fraction was assigned with a constant bubble size. Comparisons with experimental results showed that the use of a constant bubble size was a severe limitation, whilst preliminary simulations using the inhomogeneous MUSIG approach showed improvement. Janet et al. (2015) tested a variety of nucleation models (Blinkov et al., 1993; Riznic and Ishii, 1989; Rohatgi and Reshotko, 1975), including an RPI wall boiling model, in the flash boiling observed during depressurisation through a constriction or rupture (converging-diverging nozzle). ANSYS CFX was utilised with a two-fluid approach and results obtained with the RPI and Blinkov models demonstrated good agreement with experimental data following some minor parameter tuning.

5.4.4.2 Condensation

As the reverse of vaporisation, condensation plays an equally important role in a wide variety of engineering processes, most notably in systems requiring heat exchangers. It also forms an essential part of subcooled nucleate boiling in PWR’s, in the suppression pool systems of BWR’s, which can provide a large pressure and heat sink by condensing unwanted steam during a LOCA, and during a PTS scenario. Condensation appears in several configurations, including film condensation, which involves the formation of a liquid film on a wall whose temperature is below saturation, dropwise condensation, which is characterised by the presence of droplets on the walls, and internal flow condensation, which contributes to the formation of the various two-phase flow regimes (annular, slug, bubbly etc.). It can also be further categorised according to the source of the heat sink; direct contact condensation is that which occurs when the vapour directly contacts a subcooled liquid, rather than a subcooled surface.

As with boiling, the successful modelling of condensation phenomena requires accurate constitutive relations for the interphase heat and mass transfer. The mass transfer models include the Scharge and Lee models which, as discussed previously, require interfacial heat transfer coefficients for closure. These are overwhelmingly provided by empirical correlations (Akiyama, 1973; Chen and Mayinger, 1992; Hughmark, 1967; Isenberg and Sideman, 1970; Shah, 1979; Warrier et al., 2002; Zeitoun et al., 1994) which, whilst having varying levels of sophistication, ultimately rely on experimental tuning and integral parameters. Some recent studies (Apanasevich et al., 2015, 2015; Patel et al., 2017), however, have used correlations based on the surface renewal model of Hughes and Duffey (1991), which utilises local turbulent quantities.

Owing to their suitability for handling large interfacial areas, a number of studies have used interface capturing/tracking techniques to simulate the condensing of a single bubble rising though a vertical pipe/channel (Jeon et al., 2011; Liu et al., 2015; Owoeye and Schubring, 2015; Pan et al., 2012; Samkhaniani and Ansari, 2016; Sun et al., 2014). Most demonstrate satisfactory agreement with experimental results, where compared, but their use of empirical correlations tuned for such flows renders this largely unsurprising.

Lucas et al. (2011) extended the inhomogeneous MUSIG two-fluid approach to include the growing or shrinking of bubbles due to mass transfer (it previously only included bubble coalescence and breakup) and applied it to poly-dispersed steam condensation in a vertical flow of subcooled water. Results demonstrated good agreement with experiments in the TOPFLOW facility (Prasser et al., 2006). Patel et al. (2017) used NEPTUNE_CFD and OpenFOAM to model the drywell-wetwell steam suppression pool system experiment PPOOLEX at the Lappreenranta University of Technology (Puustinen et al., 2013). As well as a Hughes and Duffey based correlation, they applied a later one by Coste (2004) which demonstrated improvement. Results of this, and a similar later study by Tanskanen et al. (2014), were promising but noted that large modelling improvements are still required.

5.4.5 Summary

The ubiquity of two-phase flows within NPP systems means that their accurate numerical prediction becomes of critical importance to the development, uptake and ultimate acceptance of CFD within the NPP community. The scale and difficulty of the challenge stems primarily from the diverse variety of flow regimes present and the current lack of a 'one-size fits all' modelling approach. Currently modelling approaches generally require prior knowledge of the prevailing flow regime; something which might not be readily available or even known. This makes exploratory or 'blind' computations difficult and increases the expertise requirements of the user. The more advanced models can, in principle, handle very complex flow configurations but those, at some level, still rely heavily on regime dependent experimental and empirical correlations. These are typically used outside of their originally intended area of applicability which, as a result, can decrease the quality of results and the strength of the conclusions.

Significant investment and advancement in computational power has enabled more advanced numerical tools, such as Direct Numerical Simulation, to provide a glimpse of what might be possible in the decades ahead. That level of computational power, however, is expensive and it is reasonable to assume that routine thermal hydraulic computations and exploratory design calculations will still rely on the modelling methodologies introduced within this section for at least the foreseeable future.

In order for these models to better serve the nuclear industry, there needs to be an aim to advance the development of more mechanistic and theoretically based models which can be closed with the fitting of a few empirical constants, rather than relying wholly (or even partly) on experimental correlations. The majority of the, usually extensive, experimental work done historically in the process of supporting numerical nuclear thermal hydraulics has been directed towards the validation of system codes. The fidelity of the data is unfortunately, but understandably, too coarse to be useful for the kind of model development work needed to achieve this aim. Thus, this will only be possible if work is done to produce, or make available, high quality CFD grade nuclear thermal hydraulics experimental data.

5.5 Component Modelling

CFD is recognised as a high-computational-demand method in solving practical engineering problems, such as nuclear reactor systems, since the governing equations of momentum, mass and energy are approximated with a set of discrete equations which are solved over a domain with millions or even billions of elements. As a result of the rapid development of computer technology and computing science since the second half of the last century, great progress has been made in the development of CFD methodologies.

However, major challenges still exist, especially those associate with turbulence modelling which is believed to be the last "mountain" to climb for single phase flows, (Smith et al., 2013b). Recently, high-fidelity methods, such as LES (Large Eddy Simulation) and DNS (Direct Numerical Simulation), have become a research hotspot in turbulence studies to produce simulation of flow phenomena using minimum or no empirical models which are the fundamental limitations of the traditional RANS or URANS (Unsteady RANS) turbulence approaches (Menter et al., 2003).

As such, both in academia and industry, LES and DNS methods tend to be more and more frequently used to predict turbulence-related physical phenomena in real-world processes and equipment, and nuclear thermal hydraulics is no exception. Unfortunately, these advanced methods place great demands on computing power, and consequently are still limited to simple geometries and low Reynolds numbers. In fact, even simulating the entire reactor core with less-expensive RANS models still faces tremendous challenges in computing capability due to the complex internal geometries (Yu et al., 2015).

5.5.1 Application of Turbulence Models to Reactor Internals

The internal structure of a nuclear reactor core is extremely complex and varies from design to design. Nevertheless, the primary coolant flow inside a nuclear reactor can be mostly considered as fully developed wall-bounded turbulent flow from a perspective of basic flow regime, such as the flow in a rod bundle of a PWR. Nevertheless, the ability to predict some classic “simple” flows, such as flows through a channel or a pipe, a forward or backward facing step, or around a certain-shape obstacle (e.g. a sphere or a cylinder, etc.) is fundamental to the prediction of the reactor cooling (Benim et al., 2008; Boileau et al., 2013; Chien, 1982; Constantinescu et al., 2003; Fornberg, 1988; E.M.J. Komen et al., 2017; E. M.J. Komen et al., 2017; Liu et al., 2017; Meri et al., 2001; Piomelli et al., 1988; Tiselj and Cizelj, 2012; Travin et al., 1999; Vreman and Kuerten, 2014; Werner and Wengle, 1993).

High fidelity simulations, such as LES and DNS, (Boileau et al., 2013; DeVilliers, 2006; Liu et al., 2017; Meri et al., 2001; Piomelli et al., 1988; Tiselj and Cizelj, 2012; Vreman and Kuerten, 2014; Werner and Wengle, 1993) have also been used, but they are still limited by the high computational overhead for complicated geometric components. Hybrid RANS-LES and DES, which are comparatively less computationally-expensive than LES will develop further (Slotnick et al., 2014). However, the more traditional RANS and URANS methods are likely to continue to play a dominant role in large-scale simulations in the area of nuclear thermal hydraulics, although they provide less information than the above high-fidelity methods (Benim et al., 2008; Kawai and Larsson, 2012).

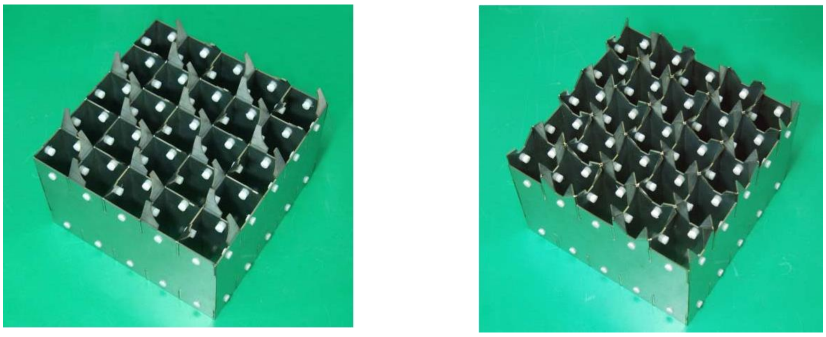
5.5.2 Fuel assembly

5.5.2.1 PWR

Spacer grids with mixing vanes are generally used to reinforce the array of the fuel rods and enhance the fuel-to-coolant heat transfer by inducing turbulent secondary flows downstream, which brings additional challenges to CFD simulations (Conner et al., 2010). Figure 20 shows two types of spacer grids used in laboratories representing some key features of spacers used in reactors. In order to test the ability of state-of-the-art CFD methods to capture the important turbulent structures in fuel bundles, benchmark experiments were designed and carried out with experimental facilities constructed in accordance with real-world fuel bundle designs. They provide accurate testing data to the CFD community, to facilitate performance improvement and assessment criteria of CFD simulations in this area.

Considering the affordability of computing costs, 4x4 and 5x5 rod bundle designs are most commonly adopted in place of a real-world 14x14 or 17x17 PWR rod bundle without losing major flow characteristics, (Denefle et al., 2017; Navarro and Santos, 2011), e.g. OECD/NEA KAERI MATiS-H, (Lee et al., 2014) and EPRI NESTOR CFD Round Robin, (Wells et al., 2015). In these benchmark experiments, velocity profiles and turbulence statistics were obtained with advanced Laser Doppler Velocimetry (LDV) (Chang et al., 2014; Fen Shen et al., 1991; Karouta et al., 1995; Rowe et al., 1974; Xiong et al., 2014a, 2014b; Yang and Chung, 1998) or Particle

Image Velocimetry (PIV) based technologies (Conner et al., 2013; Dominguez-Ontiveros and Hassan, 2009; Elvis et al., 2012; Hosokawa et al., 2012; Lee et al., 2013). Figure 21 presents a typical result of the measurements in a benchmarking experiment.



(a) (b)

Figure 20: Two types of spacer grids used in OECD/NEA KAERI MATiS-H benchmark (a) Split-type spacer grid, (b) Swirl-type spacer grid (Smith et al., 2013b)

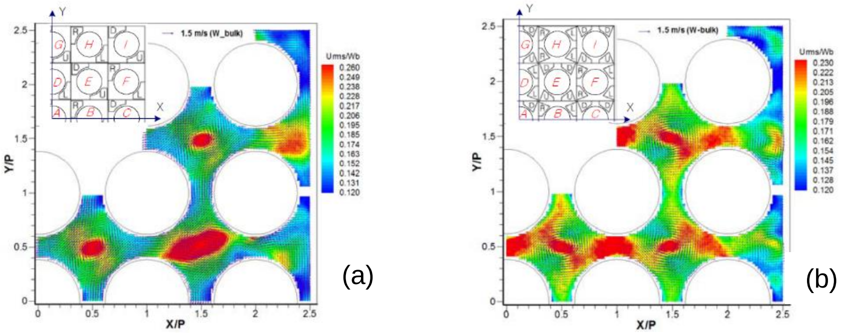


Figure 21: Distribution of measured lateral velocity vectors U, V coloured according to turbulence intensity, U_{rms}/W_{bulk} at Z=1.0 Dh (a) Split-type spacer (b) Swirl-type spacer (Smith et al., 2013b)

Since the early 1990s, researchers have begun performing CFD simulations to study the flow around PWR rod bundles with spacer grids. Due to the limitation of computing capability, these early studies mostly adopted a single sub-channel domain with symmetry assumptions at boundaries to minimise the computational mesh (Cui and Kim, 2003; Házi, 2005; Imaizumi et al., 1995; Karouta et al., 1995). However, these assumptions and simplifications cannot always lead to reliable results. Lee and Choi (2007) pointed out that the number of sub-channels in a CFD model is important for accurate predictions due to the complex interactions between sub-channels.

With the rapid development in computing power, 2-subchannel and 4-subchannel models become more popular, (G. Chen et al., 2017; Han et al., 2017; Liu et al., 2012; Liu and Ferng, 2010; Tseng et al., 2014; H. Zhao et al., 2017) and provide relatively better results than single sub-channel approaches. In the recent decade, CFD simulations of coolant flow in sub-channels were intensively performed based on 4x4 and 5x5 rod bundle arrays, (Agbodemegbe et al., 2016; Ala et al., 2017; Bieder, 2017; Bieder et al., 2014; Chen et al., 2016; X. Chen et al., 2017; Cheng et al., 2017; Conner et al., 2010; Denefle et al., 2017; Ikeda, 2014; In et al., 2017, 2001; Kang and Hassan, 2016; Lee et al., 2014; Navarro and Santos, 2011; Peña-Monferrer et al., 2012; Podila et al., 2014; Podila and Rao, 2016a, 2017; Wei et al., 2017; Zhou et al., 2017), making use of a number of benchmark experiments that have been carried out with similar rod bundle configurations. Turbulence models were carefully investigated in these studies to confirm their validity in predicting complex flows in the vicinity of the spacer grids.

In addition to the traditional two-equation eddy-viscosity models, a number of advanced RANS/URANS models (such as k-ω SST, RSM), hybrid RANS-LES models and full LES were applied to simulate the turbulent swirling flow downstream of the mixing vane. However, it is generally agreed within the CFD community that high-order turbulence models do not always guarantee a better numerical solution in rod bundle simulations, which is quite different from the conclusions from OECD/NEA Vattenfall T-junction benchmark exercise, (Mahaffy et al., 2014; Smith et al., 2011).

In general, LES performs somewhat better than RANS in predicting turbulence statistics downstream of the spacer grids, (Bieder, 2017; Bieder et al., 2014; Lee et al., 2014), but it is far from overwhelmingly superior than some RANS and URANS models, such as the k-ω SST model, which has been found to have an excellent performance in such kind of simulations (Cheng et al., 2017; Liu et al., 2012; Sohag et al., 2017; Tseng et al., 2014). Even some low computing-cost models, such as the k-ε model with standard wall function, can produce acceptable results in terms of mean velocity and pressure drop, (X. Chen et al., 2017; Podila et al., 2014). This is clearly a case that needs to be better understood.

A good proportion of the investigations reviewed above also studied the heat transfer between the coolant and the rod bundle. It has been generally concluded from these studies that heat transfer along the fuel rod is significantly enhanced by secondary flows induced by the spacer grid, (Chen et al., 2016; Cheng et al., 2017; Sohag et al., 2017; Zhou et al., 2017). RANS turbulence models can predict the axial wall temperature with reasonable agreement with experimental measurements when conjugate heat transfer is considered, (In et al., 2017; Kang and Hassan, 2016). However, these models cannot capture well the heat transfer in the corners of sub-channels, and in turn the circumferential temperature may be poorly predicted, (Podila and Rao, 2017; Tseng et al., 2014). In addition, the computational grid is another major concern in rod bundle simulations, as such the results have been found to be highly sensitive to grid quality which is of similar importance to that of gird resolution itself (Lee et al., 2014). More robust and adaptive numerical methodologies are required to deal with this issue.

5.5.2.2 HTGR/VHTR

High Temperature Gas-cooled Reactor (HTGR)/Very High Temperature Reactor (VHTR) are one of the candidate Generation IV nuclear reactor designs advanced for their inherently safe performance by using a large amount of graphite, low power density design, high conversion efficiency and integrated energy utilisation, e.g. hydrogen production, coal gasification, etc. (Wu et al., 2010).

A pebble bed of spherical fuel pellets is one of the core designs adopted in the HTGR. Due to narrow flow channels formed around the fuel pellets, the coolant flow is very complex in terms of strong anisotropic curvature near the surface of the fuel pebbles. Direct measurements of the flow field of the pebble bed is extremely difficult, hence numerical simulation is a useful tool. Shams et al. (2013a) pointed out that to simulate a full-scale pebble bed with detailed CFD methods is not feasible in the foreseeable decades, and simulations based on a limited-sized domain are a compromise between accuracy and computing cost.

Over the last decade, the RANS approach has intensively been used to model the complex flow around curved pebble surfaces (In et al., 2008; Lee et al., 2007; Taylor et al., 2002; Wu et al., 2010). However, no particular success has been achieved which may be due to limitations imposed by the various closures as explained by Wu et al. (2010). More recently, Hassan (Hassan, 2008) and Shams et al. (2015a; 2014b, 2013a, 2013b) used more advanced turbulence models, such as LES, hybrid LES/RANS and DES, to investigated the flow distribution in the pebble bed. Shams et al. (2013c, 2013d, 2012) also did q-DNS simulations and found that q-DNS data can be considered as benchmarks to validate other low-order turbulence models. By comparing the results with q-DNS data, Shams et al. (2013a) found that LES is much better than RANS and URANS in terms of predictions of RMS fields, and so may be used to validate RANS approaches in a realistic pebble bed configuration. However, URANS models such as the cubic k-ε model still seem to be acceptable to produce scoping simulations for such complex flow configurations, considering that they are much faster than LES.

Another version of the VHTR is the prismatic reactor in which the core consists of several rings of hexagonal graphite blocks drilled to accept fuel pins and provide flow channels for helium coolant. Gaps occur between adjacent hexagonal blocks to allow for tolerances in manufacturing the blocks and geometrical changes over the lifetime of the reactor, which allow bypass flow of the coolant therein. MacDonald (2003) pointed out that the bypass flow can be as high as 20% of the total coolant flow in the core, which can have a significant effect on the overall performance of the reactor.

Due to difficulties in experimental measurements, the studies of the bypass flow are largely numerical using CFD methods. In order to minimise the computing cost, most of these studies were based on a geometry of a 1/12 sector of a prismatic block for the whole core length, (Johnson and Sato, 2012; Lee et al., 2016; Sato et al., 2010, 2009; Tak et al., 2008; Tung et al., 2012). Others use geometries at core-scale of corresponding experimental facilities, (Kanjanakijkasem et al., 2016; Wang et al., 2014). These works systematically studied the effects of the gap width, wall roughness and irradiation-caused shrinkage of the graphite block on cooling effect, temperature distribution and flow regimes.

For steady state operation, the 1/12-sector model gained significant success. It seemed, however, to be too small for a natural convection-dominated situation which would appear after a loss of forced convection through the core for various reasons. Simoneau et al. (2007) employed a porous medium model to account for a 30 degree section of the reactor core and simulated the natural circulation under a laminar flow assumption. Tung et al. (2016, 2014, 2013), on the other hand, performed a staged study using a detailed CFD method, which included a 1/12-sector model, a sub-region model including several sectors and finally a 1/12-core model. In these studies, a variety of RANS turbulence models were investigated and compared against the laminar assumption of the flow in the fuel channel. The realisable k-ε model combined with a two-layer shear driven approach was finally selected for turbulence modelling in the 1/12 core model which provides the most detailed and accurate results to characterise the phenomena of natural convection with 520 million computational cells. Takamatsu (2017) and Tsuji et al. (2014) also employed detailed core-scale models to simulate forced convection and mixed convection in a High Temperature engineering Test Reactor (HTTR). Their results agreed well with the experimental measurements.

5.5.2.3 SCWR

The SuperCritical Water Reactor (SCWR) is the only water-cooled reactor in the proposed Generation IV reactors, which has a high thermal efficiency, a compact system structure and low capital cost, (Heusener et al., 2000; NERAC and GIF, 2002; Oka and Koshizuka, 2001, 2000). Different from sub-critical conditions, heat transfer behaviour of supercritical fluid shows some surprising characteristics due to drastic changes in thermal-physical properties in the vicinity of pseudo-critical temperature, such as density, specific heat, viscosity as well as thermal conductivity (Jackson and Hall, 1979a, 1979b). Hence, a comprehensive understanding of supercritical pressure flow and heat transfer, especially in the flow geometry related to the fuel assembly, is essential for the development of SCWR.

One of the most significant features of the supercritical flow is the heat transfer deterioration which may be caused by buoyancy effects resulting from sharp variation of density near the pseudo-critical line (Rahman et al., 2016). Due to great technical difficulties and high economic expense, experimental studies on heat transfer of supercritical pressure fluids are still limited. Thanks to the fast development of computational methods and increase of computing capacity, CFD methods have been used by many researchers to study supercritical flows in different geometries, e.g. circular pipes, (Bae et al., 2005; He et al., 2008a, 2008b, 2005, 2004a, 2004b; Jaromin and Anglart, 2013; Liu et al., 2013a; A Shams et al., 2015; M. B. Sharabi et al., 2008; Wen and Gu, 2011; Zhang et al., 2012), plane channels, (M.-T. Kao et al., 2010; M. Sharabi et al., 2008) and annular channels, (Liu et al., 2013b; Ma et al., 2017), which largely enhanced the understanding of this phenomenon.

However, these studies could not provide a general consensus on the choice of a suitable turbulence model for supercritical flow simulations, as it has been found that the performance of the turbulence models used in these works varied significantly from case to case, and they are flow and geometry dependent (Podila and Rao, 2016b). Among various turbulence models tested, the low-Reynolds-number k-ω SST model was believed by some researchers to have better performance than other RANS models in supercritical pressure flow simulations given the wall region is well resolved ($y{+}= \sim 1.0$), (Liu et al., 2013b; Palko and Anglart, 2008; Schulenberg and Visser, 2013; Zhu, 2010).

With the accumulation of knowledge derived from these studies, exhaustive studies have been focused on modelling of a single sub-channel of a SCWR due to its low computing cost, (Ampomah-Amoako et al., 2013; Gu et al., 2010, 2008; Podila and Rao, 2015; Rahman et al., 2016; Sharabi et al., 2009; H. Wang et al., 2016; S. Zhang et al., 2014). However, the single channel analysis could be conservative under a real SCWR condition due to the complex exchanges among channels. More recently, some researchers began to simulate the SCWR with rod bundle models, such as 2x2 square bundle and 7-rod hexagon bundle (Podila and Rao, 2016b; Shang, 2009; Shang and Lo, 2011, 2010). The results obtained indicated that both the geometry and orientation of the rod bundle can have a significant effect on the flow and thermal behaviour in a SCWR. DNS has been used to complement experiments to produce detailed information to improve our understanding of heat transfer deterioration and to improve turbulence models (Bae et al., 2006, 2005; Nemati et al., 2016, 2015; Wang and He, 2015). In the future, more work needs to be done along this direction to provide more information to guide the design of the SCWR.

5.5.3 Plenum

Typically prior to the reactor core fuel assembly, the coolant first flows through the bottom plenum, which aims to produce a uniform flow distribution in the fuel channels. After the coolant is heated up by the nuclear fuel and comes out from the fuel assembly, it flows into the outlet plenum before leaving the core. Therefore, understanding the coolant flow and mixing in the plena plays an important role in nuclear reactor design and fabrication, control at operation or accident conditions, as well as maintaining the integrity of the fuel assembly and other components (Wu et al., 2012). The internal structure is usually very complex in the plenum which aggravates the lateral flow caused by flow direction change. This brings additional challenges to CFD simulations.

For CFD simulation of the outlet plenum, one of the challenges is the non-uniformity of the inlet flow and temperature distribution. To obtain suitable inlet boundary conditions for the CFD model, some researchers carried out separate analysis using a system code e.g. Chiang's work in modelling the upper plenum of a PWR (Chiang et al., 2011), Anderson's work in modelling the outlet plenum of a VHTR (Anderson et al., 2008) and Mochizuki's work in modelling the upper plenum of a sodium-cooled reactor (Mochizuki and Yao, 2014). Xu et al. (2012) on the other hand, performed an isothermal simulation of the outlet plenum of a PWR with a uniform velocity inlet boundary condition based on previous finds of Conner et al. (2003). Kao et al. (2010; 2011) performed a CFD analysis for two different sub-domains of the upper plenum of a PWR, which were a ¼ section of one control rod guide tube and a representative unit containing two ¼ sections of adjacent control rod guide tubes and one ¼ section of a neighbouring support column, respectively. Fine meshes were used in this work, which allow capturing smaller geometries and flow details. Böttcher (2008) set up a CFD model for a complete reactor pressure vessel with some simplifications for complex structures in the core, but the outlet plenum was fully resolved.

The inlet plenum is also of great importance due to its significant influence on the flow behaviour of the coolant in the reactor core, (Jeong and Han, 2008; Watanabe et al., 2015). It has been found that the coolant flow coming from the cold leg encountered high resistance in the inlet plenum and is redistributed due to internal structures, such as Control Rod Guide Tubes (CRGT), (Frepoli, 1996; Matsumoto et al., 2007; Takahashi et al., 2003). This changes the pressure loss and flow distribution significantly depending on the specific design of the plenum.

To achieve a better understanding of the stratification and mixing behaviour of the coolant flow in various conditions, boundary conditions representative of the reactor conditions are essential in CFD simulations. Early studies (Bieder et al., 2007) used a uniform velocity field at the inlet of the cold legs, which was found to be inappropriate for the prediction of buoyant asymmetric flow in the cooling loop (Boumaza et al., 2014; Farkas et al., 2016). In addition, the strong swirl induced by the main circulation pump may also have strong effects and needs to be considered as well, (Petrov and Manera, 2011).

Due to the complexity of the geometry, detailed modelling of the inlet plenum based on a real-scale reactor is rare in the current literature. Alternatively, simplifications have been made, which have still provided some details on the unsteady flow field of the reactors (Boyd and Skarda, 2014; Brewster et al., 2017). Recently, in order to achieve more uniform flow into the core region, EDF Energy launched a research project for a new reactor design by optimising the flow diffuser in the inlet plenum. A number of research projects were carried out to investigate the effects of different designs of the diffuser based on simplified models where the core was modelled using a porous medium approach (Ge et al., 2017; Xu et al., 2017, 2016).

5.5.4 Containment

In most NPP designs, the third and the fourth levels of defence are achieved through a strong structure enveloping the nuclear reactor, which is referred to as the containment. The containment protects the nuclear reactor system against external (e.g. hurricane, earthquake, aircraft crash etc.) and internal (e.g. LOCA, Main Steam Line Break (MSLB) accident, etc.) events and accidents, and provides biological shielding of neutron or gamma radiation (IAEA, 2004). To design the containment to fulfil these requirements, it is very important to understand the thermal hydraulic characteristics of the flow within the containment under operational state and accident conditions.

Thermal hydraulic analyses of the containment have mostly been done with lumped parameter codes in the past, (Tills et al., 2009; Vijaykumar and Khatib-Rahbar, 1999), despite some inaccuracy due to larger control volumes used, (Xiao et al., 2017). Water film evaporation plays a significant role in decay heat removal from an over-heated containment vessel, (Woodcock et al., 2004). Ambrosini et al. (2002) carried out a CFD simulation on the evaporation cooling process of an experimental water film. More recently, CFD analysis has been performed to simulate natural circulation with thermal and density stratification which is believed to be not well resolved in typical system codes, especially for postulated design-base accidents (LOCA or MSLB) in a Passive Containment Cooling System (PCCS).

Jang et al. (2013) and Su et al. (2014) performed CFD analysis of the cooling system on a simplified geometry with an evaporation channel and a condensation channel. Wang et al. (2016) investigated the AP1000 PCCS outside cooling with a CFD approach incorporating the Eulerian wall film model to account for the water film evaporation. Xiao et al. (2017) performed a comprehensive simulation of the conjugate heat and mass transfer between the gas inside the containment, water film on the inner steel wall of the containment and the gas in the annular channel between the two walls of the containment. Heat conduction in the solid structure of the containment was also considered in this study.

5.5.5 Summary

Typical reactor cores contain thousands of fuel pins which result in thousands of fuel channels where the coolant circulates to remove heat generated from the nuclear fuels. Despite the complexity of the reactor core, the internal structures are spatially repetitive in the three directions. This repetition allows a CFD model for a small part of the reactor to be constructed rather than based on the entire reactor core. Such CFD models are feasible to gain local flow information contributing to an understanding of the whole picture inside. In the above section, the research progress in CFD modelling of the fuel assembly, plenum and containment has been reviewed.

The fuel assembly is undoubtedly the most important one which attracts a huge attention from the CFD community in nuclear thermal hydraulics. Regarding PWR rod bundles, validation of advanced turbulence models used in simulating the turbulent swirl flow downstream of spacer grids is currently a research hotspot. Experience shows that the use of more complicated turbulence models does not always necessarily lead to better simulation results. For instance, the MATiS-H benchmark exercise shows that the advanced LES method is not always superior to a RANS/URANS model in simulating PWR rod bundles with mixing spacers. Therefore, more work needs to be done to setup guidelines for reasonable utilisation of the turbulence models according to specific needs. This will also be helpful to improve the simulations of flow and heat transfer around the spacer grids and further optimise the design of these structures.

For the cases of other types of nuclear reactor, CFD approaches seem much less sufficient than that of the PWR. To date, some high fidelity methods (LES and DNS) have been found to be used for simulation of the pebble-bed reactor. However, RANS simulations are still the main stream for the prismatic reactor. Future studies should consider the use of more advanced turbulence models to provide more accurate predictions on flow transitions and temperature profiles in these reactor types. In SCWR, heat transfer deterioration is a major concern that has been intensively studied in simple geometries, and the k-ω SST turbulence model is found to have better performance than other RANS models in predicting flows at a supercritical pressure.

In conclusion, although significant progress has been made in the application of CFD to fuel assembly modelling, improvements are still needed to model some of the important flow physics that may occur in both normal and accident operations, including heat transfer deterioration, buoyancy effects in mixed convection, swirling flow, etc. Such improvements may result from further development of advanced wall treatments and improved meshing methodologies. Considering the limitations of the current computer capability, these advanced methods are very likely to be used for the modelling of small segments of a real-world fuel assembly.

Alternatively, the development of ‘coarse-mesh’ CFD methods, or semi-empirical approaches, can significantly reduce the mesh and computational requirements. With this kind of method, the fuel assembly or even the whole core could be simulated with much more modest computational resource and might help to bridge the gap between detailed CFD and system codes.

5.6 Whole System Modelling

To faithfully capture the detailed flow and heat transfer phenomena in a reactor core and understand the overall thermal hydraulic performance of the nuclear reactor, sufficient mesh resolution and accurate models are essential in well-resolved CFD simulations. As a result, such simulations are restricted to modelling partial sections of the key components of the nuclear reactor due to constraints in computer capacity (Viellieber and Class, 2012).

Up to now, very few studies can be found to simulate the entire reactor core using well-resolved CFD. Instead, the overall reactor has been traditionally simulated using the best-estimate system analysis codes (Section 4) developed based on 0D/1-D methods, such as COBRA2-CP (Thurgood et al., 1983), TRAC (Liles and Mahaffy, 1986), TRACE (U.S. Nuclear Regulatory Commission, 2010), CATHARE (Bestion, 1990), RELAP5 (RELAP5 Development Team, 1995), ATHLET (Lerchl et al., 2012) and MARS (Chung et al., 2010). Despite being able to provide a complete description of a NPP at various conditions, system codes are not always satisfactory in simulating 3D transients that take place in complex geometries (Corzo et al., 2015).

5.6.1 CFD Methods

With suitable simplifications, CFD methods can also be used to model the whole reactor core at an acceptable computing cost. Tsuji et al. (2014) and Takamatsu et al. (2017) simulated a natural convection-dominant circulation in a HTTR under LOCA conditions using a 1/12-core model, which was confirmed to be superior to the corresponding component modelling by Tung et al. (2016), who carried out a staged study on a similar prismatic VHTR. In these studies, the sectional core models used in place of the entire reactor core largely reduced the total computational domain taking advantage of the circumferential symmetry of this type of reactor.

Simoneau et al. (2007) made further simplifications to the 1/12-core model of a modular prismatic high temperature reactor. In their study, a porous media approach was used to model the prismatic fuel stacks. The total number of control volumes was therefore reduced by 1 and 3 orders of magnitude as compared with those of Tsuji and Tung, respectively. In the past decade, the porous media approach has been widely used in coupling with the well-resolved CFD method to simplify the core modelling. In most of these cases, the porous media simplification was used to describe the fuel assembly, (Chen et al., 2015; Fiorina et al., 2015; Skibin et al., 2017; Viellieber and Class, 2012; Yu et al., 2017, 2015), others also include the plena, (Brewster et al., 2017; R. Chen et al., 2017).

In addition, some researchers proposed other ways for modelling the core. Böttcher (2008) simulated the full RPV of a VVER-1000 PWR with geometric simplification of the core region and an additional pressure loss coefficient for the lower plenum. Corzo et al. (2015) incorporated a 1-D finite volume code to account for the complex fuel channels in a full core simulation of a pressurised heavy water reactor. Zhang et al. (2013) employed a distributed resistance model to represent the core module of a real geometry model of a PWR, whilst a detailed model was used for the downcomer and the lower plenum.

5.6.2 Coupled Methods of CFD and System Codes

In addition to the simulations applied to the reactor core and its key components, CFD can also be used for design and safety assessment of the entire NPP system. Such applications are not based on CFD modelling of the whole NPP system, which is neither necessary nor practical, but is achieved by coupling it with thermal hydraulic system codes. Best-estimate system codes have been developed to analyse system response during a wide variety of accident scenarios and transients, but they cannot capture the transients where 3-D flows play an important role in a given accident scenario. Therefore, a coupling between system codes and CFD combining both advantages is a hopeful endeavour for safety assessments in these situations (Bertolotto et al., 2009). To date, tremendous efforts have been devoted to find different ways of coupling different pairs of codes.

From a spatial point of view, two coupling methods are described in the literature, namely the domain decomposition and domain overlapping approaches. From a temporal point of view, they can be classified as implicit/semi-implicit and explicit approaches, respectively (Grunloh and Manera, 2016). Early attempts to coupling a system code with CFD include Aumiller et al. (2001) and Gibeling and Mahaffy (2002). In recent years, a number of demonstrations of coupling system codes and CFD codes have been made for applications in a variety of simple testing geometries, such as a straight pipe, bent pipe, T-junction, etc. (Bertolotto et al., 2009; Grunloh and Manera, 2016; Li et al., 2014; Papukchiev et al., 2009; Park et al., 2013). Some researchers have applied coupled simulations to nuclear systems:

- Anderson et al. (2008) analysed a VHTR-type reactor with a coupled RELAP/CFD model where the 3-D flow in the outlet plenum was accounted for by the CFD model.
- Papukchiev et al. (2011) coupled ATHLET and ANSYS CFX and validated it against a pressure thermal shock related experiment for a PWR.
- Vyskocil and Macek (2014) coupled the system code ATHLET, the neutron kinetic code DYN3D and the CFD code ANSYS Fluent. A scenario with strong 3-D phenomena referred to as ‘one steam dump to the atmosphere’ of a VVER-1000 reactor was simulated.
- Bury (2013) studied a containment system under a LOCA using an in-house system code HEPCAL-AD coupled with ANSYS Fluent, which simulated the natural circulation within an annular channel between an inner steel vessel and the containment wall.
- Bavière et al. (2014) simulated a sodium cooled nuclear system with coupled simulation of CATHARE2 and Trio_U, which allows energy and momentum feedback from CFD to the system code. The difficulties that the system code encountered in predicting evolution from forced convection to natural convection in a large pool for a sodium reactor with a complex 3D geometry can be addressed with the coupled simulation (Pialla et al., 2015).

5.6.3 Summary

In this section, the possible ways are discussed for CFD to be used in whole core modelling or even the whole NPP system modelling, which have been done with the best-estimate system codes for decades. Two methodologies have been used to apply CFD to extend the capability of the traditional system codes.

Firstly, the moderately computationally-expensive coarse-grid CFD/under-resolved CFD is an option to produce more detailed simulations of the whole reactor core compared with the system codes. Such CFD adopts geometry simplification, porous media approach or distributed resistance method. In comparison with system codes, coarse-grid CFD provide more flexibility, relies less on experimental or empirical inputs and has the potential to reproduce the results of detailed CFD simulations. However, such methods are still at their infancy and significant developments are needed to realise their potential.

Secondly, the capability of the traditional system code can be enhanced by coupling it with a CFD code, which is used to simulate components where the representation of the 3-D characteristics is required. Despite some promising results, the validation of the coupling methodology is still an imperative and challenging task for the future. Most work reported to date is for coupling of specific pairs of codes, and the methods used are still relatively primitive.

Development of advanced and generic methodologies to improve stability and efficiency of coupling will certainly see broader applications of this promising whole system modelling.

5.7 Porous Media

Flow and heat transfer characteristics in porous media are of interest in many practical applications, such as gas turbine blade cooling, metal foam heat-exchangers, cooling of electronic components, catalytic converters and fuel cells. Depending on whether the solid material of the porous matrix has high or low thermal conductivity, porous components can be used to either greatly enhance or attenuate heat transfer. Porous components are introduced to thermal hydraulic systems of current reactors and are expected to be more widely used in new generation designs. The most obvious example is the pebble bed nuclear reactor, an example of which is shown in Figure 22.

It is therefore necessary to be able to represent the flow within a porous material and also to quantify the thermal interaction between the fluid and the solid matrix. Further interest in the use of numerical models of flow through porous media in thermal hydraulics analysis arises from the current practice within the nuclear industry, mentioned in Section 5.6.1, to model flows through complex and multi-layer components as flows through porous materials. An example of this is the modelling of heat transfer and fluid flow within insulation packs used to protect the hot-box dome of advanced gas cooled reactors, which is described in Cooper et al. (2016).

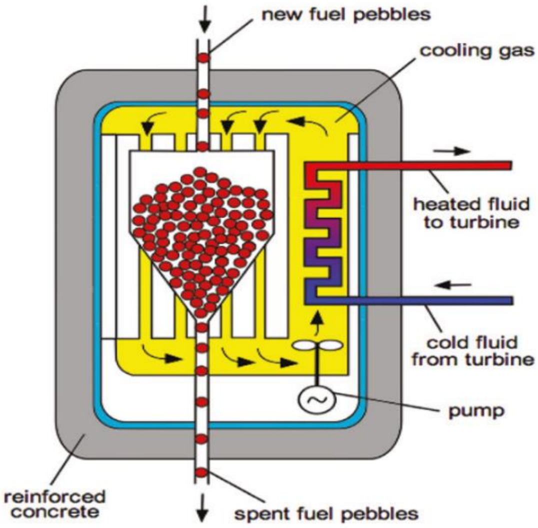


Figure 22: Pebble bed reactor (Revol, 2015)

5.7.1 Modelling Review

To describe the flow and heat transfer characteristics precisely within the pores of porous media requires huge computer resources, and in any event it is only possible in packed bed types, in which the geometry of the solid matrix is well defined and repeatable. In the case of porous foam matrices with a random structure, microscopic analysis requires techniques like x-ray tomography. Therefore, the volume-averaging theorem is usually applied to flow and heat transfer transport equations to analyse the flow through porous media. This process results in a set of the Navier-Stokes equations for the macroscopic flow, meaning the space-averaged flow, in terms of the Darcy velocity (total volume averaged velocity) and the porosity of the porous media, φ, which is essentially the void volume fraction occupied by the fluid.

The drag force that the porous structure exerts on the fluid is modelled through two terms, the Darcy term, which accounts for the extra viscous force, and the Forchheimer term, which accounts for form drag due to the porous structure. Both terms include the porosity and the latter also involves the permeability, K (m^2), which represents a measure of the interconnected pores inside the porous media, which allows fluid to penetrate within these pores.

For the thermal variation within the porous medium, two macroscopic temperature models are available; a Local Thermal Equilibrium (LTE) model, or One-Equation Energy model, and a model for separate fluid and solid temperatures called the Local Thermal Non-Equilibrium (LTNE) model, or Two-Equation Energy model. In the former approach, the average solid and fluid temperatures are locally assumed equal. The transient and conduction terms are based on a weighted average of the fluid and solid thermo-physical properties. In the second approach the average solid temperature locally differs from the average fluid temperature. There are two macroscopic transport equations, one for the energy of the fluid and one for the energy of the solid. An interfacial energy transfer term is included in both equations to account for the local transfer of thermal energy between the solid and the fluid phases, which of course can now have different local temperatures. The latter approach is more appropriate for transient cases and also cases with internal heat generation.

Turbulent flow can be detected even in the porous media when the pore length scale is larger than the turbulent length scale. When the pore Reynolds number is sufficiently high, Nakayama and Kuwahara (1999), turbulence modelling is required. Numerical modelling of turbulent flow in porous media is mainly based on the macroscopic approach in which the double-averaging (volume and Reynolds averaging) is used. Macroscopic Navier-Stokes equations can be derived by two different methodologies: either using time-averaging of volume-averaged Navier-Stokes equations, or volume-averaging.

Pedras and de Lemos (2001) and Nakayama and Kuwahara (1999) and subsequently Nakayama and Kuwahara (2008) developed macroscopic two-equation k-ε turbulence models for turbulent flow through porous media. Additional terms were introduced in the macroscopic turbulent transport equations to account for the effects of the porous forces on the generation rate of turbulence and on the production rate of its dissipation rate, with their coefficients determined by conducting microscopic analysis through spatially periodic arrays of square and elliptic bars by the former Pedras and de Lemos (2001) and latter Nakayama and Kuwahara (2008) study, respectively. These source terms were modelled based on a balance of either turbulent kinetic energy or mean kinetic energy within the pore in the former and latter, respectively. More recently, Kuwata and Suga (2015) developed a volume-averaged version of the Craft and Launder (1996) Two-Component-Limit (TCL) Reynolds Stress closure, and Mößner and Radespiel (2015) developed a volume-averaged version of the Jakirlić and Hanjalić (2002) Reynolds stress version.

The flow over a porous wall behaves differently to that over a solid wall. The slip velocity at the permeable wall is one of the characteristic features. Since the permeable wall only provides weak blocking, momentum exchanges across the fluid/porous interface region are expected and cause energy dissipation, which leads to a significant increase in the friction factor compared with that at an impermeable wall. Therefore, the porous surface enhances the onset of turbulence, and the flow is expected to be turbulent at a lower Reynolds number compared with that over a solid surface.

This is modelled by following the approach of Kuwata and Suga (2013), where a variable resistance, for a second-moment closure, across the interface region was implemented by applying variable porosity and damping functions for the extra drag forces in the governing momentum transport equations and also for the extra terms in the turbulent stresses and ε

transport equations. These damping functions have been tuned and optimised to produce reasonable results in comparison with available DNS and experimental data. This approach to the modelling of interface effects has recently been extended to k-ε models by Al-Aabidy et al. (2017), but further developments are necessary.

5.7.2 Summary

In summary, as far as nuclear thermal hydraulics is concerned, the next challenge in the modelling of flows through porous media is in the modelling of heat and fluid flow through porous regions, sometimes deliberately chosen to have a low thermal conductivity and sometimes the opposite. There is therefore a need for more reliable and cost-effective turbulence models of steady and transient turbulent heat and fluid flows through porous regions.

The scientific literature shows that the above described RANS models of turbulent flow in porous media have been applied to internal flows of considerable complexity, and validations of flow predictions have been successful, especially at high Reynolds numbers. There is, however, less validation of the turbulence modelling of the interface regions, of the thermal predictions, especially with natural convection, and what there is, it is mainly confined to air as the fluid, which has a Prandtl number of 0.7.

Moreover, existing validation is confined to steady state cases. To address the needs of the nuclear industry, the existing RANS models need to be further developed by extending the validation to unsteady flow phenomena and also to forced and natural convection cases for a range of Prandtl numbers. This is essential for the RANS models to become sufficiently general for reliable use in future reactor designs.

5.8 Fluid-Structure Interaction

Fluid-Structure Interaction (FSI) phenomena play a significant role in most engineering applications; the collapse of the Tacoma Narrows Bridge in 1940 being a well-known example. FSI analysis is equally important in nuclear engineering. An obvious example is Flow-Induced Vibration (FIV) of PWR fuel pins. As shown in Figure 23, the fuel elements consist of long slender vertical rods. The coolant fluid, in this case water, is pumped upwards in a direction parallel to the rods and the turbulence of the coolant generates flow-induced vibrations. Kim (2010) reported a systematic fuel failure occurring in a 16x16 Korean Optimised Fuel Assembly (KOFA).

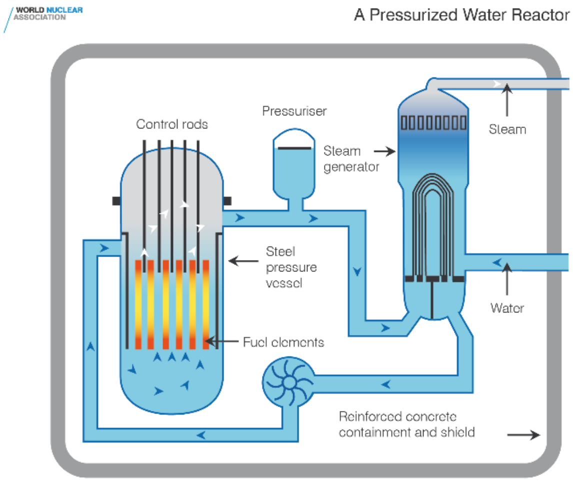


Figure 23: Schematic view of a PWR (Copyright World Nuclear Association)

Fretting phenomena due to flow-induced structural vibrations have also been identified in many other types of nuclear reactors, including lead/lead alloy cooled fast reactors, accelerator driven systems (Del Giacco et al., 2014, 2012a, 2012b) and boiling water reactors (Edsinger et al., 2011). According to Kim (2013), grid-to-rod fretting induced failure accounted for around 70% of the worldwide nuclear fuel rod failures in 2011. Other FSI-induced problems are also present such as the vibration of boiler tubes in many types of nuclear reactor. There is consequently a strong case for the development of versatile FSI solvers which can deal with a wide range of problems including the challenging topic of FIV.

5.8.1 FSI Methodologies

Traditionally the choice has been to focus on either the fluid or the solid aspect of the problem at hand and to simplify the other. Even though this approach might be useful in some situations, it is not acceptable for cases where the coupling is so intricate that the simplification of either one yields incorrect results. Several approaches are suitable for FSI modelling, depending on the degree of accuracy required, and on the characteristics of the problem under consideration. The two main existing branches according to the behaviour of the solid body are: a) deformable solid body modelling, and b) rigid-body motion modelling.

Regardless of the assumptions made about solid behaviour, a further modelling choice relates to yet another equally crucial question, namely the coupling strategy e.g. direct or segregated coupling. Coupling can be achieved in a direct manner if both solid and fluid are solved concurrently. This approach requires a powerful nonlinear numerical solver, designed with this purpose in mind. Because the engineering field has historically been segregated regarding the simulation of solid and fluid problems, domain specific solvers are currently the norm rather than the exception. It is therefore more practical to integrate existing bespoke fluid or solid solvers together to tackle FSI problems, than to create one from the ground up. This is why the segregated coupling approach is far more popular. Strong coupling can still be achieved with segregated solvers by means of outer iterations. If the interaction amongst the two media is not so intrinsic, acceptable solutions might be obtained with weak coupling techniques, and thus avoid the computational overhead inherent to segregated strong coupling algorithms.

Fluid-solid interaction phenomena are complicated by nature since they involve coupled behaviour. There are two general coupling techniques to solve FSI problems:

- Monolithic approach
- Partitioned approach

In a monolithic implementation the entire set of non-linear algebraic equations arising from the discretised governing equations of fluid flow and solid mechanics is solved as a whole (Tyković and Jasak, 2007). That way, there is no need to treat the interface section separately in order to couple the problem. This method usually exhibits a better convergence rate than its partitioned counterpart (Heil et al., 2008; Ryzhakov et al., 2010). Due to the deep-rooted interaction between the fluid and the solid while formulating and solving FSI problems with this technique, it is well suited to handle strongly coupled behaviours (Greenshields and Weller, 2005).

In contrast, the partitioned technique relies on solving the fluid and solid domains in a segregated manner. This allows for either the same or different equation discretisation method to be used for the two domains. The interaction of both domains is handled at the interface (Tyković and Jasak, 2007). From the numerical solutions of the fluid and solid domains, the resulting pressure or displacement fields are applied as boundary conditions for the respective media. In the partitioned approach context, this is the most widely applied methodology at the interface to couple the problem. However, a key factor that directly impacts the accuracy of the solution is how to handle the transfer of information from one domain to the other. If the locations where the dependent variables are stored in each region are different, which means that interpolation is required, then the accuracy of the overall model can depend heavily on the interpolation scheme.

Traditionally, the governing equations of fluid flow are derived in an Eulerian reference frame by means of the material derivative. The governing equations of solid mechanics, on the other hand, are usually presented in a Lagrangian reference frame. When solving FSI problems it is of vital importance to account for the changes in the fluid physical domain due to the deformation or rigid movement of the solid body. For the solid region, the computational domain adopts the same reference frame as the governing equations, in this case being a Lagrangian reference frame. This way, tracking free surfaces or interfaces between different materials becomes much easier. The drawback of this computational domain methodology comes when large deformations of the material arise, causing the computational domain to experience such large deformations as well which might break the underlying solver.

The Arbitrary Lagrangian-Eulerian (ALE) method implements a combination of both the Lagrangian and Eulerian descriptions to take advantage of their strengths. The result is a powerful method to solve problems in which both large deformations and tracking of surfaces or interfaces matter.

5.8.2 Deformable Solid FSI Modelling

If the problem requires the solid to be modelled as a deformable body, then the first obstacle for attacking numerically the coupled phenomena is the fact that both the solid and the fluid domains are usually discretised employing different approaches in most commercially available segregated solvers. While solid mechanics problems typically are dealt with using the Finite Element Method (FEM), fluid mechanics problems are discretised via the Finite Volume Method (FVM). Furthermore, the solution techniques employed by both methods to solve the discretised set of equations are radically different. Numerical fluid mechanics solutions are obtained with iterative methods, which are better suited to attack non-linearities. On the other hand, solid mechanics problems typically rely on direct methods for such tasks (Jasak and Weller, 2000). With plenty of FEM and FVM commercial codes available nowadays, the traditional FSI approach is to set up the solid mechanics problem with imported stress boundary conditions. The imported boundary conditions result from a flow field solution obtained by using a different software package corresponding to the fluid with which the solid interacts.

As discussed in Yates (2011), this procedure involves several factors that have to be considered before committing to solve the problem in this fashion. The aforementioned boundary condition information has to be interpolated to the locations on the boundary where the discrete values of the dependent variables are stored in the FEM. This will unavoidably lead to errors that could be significant. Computational overhead is also likely to occur since the data storage structure of both approaches is quite different; this is exacerbated when dealing with transient problems where the transfer of information has to be repeated for each time step.

An alternative to employing the two separate discretisation methods is to solve both the fluid and solid domains using a single discretisation technique. This, along with the same variable storage arrangement for both domains, eliminates the major issues mentioned above. The obvious question then becomes whether to extend the FEM method to the solution of fluid dynamics or the FVM to the solution of the solid mechanics equations.

The FEM has overcome one of its major limitations when being considered for the solution of fluid dynamics problems, namely the usage of computationally expensive direct methods for solving the resulting system of discretised equations (Reddy and Gartling, 2010). The FVM has also earned a respectable reputation amongst researchers to attack solid dynamics problems, because of its conservative properties, and the inherent nature of iterative solvers to deal with non-linearities.

The work of Farhat et al. (1995) is regarded as revolutionary in the field of FSI. It implements a partitioned FEM-FVM solver using the ALE method for the transient movement of the fluid computational domain with application to aero-elastic problems. Another early example of a partitioned FVM-FEM study is the work of Glück et al. (2001), to solve for lightweight membrane structures interacting with fluid flow. The coupling depended on the transfer of information between the two non-matching grids, and was handled by a conservative algorithm scheme pioneered by Farhat et al. (1998). To account for the mesh motion the ALE technique introduced by Demirdžić and Perić (1990), and reviewed above, was used. A novel concept to FSI modelling was presented by Slone et al. (2002). The authors implemented a single governing equation discretisation method; the FVM for both media. Furthermore, by using a vertex based FVM for the solid continuum, the transfer of information between both media was done efficiently and without the need to employ non-conservative interpolation methods. A similar approach was also successfully implemented by Yates (2011) in the simulation of bio-engineering flows.

A more general approach to elastic fluid-structure interaction using the Overset Grid method can be found in Kimura et al. (2010), Paik (2010), Nakata and Liu (2012) and Miller et al. (2014). In particular, the study of Miller et al. (2014) employs a FEM-FVM partitioned solver along with the overset grid method. Results show a significant improvement over the traditional ALE method with regard to mesh quality and the avoidance of having to re-mesh the whole fluid computational domain for transient moving bodies. A strong advantage of the overset grid method is the high quality of the near-wall mesh, which is critical in turbulent FSI analysis and also in FSI applications influenced by thermal variations.

5.8.3 Rigid Body FSI Modelling

If the problem is suitable to model the solid as a rigid body then the solid governing equations are, in general, less challenging to solve. However, the coupling is still critical to obtain accurate solutions. In these cases, the most challenging aspect to deal with is efficient fluid domain grid generation at each time step without degrading mesh quality due to solid body motion.

Fortunately there exist methodologies that allow efficient redefinition of the fluid computational domain at each time step, while preserving the original mesh quality. The Immersed Boundary Method (IBM) is a popular choice for this purpose. The overset grid method also falls under this category, with the added benefit of being particularly well-suited for problems requiring fine near-wall grids without compromising grid quality. Both approaches rely on somehow disabling or neglecting computational cells in regions occupied by the solid mass.

In terms of grid generation ease, the immersed boundary method is perhaps the simplest choice, as in most of its variants a static non-conformal Cartesian grid is used to discretise the fluid physical domain, whilst the body generated mesh comprises a set of Lagrangian nodes. The concept behind the method is to account for solid interaction on the fluid side by means of the addition of source terms that represent wall forces in the fluid momentum equations, while the solid mesh is responsible for tracking solid body motion (Peskin, 2002).

Although the original method was developed for elastic FSI problems, several modified implementations have proven its viability to resolve rigid-body FSI problems. The Immersed Boundary Projection Method (Taira and Colonius, 2007) was successfully applied to model rigid body FSI problems in which the motion of the immersed rigid structure was prescribed. More recently it was successfully applied to model strongly coupled two-way FSI of a set of articulated plates (Wang and Eldredge, 2015).

One of the earliest published studies employing overset grids for FSI phenomena is that of Freitas and Runnels (1999). They analysed the flow-induced rigid body dynamics of a square cylinder. By integrating the stress field generated by the flow over the surface of the cylinder, the resultant force and moment were fed to the rigid body dynamics equations to compute the resulting kinematics. Similarly, Prewitt et al. (2000) further extended the Chimera method to account for the six-degrees of freedom rigid body motion for purposes of aerodynamic analysis.

The overset grid technique is increasingly becoming popular within the CFD community to solve rigid-body FSI problems. Recently there has been a surge in the usage of the method to model naval applications, Carrica et al. (2007). More recently their research group has implemented a solver in the open source OpenFOAM platform that makes use of overlapping grids to model ship hydrodynamics under different operating conditions (Shen et al., 2015) . Their simulations include a free surface solver, six degree of freedom solver (6DOF), unstructured overset grids, turbulence modelling and rotating ship propellers.

The solid body motion solver is commonly based on high order numerical methods such as Runge-Kutta or Adams-Bashford, and the solution of the Euler-Newton equations of rigid body motion introduces negligibly little cost to the overall solution algorithm. Currently most commercial CFD packages offer rigid body motion solver modules which can be coupled to the fluid flow solution.

5.8.4 Summary

As demonstrated by the multiple and ever growing number of research projects involving the use of the FVM to solve solid mechanics problems, elastic FSI modelling seems to be pointing towards a partitioned single FVM formulation. The conservative properties of the FVM along with the existence of iterative solvers allow it to tackle fluid dynamics problems more efficiently than its FEM counterpart while being perfectly capable of simulating elastic solid mechanics. The use of a single integrated environment for simulating solid-deformation FSI problems avoids many of the difficulties associated with different data structures and interpolation schemes. Furthermore, readily available open source FVM CFD tools such as OpenFOAM have instilled methodical software development practices suitable for complex undertakings such as FSI simulations.

The use of the overset grid method provides considerable advantages when it comes to modelling fluid flow around moving bodies. In combination with the ALE method and unstructured grids, it allows the preservation of mesh quality even around deforming solid bodies, and enables the flexibility of introducing local mesh adaption techniques. Ultimately, a partitioned single unstructured FVM formulation, coupled with the overset grid method, proves to be a powerful modelling environment, for deformable solid FSI problems.

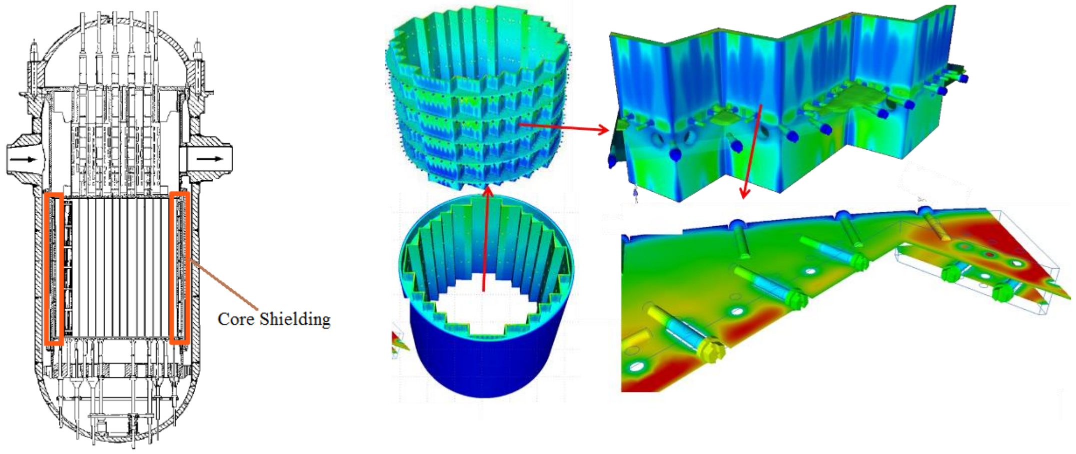
Although not as popular as the immersed boundary method, the use of overlapping grids to model fluid flow around moving rigid-bodies is definitely more established than its use to model flow over elastic bodies.

In a NPP context, it has been seen that FSI phenomena, such as flow-induced vibration, can cause serious damage to reactor components. The development of reliable and validated simulation methodologies for unsteady FSI phenomena is consequently urgently needed. Progress has so far been slow because of the multidisciplinary nature of the phenomenon, which makes the development of simulation methodologies more challenging, but also suitable validation data very hard to come by.

As far as simulation methodologies for unsteady FSI reactor phenomena are concerned, the use of a single integrated environment, combined with the use of overset meshes, offer a promising strategy. The provision of suitable and detailed validation data is essential for the development of suitable FSI algorithms in nuclear thermal hydraulics and needs to be given a very high priority.

5.9 Conjugate Heat Transfer

Conjugate Heat Transfer (CHT) is the coupling of heat conduction analysis in solids with convective heat transfer analysis in fluid regions. CHT is attracting increasing attention, and gaining importance in a diverse range of engineering applications, from geothermal energy generation to casting and solidification, including nuclear engineering. One such example is the EDF Energy thermo-mechanical study of the bolts holding the PWR core shielding, shown in Figure 24. The objective was the evaluation of the mechanical integrity of 1,000 bolts used to hold the peripheral thermal shielding part of the nuclear core, through structural mechanics analysis of the thermal stresses. A coupled CFD/heat conduction simulation, using two separate codes, one for CFD (*Code_Saturne*) and one for heat conduction (SYRTHES) was carried out. The simulated temperature field of the bolts holding the peripheral shielding was transferred to a structural analysis code.



(a) PWR schematic diagram (b) Core shielding

Figure 24: Conjugate heat transfer simulation of PWR core shielding to compute fields in 1000 bolts (Solid Code_Syrthes, Fluid Code_Saturne).

5.9.1 Modelling of Conjugate Heat Transfer

As indicated in Section 2.2, the successful modelling of CHT phenomena requires simultaneous thermal analysis in the fluid and solid regions, which in addition to the mean temperature field also extends to the temperature fluctuations. It is thus essential, for nuclear thermal hydraulic applications, to develop cost-effective RANS models, which can reliably simulate how turbulence-generated thermal fluctuations penetrate into solid regions. However, as shown by the brief overview below, this research area is still in its infancy.

The earliest research of conjugate heat transfer was conducted by Polyakov (1974). In his studies, an analytical solution for temperature fluctuations in the viscous sub-layer adjacent to a semi-infinite solid was obtained. The results showed that temperature fluctuations at the fluid-solid interface are dependent on the specific fluid and solid properties.

Only a few studies have employed experimental methods. Chiu et al. (2001) investigated the channel flow which is heated from below and showed that the conjugate heat transfer has a strong impact on heat transfer. Dees et al. (2012) studied an internally cooled turbine blade. The mean temperature distributions at both internal and external faces were obtained. Mensch et al. (2014) and Mensch and Thole (2015) studied the blade end-wall with film cooling and impingement.

Physical insight and validation data for the development of cost-effective RANS models of conjugate heat transfer have so far been generated by DNS studies. These have mainly focused on conjugate heat transfer in heated channels. Kasagi et al. (1989) showed that the near-wall behaviour of the temperature variance, turbulent heat flux and turbulent Prandtl number are dependent on the thermal properties and the wall thickness.

Sommer et al. (1994) introduced two limiting thermal wall-boundary conditions, isothermal and iso-flux respectively. Mosyak et al. (2000) demonstrated that the wall temperature fluctuations are affected significantly by the type of thermal wall-boundary condition. Tiselj et al. (2001b) investigated the effect of these two ideal boundary conditions on heat transfer for friction at a Reynolds number of 171 and Prandtl numbers 1.0 and 5.4. Their results showed that the type of boundary condition has no effect on the mean temperature profile, but confirmed the findings of earlier studies, that they have a significant effect on the temperature fluctuations within the viscous wall sub-layer.

There then followed a series of further DNS studies by Tiselj and co-workers, which include Tiselj et al. (2013, 2004, 2001a), Tiselj and Cizelj (2012) and Tiselj (2014). They further explored conjugate heat transfer in a heated channel of walls of different thicknesses and over a range of Reynolds numbers, Prandtl numbers and wall thermo-physical properties. They demonstrated that two dimensionless parameters play an important role in determining the strength of temperature fluctuations in the fluid near-wall region and also within the wall; the thermal activity ratio, K and the diffusivity ratio G. These are defined as:

$$K = \frac{\left(\rho_f c_{Pf} \lambda_f\right)^{\frac{1}{2}}}{\left(\rho_s c_{Ps} \lambda_s\right)^{\frac{1}{2}}}, \qquad G = \frac{\alpha_f}{a_s}$$

where ρ, c_P, λ and α are the density, specific heat capacity, thermal conductivity and thermal diffusivity ($\propto = \lambda/\rho C_P$) respectively and subscripts f and s denote fluid and solid respectively.

More recently Flageul et al. (2017, 2015) in their DNS study of conjugate heat transfer in a heated channel provided information on the variation of the dissipation rate of the temperature variance. They demonstrated that due to the changes in thermo-physical properties, the dissipation rate is discontinuous across the surface of the solid wall.

In a departure from the practice of focussing on conjugate heat transfer in basic channel flow cases, Wu et al. (2017) have applied DNS analysis to the more complex conjugate heat transfer case, of a jet in a cross-flow, shown in Figure 25. They demonstrated for such complex cases the effective diffusivity approximation of the turbulent heat fluxes becomes inadequate.

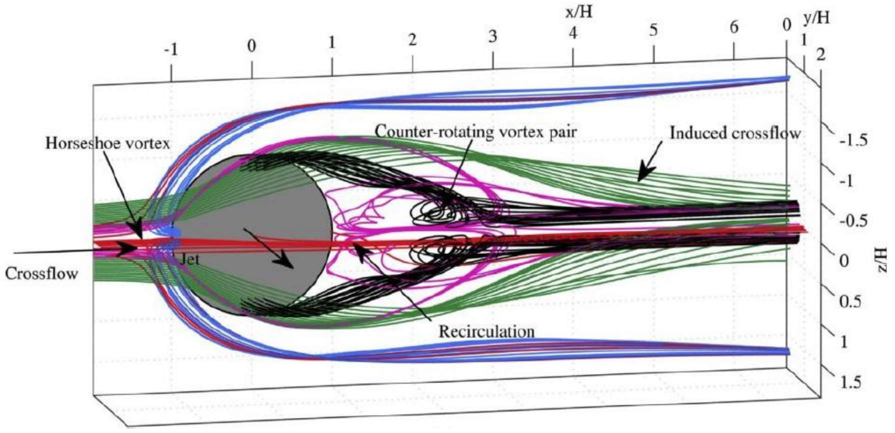


Figure 25: Flow structures of jet in crossflow. From (Wu et al., 2017)

Compared to the above-mentioned DNS studies, RANS simulations of conjugate heat transfer must not only be able to reproduce the mean temperature variation within the fluid and solid domains, but also the temperature fluctuations within the solid. This in turn requires the inclusion of transport equations for the temperature variance and its dissipation rate. Such model equations have been proposed by Hanjalić et al. (1996), but not within the CHT context. The work of Craft et al. (2010) has made some progress in the development of RANS models which can reproduce the correct variation of the temperature variance and its dissipation rate within the fluid and also across the solid. More extensive validation is however needed before this approach can be more widely applied.

5.9.2 Summary

Conjugate heat transfer (CHT) analysis is assuming increasing importance in reactor design and safety analysis. There is consequently a need for the development of simulation methods which can not only reproduce the mean temperature variation in the fluid and solid regions simultaneously, but which can also predict how turbulence-induced thermal fluctuations penetrate into the solid.

So far, experimental investigations have made only a modest contribution to the advancement of our understanding of CHT, and these are mostly for turbine blade cooling applications. Combined fluid/solid DNS has proved a valuable tool in improving our knowledge and understanding of this phenomenon, but inevitably such a computationally expensive approach, with one or two notable exceptions, has so far been limited to simple test cases. For CHT analysis of more complex cases, the development of suitable and cost-effective RANS is necessary.

The development of RANS thermal models suitable for CHT analysis is still in its early stages, with very few researchers involved in such efforts. A more concerted research effort is needed.

5.10 Liquid Metals

It is worth first noting some recent review papers providing a useful overview on international activities on the thermal hydraulics of liquid metals.

- Cheng et al. (2015) and Papukchiev and Buchholz (2017) provided an overview of a recently completed European project, THINS, on modelling of next generation nuclear power systems.
- Roelofs et al. (2015; 2017) described two ongoing European consortia on LMFR thermal hydraulics, that is, the Horizon 2020 SESAME and MYRTE projects.
- Merzari et al. (2017) discussed issues and perspectives of applications of LES in nuclear reactors from the point of view of a US consortium, the Centre for Exascale Simulation for Advanced Reactor (CESAR).
- Kamide et al. (2017) provided an overview of activities in SFR in Japan and Chellapandi and Velusamy (2015) in India.
- Tenchine (2010), Grötzbach (2013) and Roelofs et al. (2013) discussed some fundamental challenges in simulating heat transfer to liquid metals.

5.10.1 Fundamental Studies on Heat Transfer to Fluids of Low Prandtl Number

Heat transfer to liquid metal is special because the Prandtl number of liquid metal (sodium, lead) is significantly lower than one (around 0.01 to 0.001) as opposed to of order unity for air and water where most heat transfer research has been carried out. As a consequence, the process of heat transfer in liquid-metal turbulent flow exhibits significantly different characteristics from those of ‘common’ fluids, having a very thick thermal boundary layer, for example.

Specific correlations have been found to be necessary for such fluids, normally based on Peclet number ($RePr$). A recent review of experimental data and correlations for turbulent forced convection of liquid metals in pipes can be found in Pacio et al. (2015). For CFD and turbulence modelling, the key challenge is the invalidity of the Reynolds analogy, as the turbulent Prandtl number, which is often taken as a constant, varies significantly in the boundary layer. Improving turbulent heat flux ($\overline{u_\iota T'}$, appearing in the Reynolds-averaged energy equation) is a key topic in the CFD modelling of liquid metal. Grötzbach (2013) provided a comprehensive overview of challenges in low-Prandtl number heat transfer simulation and modelling.

As part of a European consortium project, THINS, a number of approaches have been developed and/or tested for the modelling of turbulent heat flux (Cheng et al., 2015; Papukchiev and Buchholz, 2017; Ferry Roelofs et al., 2015). As a basic approach deviating from the constant turbulent Prandtl number (Pr_t), Duponcheel et al. (2014) assessed the performance of turbulent heat flux models using variable Pr_t based on LES channel-flow data at a reasonably high Reynolds number ($Re_\tau = 2000$). The models examined include (i) Reynolds (1975), which is dependent on global flow parameters; (ii) Weigand et al. (1997), which is partly dependent on global flow parameters and (iii) Kays (1994), which is dependent on local flow parameters. They also proposed a new expression, the so-called mixed-law-of-the-wall.

Kenjereš and Hanjalić (2000) proposed an algebraic heat transfer model (not specifically for low Pr fluids), which has been widely used and implemented in STAR-CCM+ (Kenjereš et al., 2005). Shams et al. (2014a) assessed and recalibrated such models for heat transfer to liquid metals. A shortcoming of the original model (Kenjereš et al., 2005) is that different sets of constant coefficients were used for different flow regimes. Shams et al. (2014a) replaced one of the constant coefficients with a correlation based on the Peclet number, which has achieved much improved performance. Additionally, a four equation turbulence model has been developed and used for forced convection heat transfer to liquid metals in Manservisi and

Menghini (2014). Marocco et al. (2017) performed a careful assessment of the correlation model of Kays (1994) and the four equation model of Manservisi and Menghini (2014) in the simulation of mixed convection in a vertical concentric annulus. They have rather interestingly found that the former simpler model performs much better than the latter more sophisticated four-equation model in capturing the heat transfer deterioration due to buoyancy.

5.10.2 Fuel Assembly

In addition to the ‘peculiar’ heat transfer characteristic due to low Prandtl number, other challenges involved in the SFR sub-assemblies include transverse flows, the effect of the spiral spacer wires, blockage and the so-called gap instability (e.g. Meyer & Rehme (1994) and Duan & He (2017)) associated with the small pitch-to-diameter ratio used in SFRs, which potentially lead to strong flow instabilities and fuel pin vibrations.

ANL has developed a fluid and thermal simulation computer package Nek5000, which is aimed at tackling transitional and turbulent flows in complex domains based on the spectral element method (not specifically for liquid metal). The package is particularly suitable for LES and DNS. As part of the US NEAMS and CESAR programs, Nek5000 was used to perform various LES simulations for SFR cores providing valuable detailed data required for improvement/validation of simulation tools (Pointer et al., 2009).

Merzari et al. (2017) described their methodology and LES in simulations for both fuel channels and reactor core natural circulations, including a 37-pin bare rod bundle and a 19-pin SFR bundle with a pin-to-diameter ratio of 1.08 and Re=15,000. In the current European SESAME and MYRTE projects, DNS and LES are also identified and used as a key approach to generate detailed validation data on LMFR thermal hydraulics alongside physical experiments (Roelofs et al., 2017). Earlier work using DNS and LES for Lead-Bismuth Eutectic (LBE) was reported in Bricteux et al. (2012). The reliance on such high fidelity CFD is due to the rapid development in computer technology as well as the fact that physical experiments are technically challenging and liquid metal is opaque, making advanced flow measurement techniques inaccessible.

Merzari et al. (2016) summarised a benchmarking exercise based on a collaboration between Argonne and some European organisations (NRG, SCK-CEN and UGent) examining the performance of RANS simulations in reproducing a LES simulation of an isothermal flow in a 7-pin SFR assembly with wire-wrapped spacer. It was found that all models tested (including the k-ω SST, a cubic k-ε model and a k-ε realisable model) were able to capture somewhat the cross flow, with the k-ω SST performing marginally better than other models. Jeong et al. (2017) reported a separate study of a 7-pin wire wrapped rod bundle with heat transfer and again to some extent endorsed the reasonably good performance of the k-ω SST model in producing a good level of cross flow. Doolaard et al. (2015) reported some preliminary results of a benchmark of RANS models against a LES with conjugate heat transfer for a 19-pin wire-wrapped rod bundle with characteristics representative of MYRRHA. Pacio et al. (2015; 2017, 2016) described comparison between experiments and simulations of an LBE cooled fuel assembly in a hexagonal rod bundle with spacers and the MYRRHA reactor respectively.

Zhao et al. (2017) carried out CFD simulations of an isothermal flow in a wire-wrapped hexagonal 7-pin enclosed bundle and found that the transverse flow does not vary significantly with the Reynolds number, but rather strongly with the pitch-diameter ratio.

Manservisi and Menghini (2015) simulated liquid metal flowing in a square lattice bare rod bundle geometry using a constant turbulent Prandtl number as well as a two-equation turbulent heat flux model. The constant turbulent Prandtl number clearly did not capture the expected behaviour whereas the conclusion regarding the two-equation model was inconclusive due to the lack of data for comparison, but these authors believe such a model was tested favourably in simpler flow configurations. Ge et al. (2017) performed simulations of flow of heavy liquid metal in triangular and square lattices using the low Reynolds number Launder-Sharma turbulence model coupled with various turbulent-Prandtl-number models to assess their performance. The assessment was based on heat transfer correlations for such sub-channels. Among the models tested, Kays (1994) and Aoki (1963) were found to produce predictions that are close to the empirical correlations.

Finally, it is worth noting the work by Hu and Fanning (2013), who developed a momentum source model for a wire-wrapped rod bundle to simplify mesh generation to resolve the geometry of the wire spacers which remains a major challenge. They have demonstrated the advantage and reliability of this method in simulating 7-pin and 37-pin bundle configurations.

5.10.3 Pool Thermal Hydraulics

A principal safety concern in the top plenum is the mixing of the sub-assembly jets with various fluid temperatures in the core outlet region, which may potentially cause high-cycle thermal fatigue resulting in thermal striping or cracks. The temperature variation may be several tens of degrees and the frequency is between 1 Hz to 50 Hz (Velusamy et al., 2010). Recent studies include:

- A detailed experiment has been carried out using a sodium experimental facility with parallel triple-jets at JAEA (Kimura et al., 2007). LES was performed to simulate the jet mixing and compared with experiments by Kiruma et al. (2002), Chacko et al. (2011) and some others.
- Tenchine et al. (2013b) described experimental studies at CEA based on two identical test sections, one with air and one with sodium based on two co-axial jets at different temperatures emerging from a large tank. Numerical simulations using both RANS and LES (using the CFD package TRIO_VF developed at CEA) were compared with their experimental data as well as those of Kimura et al. (2007) mentioned above. It was concluded that the LES expectantly performed better than the RANS, but the former still needs improving.
- More recently Varol et al. (2017) reported a combined experimental and numerical study using LES of parallel jets mixing about perforated obstacles. Good agreement between them was found which illustrated the mixing characteristics.
- LES was also performed to study the thermal striping in the upper plenum of the Korean PGSFR at KAERI (Choi et al., 2015). Nouali and Mataoui (2014) studied horizontal jets of different patterns using URANS.
- Ward et al. (2018) discussed the scaling of thermal stratification and mixing in the outlet of the plenum of SFRs to address the issue encountered when scaled-down experiments are designed to study such phenomena in real reactors.

The sodium-argon free surface in the primary sodium circuit is an important source of gas entrainment which may present a safety problem. Tenchine et al. (2014) described several water tests in relatively simple flow conditions to study vortex formation and gas entrainments. This was accompanied by numerical simulations using a front-tracking method coupled with a LES using TRIO_U (a CFD package developed at CEA) to study surface instabilities and vortex occurrence.

Anderson and Jackson (2017) summarised studies of experimental investigations at the University of Manchester into radiative heat transfer between the pool free surface and the roof, and the characteristics of the sodium aerosols formed in the argon cover gas above the pool. Numerical simulations of these experiments are currently being carried as part of project FORTE.

5.10.4 Whole Core and System Thermal Hydraulics

Tenchine et al. (2013a) described an international benchmark organised by an IAEA Coordinated Research Project (CRP) on the natural convection in the primary circuit of PHENIX which was performed before its shutdown in 2009 (see also Tenchine et al. (2012c) describing the test in detail). Some eight organisations participated in the benchmark using 1D or 3D system/sub-channel codes. The rapid onset of natural circulation was demonstrated when the primary pumps were tripped, together with other phenomena including significant heat removal through thermal mass and heat losses, efficient heat removal through steam generator natural convection air cooling. Overall the different codes seemed to show coherent qualitative results, but significant discrepancies were demonstrated. It was shown that the use of 3D or 1D/3D coupling were necessary to resolve natural circulation. Additionally, the THINS project also used this data for validation of system and system/CFD coupling approaches (Pialla et al., 2015), which also concluded that system/CFD coupling is necessary to resolve the three-dimensional circulations.

The CATHARE system code, which was initially developed for PWRs, was adapted for SFR starting from 2006 and has become the French reference code for SFR applications (Tenchine et al., 2012b). The coupling between CATHARE and a CFD code TRIO_U (now TRIO_CFD) was also noted in this paper and in Tenchine et al. (2012a), but is further described in detail in Bavière et al. (2014) in which the approach was applied to simulating the PHENIX natural circulation test. TRIO_U is capable of simulating the whole core as well as the sub-assembly and the fuel channels (Tenchine et al., 2012a).

Hu and Yu (2016) reported the development of a 3D full core conjugate heat transfer capability of a sub-channel modelling type for SFRs at ANL. The hexagon lattice core is modelled as 1D parallel channels, with 2D models for the duct walls and inter-assembly gaps with the six sides modelled separately accounting for asymmetric temperature distribution such as in edge channels. The Jacobian Free Newton Krylov solution was applied to simultaneously solve the fluid/solid fields in a fully coupled manner. The model was compared with a full CFD solution favourably.

Finally, a 3D CFD model has been used to simulate the natural circulation in the main vessel of a pool type reactor in India as part of their SFR development activities (Vivek et al., 2013).

5.10.5 Decay Heat Removal

An important feature of SFRs is that it can naturally include passive decay removal in its design and some rather preliminary CFD attempts have been made to demonstrate such capabilities. Hung et al. (2011) performed a rather straightforward simulation of decay heat removal using a k-ε turbulence model (Launder and Spalding, 1974) with a wall function implemented in Fluent with no special treatment for turbulent Prandtl number. The model seemed to be able to demonstrate the decay heat removal principle and compare the performances of different configurations.

Parthasarathy et al. (2012) carried out a much more detailed CFD model for the Indian Prototype Fast Breeder Reactor (PFBR) to resolve the various parts of the core coupled with a 1D code to simulate other sub-systems of the decay removal circuit. They validated their model against the plant data from PHENIX. However their turbulence and heat flux models are the same as those of Hung et al. (2011). Again, the basic principle has been well demonstrated but it would not be surprising that the detailed natural circulation is not well resolved by such simple treatments such as the use of a standard wall function as well as a constant Pr_t. More recently, David et al. (2017, 2015) extended the above work, studying the decay heat removal under natural circulation in a typical SFR pool under a core meltdown scenario with part of the core debris settling core catcher, again using the Launder-Sharma model.

5.10.6 Summary

The most special feature of liquid metals is the low Prandtl number, which necessitates the development and testing of advanced turbulent heat flux models (beyond the conventional constant turbulent Prandtl number). Models of various complexities have been developed, including for example, the relatively simpler turbulent-Prandtl-number correlations and the more sophisticated models using transport equations for mean-square temperature variance and its rate of destruction. These models have up to now mostly been tested in simple conditions.

Validation using more complex geometry/conditions including for example, jet mixing, flow separation and flows around wire-spacers are ongoing. Simulations of the fuel assemblies have been undertaken using various turbulence models and the effects of blockage, wire-spacer, flow instability and inter-wrapper flows are being investigated using various turbulence models. The k-ω SST turbulence model seemed to be singled out as performing better than others, but few investigations used advanced turbulent heat flux models in simulations of assemblies. Various preliminary attempts have been made to simulate the plena flow with strong buoyancy using CFD. In addition, coupling CFD with system codes is an area of development to improve the predictions for the whole systems.

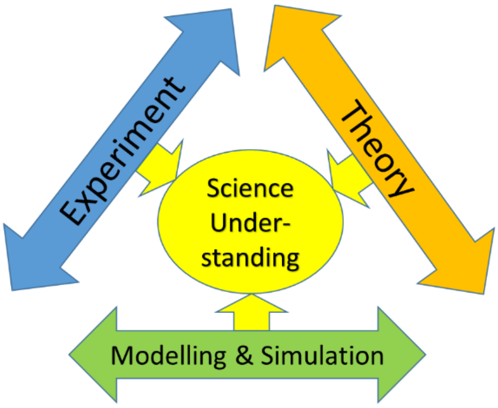
Finally, it is noted that experiments using liquid metal are extremely difficult and therefore very limited data are in existence for model testing and validation. Various international campaigns are in progress in developing liquid metal experimental facilities, but many experimental validations for liquid metal fast reactors (including assemblies and the pool) use simulating fluids such as water to reduce experimental difficulties as well as to produce detailed information that is difficult to generate with the opaque liquid metals.

In addition, high fidelity CFD (DNS and LES) is now used in the liquid metal thermal hydraulics community (including in the US and Europe) as an important and ‘routine’ complimentary way to physical experiments to generate data with which modelling tools can be validated against. Currently, such high fidelity CFD provides data for both fundamental phenomena, such as channel flow, separations and jets, and fuel assemblies with and without wire spacers.

6 Advanced Simulation and Modelling Packages

6.1 Computing and simulation as the Third leg of scientific methods

It is now 20 years since the US Department Of Energy's (DOE) Accelerated Strategic Computing Initiative (ASCI) program was introduced to "eliminate reliance upon nuclear testing in the US nuclear weapons program and achieve high confidence in the use of simulations for stockpile assessment and certification". As illustrated by the DOE director in Figure 26: "(ASCI) established computational simulation into a third fundamental piece of the scientific method, on a par with theory and experiment. [in 10 years] astounding advances were made in simulation applications, computing platforms, and user environments" (Larzelere, 2007).



Addition of Science Based Modelling and Simulation

- Science (1st principles) based modelling and simulation used to extrapolate and predict beyond tested states.
- Can quickly confirm or disprove Theory hypotheses.
- Improve experiments by predicting 'areas of interest' and expected results.

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

Figure 26: Enabling the Shift to a Science Based Approach (Larzelere, 2010)

A 10,000-fold increase in system performance in 15 years was seen in the US from the first tera-scale system, ASCI Red in 1997 to peta-scale systems 2012: Sequoia, Cielo, and Roadrunner. Hoang (2013) explains how the Office of Advanced Simulation and Computing (ASC), Nuclear National Security Administration plans for the next stage with a focus on collaboration and end user productivity in view of the increasing complexity. V&V also figures prominently alongside HPC technology.

While the traditional scientific method (experimental and theoretical) did not yet acknowledge the role for computing and simulation, Ang et al. (1998) established the model verification and simulation validation from first Principles simulations in the ASCI program. This practice of using first Principles simulations to validate CFD models is now ubiquitous in academic circles. In thermal hydraulics turbulence modelling, DNS databases are used extensively to improve and validate RANS models.

As stated in Merzari et al. (2016), as part of a U.S. DOE International Nuclear Energy Research Initiative (I-NERI), ANL is collaborating with the Dutch and Belgian Nuclear Research (NRG, SCK·CEN) to perform and compare a series of fuel-pin-bundle calculations representative of a wire-wrapped fuel bundle for which little data is available for verification and validation of new simulation tools.

Ghent University and NRG performed their simulations with commercially available CFD codes. The high-fidelity ANL LES code Nek5000 from the Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) suite was also used. It was intended to serve both as a surrogate for physical experiments and provide insight into experimental results.

As part of the NEAMS program, ANL has performed several wire-wrapped analyses with Nek5000. The geometry is related to the assembly design of MYRRHA. A 19-pin wire-wrapped conjugate heat transfer benchmark is also open to international participants.

6.2 High Performance Computing and Thermal Hydraulics

Using commercially available hardware, ASCI boosted the development of teraflop HPC components which has now increased by 10^5 to hundreds of petaflops. Later Japan, then China competed for leadership[23], but also EU with Switzerland (currently 3rd), UK (11th), Spain (13th), Italy (14th) and industry such as Total (19th). EDF Energy, in the top 50 for a decade has fallen behind. The UK has 10 machines in the Teraflop range (5 in the Met Office and ECMWF, EPSRC and STFC, Edinburgh, Cambridge and AWE). In 2016, DOE's HPC (TITAN, MIRA) peaked at 10-27 petaflops, upgrading to 150-180 petaflops by 2019 (National Academies of Sciences, Engineering and Medicine, 2016).

Bell (2015) shows a 1,000 Million times increase in computing speed over last 30 years, and so Moore's law of power doubling every 18 to 24 months (x 1,000 per decade) is in-fact exceeded. The development of desktop computing power that could be bought for $1,000 is equally astonishing. Radical changes of algorithms from Navier-Stokes equations solvers to Monte Carlo simulations where processes are identical and better suited for cheaply available GPUs bring another dramatic price drop and could make first principles thermal hydraulics simulations available to all.

6.3 Direct Numerical Simulation

Discrepancies with fine experiments could entirely be removed by spatially averaging the DNS to match the viscous-scaled length of the hot-wire sensor, thereby explaining observed differences solely by insufficient spatial resolution of the sensor. For simple RMS fluctuation measurements, DNS is now more accurate than experiments (Örlü and Schlatter, 2013).

The number of cells needed for DNS scales with Re to the power of 9/4. Laminar to turbulent flow transition occurs at mean flow Reynolds numbers of roughly $Re_M = 3000$. DNS Re numbers are reported using turbulent scales (Re_t), but if we re-scale them in terms of mean flow parameters we see that around 2001, DNS with several million cells only focused on laminar-turbulent transition and viscous-log layer interaction for small lab-scale experiments. With million cell simulations possible since around 2010, DNS is relevant to industrial scale flows. A Reynolds number around a million becomes possible with 10^{12} grid points.

The Gordon Bell 2013 HPC prize was awarded for a thermal hydraulics simulation cloud cavitation collapse of 15,000 bubbles on a mesh of 13.2 Trillion cells, at a throughput speed of 721 billion points per second on Lawrence Livermore National Laboratory's (LLNL) "Sequoia" IBM BlueGene/Q (1.6 Million core in 96 racks).

DNS now includes heat transfer and curved geometries. With ANL's Nek5000 DNS code, oblique flow over a wire mounted flat wall served as a benchmark case to study fundamental flow physics as in wrapped fuel pins in SFR designs (Ranjan et al., 2011).

The actual geometry of a 19-Pin SFR rod bundle was simulated only 5 years later with 250 billion colocation points (Merzari et al., 2017).

In the cornerstone test-case of a hot jet impinging on a cold plate, the maximum mean heat transfer (Nusselt number) occurs under the nozzle slightly off axis, but with a smaller secondary

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[23] https://www.top500.org

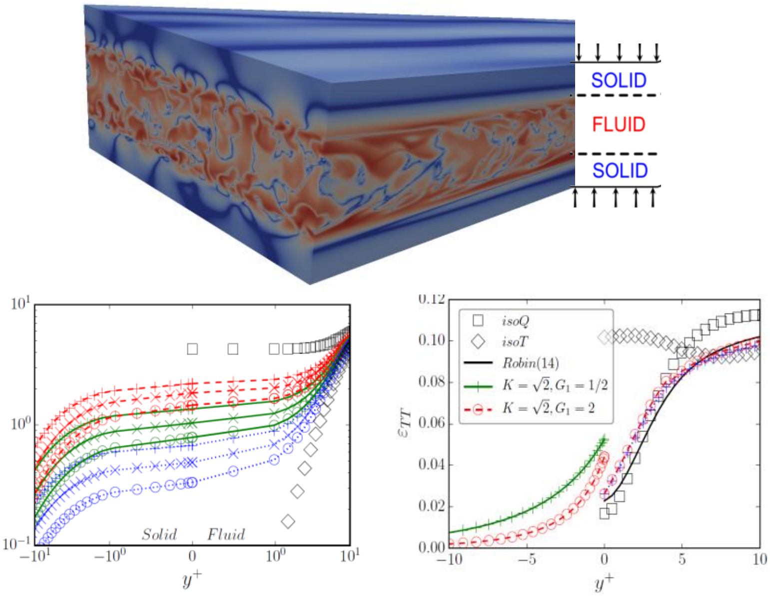
peak four pipe radius away, which has been difficult to capture with RANS models. The DNS of Dairay et al., (2015) shows that the highest-heat-transfer regions are located in this region as a result of formation of larger secondary vortices whose induced velocity generates a convective flux of cold fluid towards the impingement plate.

This shows that engineering models derived from simple pipe flow aligning and extrapolating RMS values from mean values of Nu are certainly erroneous for fatigue studies and could lead to placing conservative margins in the wrong places.

In conjugate heat transfer, mentioned in Section 2.2, unsteady heat transfer coefficients are generally evaluated based on a 1D method normal to the solid. This doesn't account for wall parallel attenuation, as could be seen in Figure 3 where small scale hot and cold spots annihilate each other by conduction in the wall parallel directions. The TEE flow introduces added complexity of separation and reattachment and there are a vast number of configurations in terms of pipe diameters and relative flow-rates to explore. RANS models extended to fluctuations inside the solid such as proposed by Craft et al. (2010) are a more practical engineering approach permitting parametric studies, even with some uncertainty margins, as long as they are well identified.

Figure 27 illustrates a simple heated channel flow DNS yielding the 4D thermal field (x, y, z, t) that allows better understanding jumps in statistics due to conductivity and volumetric heat capacity discontinuities between the fluid and solid (Flageul et al., 2015).

However, for this simplest conjugate heat transfer benchmark, thousands of DNS simulations will be needed to fully calibrate the models for the four characteristic parameters; conductivity, diffusivity, Re number and plate/channel thickness values. Machine learning could provide this on much shorter timescales than the previous decades of sporadic human benchmarking of temperature variance models on very scarce and integral data.



(Courtesy of Cedric Flageul, HAL-01162346)

Figure 27: Conjugate heat transfer channel flow DNS: T fluctuation snapshot, variance and its dissipation. Open symbols correspond to the limiting adiabatic and isothermal cases for minor differences in conductivity and capacity. Data reduction: POD, Dynamic mode decomposition

Reporting thermal hydraulic studies (experimental and computational) has long been limited to mean and RMS values and at best spectrum of time series at few (x, y, z) locations and arbitrary snapshots. This is clearly insufficient for analysis and validation.

It is certainly wasteful when the 4D fields e.g. $T(x, y, z, t)$, are available from DNS, but only for a millisecond in between timesteps. Storage space is the bottleneck of HPC. The Johns Hopkins Turbulence Database (see Section 7.3.5) with terabytes of DNS data available to all online is an exception. It is sponsored by US NSF who's wider objective is supporting Big Data research efforts.

Modern experimental techniques can also provide such thermal hydraulic fields 4D (x, y, z, t) in more limited windows, but CFD-experimental comparisons in publications too often include a couple of arbitrary snapshots side by side for illustration only. Fortunately, data-driven algorithms can now be used to determine characteristics of the vortices buried in turbulent flows.

Proper Orthogonal Decomposition (POD) takes an expansion basis of the eigenvectors of the auto-covariance matrix (computed on the fly from the snapshots) and ranks the modes according to their energy content.

Contrary to POD, Koopman modes are not based on the energy content of the flow, but rather on its spectral content. They are infinite-dimensional but can be reduced and approximated, for example, using the Dynamic Mode Decomposition (DMD) algorithm proposed by Schmid (2010) and Schmid et al. (2012). Individual POD modal coefficients can carry several dominant frequencies while the DMD coefficients only carry one frequency by nature and are preferable in some cases where POD would eliminate dynamically relevant modes because of their relatively low energy content while DMD accurately capture the dominant frequencies and spatial structures (Mezić, 2013; Rowley et al., 2009; Q. Zhang et al., 2014).

Many aspects of NPP flows (tube bundles, bends, TEE junctions, jet in crossflow, natural convection and others) exhibit multi-dominant structures with spatial-temporal features of each coherent structure that are challenging to identify, but play a significant role in the study of various physical processes e.g. heat and mass transfer vibrations. Proper orthogonal decomposition and dynamic mode decomposition, for example, should now be part of any CFD-experimental comparison project.

6.4 Artificial Intelligence and Machine Learning

On 19 Oct 2017, Google's DeepMind new neural network program beat the original AlphaGo program by 100 games to zero after only 72 hours of learning by playing games against itself and being given only the very simple set of game rules[24]. The original program had already defeated the world's number one Go player but after months of learning from, and improving upon, human strategies. The new AlphaGo needed only three days and a fraction (8%) of the previous computing power. "It shows that it is the novel algorithms that count, neither the computing power, nor the data. We've actually removed the constraints of human knowledge and it's able, therefore, to create knowledge itself from first principles, from a blank slate" said David Silver from London based Deep Mind[25].

"This approach, without the benefit of any training data, resulted in a significantly smarter Go player than Artificial Intelligence (AI) programs that were able to analyse reams of human matches. As the DeepMind article points out, if similar techniques could be used to attack other

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[24] http://www.bbc.com/news/technology-41668701

[25] http://www.deepmind.com/

structured problems, like protein folding or materials design, it could result in breakthroughs across many domains. And removing the impediment of relying on large datasets, means that this technology has the potential to be much more broadly applied" (Feldman, 2017).

Undoubtedly this applies to thermal hydraulics model development and validation from first principles DNS and AI, then will be integrated into design optimisation by virtual power plant simulators (DOE NEAMS, Section 8.2). This will be Machine Learning by itself from first Principles without human intervention nor even using Big Data, e.g. running and using DNS data "on the fly" rather than recourse to huge DNS databases, which are near impossible to store and rapidly obsolescent as HPC power increases relentlessly enabling bigger, finer DNS.

Current physical experiments will serve as milestones with PIRT checkpoints for complex designs. Future experimental programs need careful planning to provide added value between DNS and NPP scale models.

6.4.1 Machine learning for turbulence modelling

At Sandia National Laboratory Ling and Templeton (2015) demonstrated the ability of data-driven algorithms to provide substantial improvements over the current state-of-the-art in RANS error detection. The 3 algorithms, learning algorithms to identify regions of high RANS uncertainty were trained on a database of DNS or LES results, and then used to classify RANS results uncertainty and the breakdown of specific RANS modelling assumptions in 7 test cases.

Following that, Ling et al. (2016) included fundamental invariance principles (tensor basis neural network) towards automatic improved RANS predictive accuracy. This approach seems to make obsolete decades of turbulence modeller's efforts, but it could lead to more general acceptance of "improved" RANS models in industrial applications and commercial CFD codes.

This area is rapidly attracting interest in the academic turbulence model community e.g. at Stanford's Centre for Turbulence Research:

- A return to eddy viscosity model for epistemic uncertainty quantification in RANS closure (Edeling et al., 2017).
- Data-driven dimensional analysis: algorithms for unique and relevant dimensionless groups (Constantine et al., 2017).
- Physics-informed machine learning approach for reconstructing Reynolds stress modelling discrepancies based on DNS data (Wang et al., 2017).
- A Comprehensive Physics-Informed Machine Learning Framework for Predictive Turbulence Modelling (Wang et al., 2017).

The method is also invaluable for uncertainty quantification, now an imperative in NPP Design and certification by CFD.

7 Databases and Benchmarking

CFD as a technology has seen significant growth and uptake within a wide range of industrial contexts over the past few decades. Commercial CFD vendors now provide general, state-of-the-art, robust packages which are user-friendly and well supported. This reduction in the barrier to entry rightly raises questions about quality and trust in the outputs that users produce.

CFD packages are as internally complex as the problems they are applied to; the adage “garbage-in garbage-out” remains ever relevant. In response, a number of groups and organisations have produced “best practice” guidelines, which combine decades of practice and experience. A central theme within these is the Verification and Validation (V&V) processes, steps which aim to build trust and increase quality by assessing the predictions of the virtual world (i.e. CFD computations) against real-world (i.e. experimental) results. Quantifying and understanding the differences between the two is the primary outcome of the validation process.

Thermal-hydraulic systems within a NPP, as with most engineering systems, involve many different interacting physical phenomena within complex geometries. Attempting to validate CFD models against such a system as a whole is impractical and counter-productive, since deficiencies cannot be easily attributed to any one particular model and, at worst, may even cancel out. A tiered strategy is generally applied, in which a system is broken down into progressively simpler subsystems which can be validated (Oberkampf et al., 2004; Oberkampf and Trucano, 2002):

- Complete system;
- Subsystem cases;
- Benchmark cases; and
- Unit problems.

This tiered, hierarchical approach builds confidence and allows modelling problems to be more easily isolated and addressed.

The following sections identify major sources of CFD-grade (and, to a lesser extent, near-CFD grade) experimental and numerical data which might be suitable for validation purposes. The majority of existing databases are focused towards aerospace and aerodynamics applications, with a number of sources offering cases which could be considered as more academic. Whilst these cases do not directly address specific nuclear thermal hydraulics problems, they nevertheless represent cases a CFD code should be able to solve and are useful for core model development.

The majority of these databases have already been highlighted as outcomes of other projects. In January 2015, the OECD/NEA published a report assessing the use of CFD codes for Nuclear Reactor Safety problems (Smith et al., 2015) which identified four major CFD benchmark cases in addition to more general sources.

7.1 OECD/NEA

The role of the OECD/NEA is to assist member countries in maintaining and further developing the scientific, technological and legal bases required for a safe, environmentally friendly and economical use of nuclear energy. Within this, the NEA Committee on the Safety of Nuclear Installations (CSNI) holds broad responsibility for safety technology and research programmes and was set up to develop and co-ordinate NEA activities concerning technical aspects of the design, construction and operation of nuclear installations.

Since its inception in 1958 (and the CSNI in 1973), the NEA has conducted and coordinated a large number of nuclear safety related projects. The data and reports produced through these projects form a substantial body of knowledge and experience. The various databases and project lists are discussed below.

7.1.1 OECD/NEA Sponsored CFD Benchmark Exercises

In 2008, the OECD/NEA used the Special CFD Group of the Working Group on the Analysis and Management of Accidents (WGAMA) to undertake a series of international benchmark exercises. Both single-phase and two-phase flow options were considered. It was generally agreed that this would be a blind benchmarking activity, in which participants would not have access to measured data, apart from what was necessary to define initial and boundary conditions for the numerical simulation, until they had submitted their numerical predictions for evaluation.

This entails finding a completed, or nearly completed, experiment for which the data had not yet been released, or encouraging a new experiment (most likely in an existing facility) to be undertaken especially for this exercise. The group took on the responsibility of finding a suitable experiment, for providing the organisational basis for launching the benchmark exercise, and for the subsequent synthesis of the results.

The following CFD benchmark exercises have been completed or are underway:

1. OECD/NEA Vattenfall T-Junction benchmark exercise (high-cycle thermal fatigue)[26]. This was based on previously unreleased test data from a very careful experiment carried out at the Älvkarleby Laboratory of Vattenfall Research and Development in Sweden in November 2008.
2. OECD/NEA KAERI Rod Bundle CFD benchmark exercise (turbulent mixing downstream of a spacer grid)[27]. Special tests were carried out in the MATiS-H cold-flow facility at the Korea Atomic Energy Research Institute (KAERI) in early Spring 2012. Two spacer grids (of generic design), of the split type and swirl-type, were featured in the study. Computer Aided Design (CAD) files of the spacer grids were made available by KAERI to aid CFD mesh generation.
3. OECD/NEA PSI CFD benchmark exercise (jet erosion of a stratified atmosphere)[28]. A new test was carried out during February-March 2013 within one, comprehensively-instrumented vessel of the PANDA integral containment facility, located at PSI in Switzerland. This benchmark was specifically aimed at examining the erosion of a hydrogen-rich, stratified layer, occupying the upper reaches of a containment volume. This was accomplished by the impingement of a buoyant, vertical jet, placed off-centre with respect to the axis of the vessel, in order to induce significant three-dimensional motions in the flow.
4. OECD/NEA CFD benchmark with Uncertainty Quantification (turbulent mixing). This exercise started in 2015, and has not yet been formally reported. The experiments in the GEMIX (GEneral MIXing experiment) facility located at PSI in Switzerland focus on the mixing in the wake of two water streams (having identical or different densities and identical velocities) generated downstream of a splitter plate. This facility includes detailed flow measurements using Particle Image Velocimetry (PIV), Laser Induced Fluorescence (LIF) and Wire Mesh Sensors (WMS).

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[26] http://www.oecd-nea.org/nsd/docs/2011/csni-r2011-5.pdf
[27] http://www.oecd-nea.org/nsd/docs/2013/csni-r2013-5.pdf
[28] http://www.oecd-nea.org/nsd/docs/2016/csni-r2016-2.pdf

5. OECD/NEA CFD benchmark with Uncertainty Quantification (cold leg mixing). The 5th benchmark of CFD applications to Nuclear reactor safety has been approved by CSNI and is currently underway. Its main objective is to go a step further in the application of single-phase CFD to nuclear safety issues with mixing problems possibly in presence of buoyancy effects. The Pressurized Thermal Shock (PTS) facility located at Texas A&M University in the US can simulate some mixing phenomena of cold water and hot water in geometry representative of a horizontal cold leg of a PWR, as encountered in some accidental situations with ECCS injection. The facility is equipped with state-of-the-art instrumentation and measurement techniques to provide high resolution measurements of velocity, concentrations, and pressure drops at different locations within the leg, nozzle, and downcomer.

7.1.2 CSNI Code Validation Matrix

System codes have been the primary tool for analysing LWRs over the past 30 years. In order to validate the codes and the sub-models used within them, data is collected both from commercial plant operators and through conducting specifically designed experimental tests. A significant amount of test data has been accumulated over the years and the CSNI Code Validation Matrix is an attempt to collate and organise the data to be more conducive to validating system codes.

The result is a collection of internationally agreed matrices which guide code validation and present a basis for comparisons of predictions amongst the various system codes. The matrices identify the main physical phenomena that occur during LOCA and reactor transients and cross-reference these against the test facilities identified as suitable for reproducing those phenomena. The tests are categorised as being either integral tests, which capture the behaviour of the reactor system as a whole, or separate tests, which focus on the behaviour of a single component or thermal-hydraulic phenomenon. The phenomena, identification criteria and matrices are documented in a number of OECD/NEA reports (Glaeser et al., 1996; OECD/NEA, 1994).

The OECD/NEA has recently developed The International Experimental Thermal Hydraulics Systems Database (TIETHYS)[29]. TIETHYS is an online searchable database that collates all of the separate effects (Section 7.1.2.1) and integral effects (Section 7.1.2.2) test matrices.

7.1.2.1 Separate Effects Test Matrix

https://www.oecd-nea.org/dbprog/ccvm/indexset.html

The Separate Effects Test (SET) validation matrix is representative of the major part of the experimental work which has been carried out in LWR-safety thermal hydraulics fields, covering a large number of phenomena over a large range of useful parameters. A total of 2,094 tests are included in the SET matrix and phenomena tested include critical flow, phase separation/vertical flow, horizontal stratification, entrainment, liquid-vapour mixing with condensation, spray effects and heat transfer.

The website separates the tests according to the facility they were conducted in and provides an abstract for each experiment or test. The level of detail in each abstract varies, but most include at least a description of the test facility, a description of the test, the phenomena tested, the current status of the test and some references. Data available also varies; some experiments only offer a report whilst others provide some amount of test data. The data needs to be formally requested and this is subject to a non-disclosure agreement and to certain restrictions.

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[29] https://www.oecd-nea.org/tiethysweb

7.1.2.2 Integral Effects Test Matrix

https://www.oecd-nea.org/dbprog/ccvm/index.html

The Integral Effects Test (IET) matrix data is suitable for the validation of best estimate thermal-hydraulic computer codes. It consists of phenomenologically well founded experiments, for which comparison of the measured and calculated parameters form a basis for establishing the accuracy of the test predictions. Test types include core re-flooding, steam generator tube rupture, loss of feed water and transients at shutdown. The available data is organised as described above for the Separate Test Effects Matrix.

The volume of tests and accompanying data makes a complete assessment of the quality of the data impractical but the intended purpose of the test matrices (the validation of 1D system codes) implies that the fidelity of the data is not likely to be high enough to serve as validation data for 3D CFD codes. Nonetheless, they represent tests which a CFD code should be able to accurately reproduce.

7.1.3 NEA Computer Program Services

http://www.oecd-nea.org/tools/abstract/list/category

The NEA Computer Program Services provides a centralised repository of software libraries and programs relating to nuclear energy applications. The service collects, compiles and verifies the programs are suitable, complete and adequately documented.

The program categories include neutronics, hydrodynamics, shield design, experimental data processing, but most relevant is those on heat transfer and fluid flow. Many of the tools are very old.

7.1.4 Safety Joint Research Project Database

https://www.oecd-nea.org/dbprog/safety-joint-research-databases.html

The NEAs Safety Joint Research Project database maintains a list of projects which have been undertaken by participants within the OECD/NEA group in collaboration with other external agencies, companies and countries.

An overview, list of participants, the dates and budget are provided for each project. Data abstracts are also provided in a similar form to those listed for the CSNI Code Validation Matrix. Some of these abstracts provide varying levels of project data to download, though a formal request for access is required.

7.1.5 Storage of Thermal REactor Safety Analysis (STRESA)

https://stresa.jrc.ec.europa.eu

STRESA was initially an information system developed in 2000 by the EU Commission’s Joint Research Centre (JRC) to disseminate documents and experimental data from large in-house JRC scientific projects on severe accidents. It now forms the main secure experimental data repository for the JRC. STRESA was considerably upgraded and improved by the Nuclear Reactor Safety Assessment Unit (NRSA) of the JRC in 2009 in order to take advantage of more modern software solutions.

This tool provides secure storage for severe accident experimental data and calculations conducted through the European Union. The public facing section of the website provides details on all of the experimental facilities, including the organisation, the type of facility and the number of experiments conducted at the facility which have been entered into the database. Of the 58 experimental facilities listed in the database, 12 are categorised as being relevant to nuclear thermal-hydraulics.

The restricted section of the website contains further features and tools for accessing and manipulating the experimental data available. Whilst it appears a straightforward registration form is all that is required to access the restricted section, the experimental groups and funding agencies are able to restrict access to organisations and users of their choosing. The experimental data appears to be geared towards validation and verification of system-codes. Nevertheless, it provides a valuable, easily accessible, central repository in which to request further details or experimental data.

7.2 ERCOFTAC

In the 1990’s, the UK’s CEGB, EDF R&D, EU aerospace industry and turbulence modelling academic groups launched the European Research Community on Flow, Turbulence And Combustion (ERCOFTAC[30]), reporting progress in the predominantly applied, industrially-oriented areas of turbulence research. ERCOFTAC was the first to publish Best Practice Guidelines[31] for CFD and turbulence and later a more specialised one on two-phase flows.

It also has a Bulletin[32] (100th Edition), ERCOFTAC Book Series[33] and Journal of Flow, Turbulence and Combustion. Activity is organised via 30 Special Interest Groups[34] (SIG) which, alongside the historic Turbulence Modelling SIG now includes Large Eddy Simulation, Variable Density Turbulent Flows, Design Optimisation, Uncertainty Quantification in Industrial Analysis and Design. A major overarching objective is the coordination and maintenance of databases suitable for code verification and validation and a number of resources are currently active.

7.2.1 Classic Collection

http://cfd.mace.manchester.ac.uk/ercoftac

The ERCOFTAC “Classic Collection” was established in 1995 and is now administered by the Turbulence Modelling research group at The University of Manchester. It currently contains 93 test-cases is recognised as an excellent source of experimental, LES and DNS data for verification and validation of turbulent flow. Each case contains at least a brief description, downloadable data and references to published work with some containing significantly more.

The database is open to the public, but (free) registration is required to download the data. A number of cases are relevant to nuclear thermal-hydraulics, including mixing layers, turbulent flow over curved surfaces, flow past tube bundles and turbulent Rayleigh-Bénard convection.

7.2.2 SIG-15 Test Case Database

https://www.ercoftac.org/special_interest_groups/15_turbulence_modelling

The Special Interest Group on Refined Turbulence Modelling organised its 15th benchmarking workshop in Chatou, France in October 2011 and presented a series of benchmark calculations for heat transfer in a suddenly expanding pipe and thermal mixing in a T-junction.

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[30] http://www.ercoftac.org
[31] http://www.ercoftac.org/publications/ercoftac_best_practice_guidelines/
[32] http://www.ercoftac.org/publications/ercoftac_bulletin/
[33] http://www.ercoftac.org/publications/ercoftac_book_series/
[34] http://www.ercoftac.org/special_interest_groups/

7.2.3 Knowledge Base Wiki

http://www.ercoftac.org/products_and_services/wiki

The Knowledge Base Wiki, formerly known as the QNET-CFD Knowledge Base, originated from a four year EU Network on Quality and Trust in the industrial application of CFD. This was a four year project which brought together the expertise of 43 participating organisations across Europe and aimed to improve the level of trust that could be placed in industrial level CFD computations.

Members were principally from industry, but universities, national research organisations and major European CFD code vendors were also strongly represented. Following the end of the EU Network in 2004, responsibility for the Knowledge Base was passed to ERCOFTAC.

The network is organised into six applications areas. Spanning those areas were *application challenges*, which consisted of realistic test cases suitable for CFD assessment, and *Underlying Flow Regimes*, which contained well studied academic test cases suitable for assessing the key physical elements which make up the application challenges. The six current application areas include:

- External Aerodynamics;
- Combustion;
- Chemical, Process, Thermal and Nuclear Safety;
- Civil Construction and HVAC;
- Environmental Flow; and
- Turbomachinery Internal Flow.

Within the Chemical, Process, Thermal and Nuclear Safety application area there are 7 test cases:

- Buoyancy-opposed wall jet (contributed by Magnox Electric);
- Induced flow in a T-junction (EDF R&D), cyclone separator (Fluent Europe);
- Spray evolution in turbulent flow (Martin-Luther-Universitat Halle-Wittenberg);
- Combining/dividing flow in Y junction (Rolls-Royce);
- Downward flow in a heated annulus (British Energy); and
- Particle-laden swirling flow (Martin-Luther-Universitat Halle-Wittenberg).

Each case contains a detailed description, sets of test data, details of CFD simulations, an evaluation of the results and some best practice advice. Some, but not all, data is available to download.

7.3 Research Group Databases

A number of fluid dynamics research groups host some of the data they produce during their research either through their institutions or on personal sites. Thus, they are not necessarily formal products or offerings from the institution; rather, they are managed by the research group members themselves.

7.3.1 DATHET - Thermal Engineering Division, JSME

https://www.jsme.or.jp/ted/HTDB/dathet.html

DATHET (Database on Turbulent Heat Transfer) is a heat transfer focused database hosted by the Thermal Engineering Division of the Japanese Society of Mechanical Engineers. Details on the governance and history of the database are not presented but the site contains a mix of experimental and DNS cases on forced convection, natural convection and combined convection (typically mixing layers, backwards facing step and swirling flows).

Each case has a downloadable CSV file which contains details on the experimental/numerical method, the flow parameters, uncertainty and the flow data itself.

7.3.2 DNS Database of Wall Turbulence and Heat Transfer - Kawamura Lab

http://murasun.me.noda.tus.ac.jp/turbulence[35]

Hosted by the Kawamura Lab in collaboration with the Japan Aerospace Exploration Agency (JAXA), the DNS Database of Wall Turbulence and Heat Transfer contains turbulent channel flows, boundary layer flows and channel flows with two-dimensional slits. Both isothermal and thermal flows are considered.

Each DNS simulation consists of a downloadable text file with details on flow parameters, mesh refinement, references and the flow data itself. Access is freely open to the public.

7.3.3 Fluid Dynamics Group – Technical University of Madrid

https://torroja.dmt.upm.es/turbdata

The Fluid Dynamics Group at the Technical University of Madrid has published a number of detailed DNS studies on a range of fundamental fluid flow (Cardesa et al., 2017; Hoyas and Jiménez, 2008, 2006). Processed data produced for those, and many other, studies is made available at the group's website. The database contains cases on isotropic turbulence, high Reynolds number channel flows (up to $Re_\tau = 4200$), boundary layer flows and homogeneous shear layers. The database is freely accessible to the public, and each case contains a detailed description, a selection of processed data, explanations of the data files and references to publications. Additionally, the raw data produced from a selection of those cases is also available to download (a collection totalling nearly 100TB).

Hosted on the same website is a database containing the results of Working Group 21 of the Fluid Dynamics Panel of AGARD (Advisory Group for Aerospace Research and Development). AGARD was an agency of NATO that existing from 1952 to 1996 with the intention of bringing together expertise in aerospace science and technology from across NATO nations. The primary outcome of the Working Group was a report and database intended specifically for the validation of LES computations.

The database contains a mixture of DNS and experimental data and is organised into six sections: homogenous turbulence, shock wave interaction with grid turbulence, pipes and channels, free shear flows, turbulent boundary layers and a section for more complex flows. A detailed report accompanies the data, which provides a short article like description of each section and some sample plots. A total of 66 cases are presented. Flows of interest include mixing layers, flows in square ducts and flows with surface curvature.

7.3.4 Institute for Computational Engineering and Sciences - The University of Texas

http://turbulence.ices.utexas.edu

Data produced by the research groups at the University of Texas' Institute for Computational Engineering and Sciences will be well known to a large majority of turbulence modelling practitioners; the channel flow data published by Kim et al. (1987) has accrued well over 4,000

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[35] At the time of writing this website was unavailable at this address, but a mirror can be found at http://www.rs.tus.ac.jp/~t2lab/db/index.html

citations. The group continues to publish hi-fidelity DNS simulations for a range of wall-bounded and boundary layer flows and the data produced is made available online.

Processed data (profiles, statistics, balances etc.) exists for channel flows over a large range of Reynolds numbers $(180 < Re_\tau < 5200)$ and is freely downloadable through links on the site. Arrangements for full datasets can also be made providing the recipient can supply a hard drive suitable for transfer and make delivery arrangements. The site also hosts a mirror of some of the data produced by Fluid Dynamics Group at the Technical University of Madrid (Section 7.3.3). Whilst the data is of a more fundamental nature, it provides an essential starting point for the development of turbulence models.

7.3.5 John Hopkins Turbulence Database

http://turbulence.pha.jhu.edu

The John Hopkins Turbulence DataBase (JHTDB) is a publically accessible DNS data archiving database system, hosted by the John Hopkins University, USA, under the sponsorship of the US' National Science Foundation. In contrast to the majority of the databases considered here, access to the data is facilitated by a Web services interface that permits numerical experiments and database queries to be run across the internet. Clients utilise a freely available web services library to allow their own programs (written in C, Fortran or Matlab) to directly query the dataset without having to download it. The technical details of the open access implementation can be found in a number of published papers (Graham et al., 2016; Li et al., 2008).

The datasets available include forced isotropic turbulence, forced magnetohydrodynamic turbulence, channel flow, homogenous buoyancy driven turbulence and forced isotropic turbulence. The database is accompanied by detailed documentation and sample code to help researchers incorporate the dataset into their own analysis programs.

7.4 NASA

The American National Aeronautics and Space Administration remains a major developer, user and contributor of CFD technology. Its efforts are spread amongst a number of technical groups and divisions, but there are some available CFD resources of value.

7.4.1 NPARC Alliance

https://www.grc.nasa.gov/www/wind/valid/archive.html

The National Project for Applications-Oriented Research in CFD (NPARC) was formed in 1993 by the US Air Force Arnold Engineering Development Center (AEDC) and the NASA Glenn Research Center (GRC) in response to requests from industry and academic for the formal support and development of a common CFD code.

As part of the verification and validation of that code, called WIND, the NPARC collated a data archive of a number of primarily aerospace related test cases. Each case contains a detailed description, data files available to download, references and general "best practice" guidelines.

7.4.2 Advanced Supercomputing Division

https://www.nas.nasa.gov/publications/datasets.html

The Advanced Supercomputing Division is primarily concerned with the development and advancement of high-end supercomputing technologies and modelling and simulation methods. There is, however, a small database of freely available CFD datasets which include viscous flow around a tapered cylinder, a blunt fin and a space shuttle launch vehicle.

7.4.3 Langley Research Center

https://turbmodels.larc.nasa.gov/index.html

As part of an effort by The Turbulence Model Benchmarking Working Group (a working group of the Fluid Dynamics Technical committee of the AIAA), a number of verification cases are hosted as a Turbulence Modelling Resource at NASA's Langley Research Center.

The cases are again predominantly aerospace related, but with a focus on the development of Reynolds-averaged Navier-Stokes turbulence models. Some cases which may hold relevance to nuclear thermal-hydraulics include mixing layers, jets and internal flows.

7.5 Commercial CFD code Validation Cases

General purpose commercial CFD code vendors, such as ANSYS (Fluent, CFX), Siemens PLM (STAR-CCM+), EDF R&D (Code_Saturne) and Cham (PHOENICS) amongst others, are keen to demonstrate the accuracy and effectiveness of their products and thus a number of benchmark results have been conducted during the development and testing of their codes. All of these code vendors have customers within the nuclear industry.

The sensitive and commercial nature of their operations means, however, that publically available information can be limited. The primary resource for specifics on validation cases is the websites of the respective vendors and details are usually restricted to licensed users of the software.

7.5.1 ANSYS-Fluent and ANSYS-CFX

http://www.ansys.com

The Fluent & CFX codes developed and marketed by ANSYS have seen considerable use in both academia and industry. No validation details are publically available but licensed users have access to a "Fluid Dynamics Verification Manual" which contains brief simulation results for 70 different test cases.

The results are not intended to demonstrate validation and, whilst comparisons with experimental results are presented, only a single run on a single mesh with a single modelling approach is typically presented. Example cases of relevance include turbulent natural convection in a tall-cavity, anisotropic conduction heat transfer, boiling in a pipe-critical heat flux and two-phase stratified wall-bounded flow.

7.5.2 STAR-CCM+

https://mdx.plm.automation.siemens.com/star-ccm-plus

Internally, Siemens PLM conducts verification cases using the STAR-TEST suite which contains more than 30,000 individual test cases. These include both unit tests and application verification tests based on standardised validation cases. A subset of the STAR-TEST suite is provided to licensed customers of the software.

Whilst this is primarily intended to confirm the local installation of the software is correct, the set includes a number of cases relevant to nuclear thermal hydraulic. These include bulk boiling, bubbly flow, turbulent natural convection in tall cavities and axisymmetric impinging heated jets.

7.5.3 Code_Saturne

https://www.code-saturne.org

Code_Saturne, developed by EDF R&D, is open source software and thus anyone is free to audit and verify that the code implementation is correct. A V&V program is conducted internally on each version of the code. A validation manual is produced, but this is only available for the core development team and internal users.

The manual covers both separate and integral effects, with the separate effects manual including a range of approximately 40 test cases. The data used for each case is either sourced from published literature or from experiments/DNS conducted by EDF or their partners.

7.5.4 PHOENICS

http://www.cham.co.uk/phoenics.php

PHOENICS provide a publically available online Encyclopaedia[36] which provides a set of validation examples. The cases are relatively academic in nature, but do include some cases of relevance, such as two-phase flows in bubble-columns, buoyancy driven cavity flow and heat transfer in damaged AGR fuel stringers.

7.5.5 Nek5000

https://nek5000.mcs.anl.gov

Nek5000 is open source and freely available from the source code hosting website GitHub. The GitHub site contains a repository with a number of simple example cases, including Rayleigh-Bénard convection and free-surface channel flow.

A significantly more relevant V&V exercise, presented at NURETH15, concerns high-fidelity LES reference simulations conducted with Nek5000 on the OECD/NEA T-Junction and MATiS-H benchmark experiments and for the Novosibirsk “SIBERIA” and ANL MAX con-current validation experiments (Obabko et al., 2015).

7.6 FLOWNET

FLOWNET (Flow Library On the Web NETwork) was an EU initiative aimed at providing the scientific and industrial communities with a code validation tool for use with flow modelling and computational/experimental methods. This was to be achieved by the establishment of a database network, which would enable scientists, academics and industrial experts to share technical complements (test cases, experimental models and codes).

The project was active between 1998 and 2001 and primarily aimed at aerospace applications. Unfortunately, aside from the EU funding record, very little evidence of the project remains.

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[36] http://www.cham.co.uk/phoenics/d_polis/d_applic/appval.htm#250

8 Major Projects Worldwide

In this section we briefly review some major thermal-hydraulics-related projects in Europe, US as well as some relevant Coordinated Research Projects (CRPs) of the IAEA, to provide an appreciation of the main activities in thermal hydraulics worldwide.

8.1 Europe

The EU 7th Framework Programme funded a major project - Thermal-Hydraulics of Innovative Nuclear Systems (**THINS**), which was active between 2010 and 2015 Cheng et al. (2015). The project focused on a number topics, including:

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

The project aimed at establishing an experimental database and the development of new and more accurate physical models and numerical simulation tools. Some twelve experimental facilities were included in the project. New correlations or models were developed such as for heat transfer coefficient, friction factor, turbulent Prandtl number and an algebraic heat flux model. They were (partially) validated, based on the established test data and also implemented in numerical codes.

Currently in Europe, there are a number of consortia in Generation IV reactors supported through the Horizon 2020 program, including SESAME, MYRTE, 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.

The **SESAME** (Simulations and Experiments for the Safety Assessment of MEtal cooled reactors) is solely concerned with thermal hydraulics, focusing on pre-normative, fundamental, safety-related, generic challenges. This is complemented by the **MYRTE** (MYRRHA Research and Transmutation Endeavour) project, which focuses on the further development of the MYRRHA reactor in Belgium, with a large part devoted to thermal hydraulics (F. Roelofs et al., 2015; Roelofs et al., 2017). The two projects work closely together and identified the following key areas of development: Liquid metal heat transfer, fuel assemblies, plenum and system thermal-hydraulics. The projects aim to validate analytical and simulation methods with reference data. If possible and affordable, such reference data will be based on experimental results. However, the projects recognise that there are significant limitations/difficulties in physical experiments with liquid metals due to the accessibility to the flow area and level of details that experiments can provide. High fidelity simulation data (typically DNS or LES) are used to generate data to complement or replace experimental data for model validation.

The **SAMOFAR** (Safety Assessment of the Molten Salt Fast Reactor[37]) project aims to achieve a number of objectives, including to:

- Deliver the experimental proof of concept of the safety features of the MSFR;
- Provide a complete safety assessment of the MSFR and associated chemical plant; and
- Update the conceptual design of the MSFR with all input gathered during the project.

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[37] http://samofar.eu/

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 multi-physics codes including uncertainty propagation for transient calculations.

8.2 US

Currently, there are three major national R&D projects in nuclear modelling and simulation in the US; **CASL** and **NEAMS** funded by the US DoE Office of Nuclear Energy and **CESAR** funded by the US DoE Office of Science. Figure 28 illustrates the relationship between the three programs and how they contribute to the US nuclear energy program.

The Consortium for Advanced Simulation of Light Water Reactors (**CASL**)[38] - A DoE Energy Innovation Hub aims at delivering solutions to industry-defined challenges in the current LWR technology. It is a consortium between industry, national labs and universities with a vision to provide leading edge modelling and simulation capabilities to deploy within US nuclear energy industry to improve LWR operation performance. One of its key outputs is to develop and validate the so-called 'virtual reactor' package (**VERA**) to proactively address critical performance goals for nuclear power. The thermal hydraulic analysis is based on a coupled approach between the system/sub-channel codes and CFD. Developments in the VERA tools are increasingly based on Idaho National Laboratory's **MOOSE**[39] which is a modern, open-source, actively developed, parallel finite element framework for coupling a wide range of physical phenomena.

The Nuclear Energy Advanced Modelling and Simulation Program[40] (**NEAMS**) develops and validates predictive analytic computer methods for the analysis and design of advanced reactor and fuel cycle systems including Generation 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 Reactors[41] (**CESAR**) focuses on the two key physics components of reactor core modelling - CFD and neutron transport - with particular focus on parameter regimes required for robust, coupled reactor core modelling. The program has an ambitious long term mission to enable exascale reactor simulations, which will fundamentally change the paradigm of how nuclear reactors are built, tested and operated. This is 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.
- To develop a new generation of underlying algorithms which successfully exploit exascale computing to solve significant reactor simulation problems.

Both NEAMS and CESAR develop and use a common simulation Nek5000 package for thermal hydraulics. Nek5000 is based on a high order, high efficiency spectral element incompressible solver aimed at producing high fidelity simulations (i.e. DNS and LES) for complex geometries. The code however also provides options for 'intermediate' fidelity URANS and reduced fidelity CFD such as a porous medium approach.

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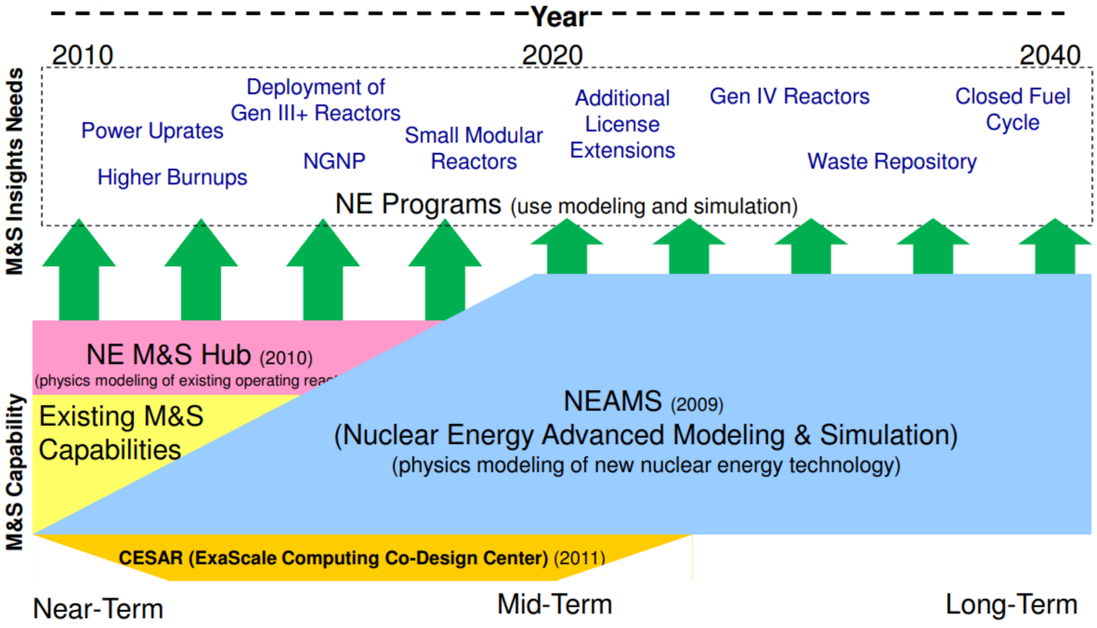
[38] https://www.casl.gov
[39] http://mooseframework.org
[40] https://energy.gov/ne/nuclear-reactor-technologies/advanced-modeling-simulation
[41] https://cesar.mcs.anl.gov/content/about-cesar



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

Figure 28: US nuclear Modelling and Simulation (M&S) programs (Larzelere, 2011)

8.3 IAEA CRPs

IAEA's Coordinated Research Activities (CRAs) aim at simulating and coordinating research activities of its member countries in selected nuclear fields. These are carried out through Coordinated Research Projects (CRPs), which bring together an average of 15 scientific institutes from different member countries to work on problems of common interest[42]. A number of such active CRPs deal with thermal hydraulics for Generation IV reactors: HTGRs (Section 8.3.1 and 8.3.2), SCWRs (Section 8.3.3) and SFRs (Section 8.3.4), SMRs (Section 8.3.5) and application of CFD to NPP design (Section 8.3.6).

8.3.1 HTGR Reactor Physics, Thermal-Hydraulics and Depletion Uncertainty Analysis (1000154) 2012-04-19 to 2019-04-18

The continued development of High Temperature Gas Cooled Reactors (HTGRs) requires verification of HTGR design and safety features with reliable high fidelity physics models and robust, efficient, and accurate codes. The predictive capability of coupled neutronics/thermal-hydraulics simulations for reactor design and safety analysis can be assessed with sensitivity analysis (SA) and uncertainty analysis (UA) methods. Uncertainty originates from errors in physical data, manufacturing uncertainties, and modelling and computational algorithms. SA is helpful to partition the prediction uncertainty to various contributing sources of uncertainty and error.

SA and UA is required to address cost, safety, and licensing needs and should be applied to all aspects of reactor multi-physics simulation. SA and UA can guide experimental, modelling, and algorithm research and development. Current SA and UA rely either on derivative based methods such as stochastic sampling methods or on generalised perturbation theory to obtain sensitivity coefficients. Neither approach addresses all needs.

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[42] http://cra.iaea.org/cra/index.html

In order to benefit from recent advances in modelling and simulation and the availability of new covariance data (nuclear data uncertainties) extensive sensitivity and uncertainty studies are needed for quantification of the impact of different sources of uncertainties on the design and safety parameters of HTGRs. Only a parallel effort in advanced simulation and in nuclear data improvement will be able to provide designers with more general and well validated calculation tools to meet design target accuracies.

8.3.2 Modular High Temperature Gas Cooled Reactor Safety Design (I31026) 2014-12-12 to 2018-12-11

The CRP will investigate and make proposals on modular high temperature gas cooled reactor (HTGR) safety design criteria. It is expected that these criteria would refer to light water reactor safety standards (e.g. Safety of Nuclear Power Plants: Design (IAEA Safety Standards Series No. SSR-2/1, Vienna, 2012)), and the deterministic and risk-informed safety design standards under development for existing and planned HTGRs worldwide that apply to the wide spectrum of design basis and beyond design basis events.

The CRP would also take into account the effect of the Fukushima Daiichi accident, clarifying the safety requirements and safety evaluation criteria for design extension conditions, especially those events that can affect multiple reactor modules or are dependent on the application (such as process heat or hydrogen production) on the plant site. The logical flow of criteria is from the fundamental inherent safety characteristics of modular HTGRs and associated expected performance characteristics, to the safety functions required to ensure those characteristics, and finally to specific criteria related to those functions.

The initial focus will be on the criteria for a specific HTGR concept (e.g. steam cycle) but other concepts (e.g. gas turbine and process heat) will also be looked at. Both prismatic and pebble bed modular HTGR designs will be considered. Several publications and presentations were identified as important input to the CRP and will be used as the point of departure. The results of the CRP will be documented in an IAEA Technical Document (TECDOC) to be made available to the entire HTGR community. The CRP could also provide technical information for future separate activities on the development of IAEA safety standards for HTGRs with the cooperation of the IAEA Department of Nuclear Safety and Security.

8.3.3 Understanding and Prediction of Thermal Hydraulics Phenomena Relevant to Supercritical Water Cooled Reactors (I31025) 2014-06-19 to 2019-06-19

The supercritical water cooled reactor (SCWR) is one of the innovative water cooled reactor (WCR) concepts mainly for large scale production of electricity. By utilising its high coolant temperature, the SCWR is expected to achieve much higher thermal efficiencies than those of current WCRs, and thereby promise improved economics.

The objective of the CRP is to improve the understanding and prediction accuracy of thermal hydraulics phenomena relevant to SCWRs and to benchmark numerical toolsets for their analysis. Several key phenomena, such as heat transfer, pressure drop and flow stability, have been identified as crucial to the successful development of SCWRs. This CRP will enhance understanding of thermal hydraulics phenomena, sharing of experimental and analytical results, prediction methods for key thermal hydraulics parameters, and cross-training of personnel between participating institutes.

8.3.4 Sodium Properties and Safe Operation of Experimental Facilities in Support of the Development and Deployment of Sodium-cooled Fast Reactors (NAPRO) (I31024) 2013-09-05 to 2018-09-05

The CRP addresses the need of standardisation of sodium (Na) physical, physio-chemical and thermo-dynamic properties, main rules for design, construction and operation of Na experimental facilities, as well as good practices and safety guidelines for Na experiments.

8.3.5 Design and Performance Assessment of Passive Engineered Safety Features in Advanced Small Modular Reactors (I32010) 2017-07-19 to 2020-07-18

The majority of Small Modular Reactor (SMR) designs for near-term deployment adopt advanced passive safety system technology to cope with both design basis- and design extension conditions.

The goal of the CRP is to develop a common novel approach for designing passive engineered safety features for SMRs and offer methods or good practices for assessing their performance and reliability. Design safety considerations on appropriate and practical countermeasures to incorporate and address lessons learned from the major accidents to enhance the design of engineered safety systems of SMRs (particularly of the integral-PWR type currently under development) will be developed.

8.3.6 Application of Computational Fluid Dynamics (CFD) Codes for Nuclear Power Plant Design (I31022) 2013-02-22 to 2018-02-21

The CRP addresses the application of CFD computer codes to the process of optimising the design of water cooled NPP. Following a number of initiatives within IAEA where CFD codes are applied to a wide range of situations of interest in nuclear reactor technology, the CRP intends to constitute a systematic framework for the consistent application of those codes.

Namely, the CRP will contribute to establish a common vision in relation to the capabilities of CFD codes and their qualification level. The CRP is also expected to provide a roadmap strengthening the application domain of the related technology. Blind analyses (i.e. code calculations performed without having access to experimental data) performed by participants will allow the achievement of the proposed objectives.

9 Closing Remarks

This report presented an overview of recent research and current practices and provided a background to recommendations for investment in the UK's thermal hydraulics modelling capability. The topic is so broad and the activity so international, that rather than presenting just a lists of projects and references, a few of the challenges have been highlighted using selected examples.

Focusing on most recent and, where possible, UK related references, the process of evaluating the state of the art led the senior academic investigators to recognise that the impact of continued exponential growth of high performance computing power, combined with novel algorithms such as AI and machine learning is much broader than was perceived in their field of specialisation. It was realised that, in certain thermal hydraulics topics, including one of our own fields of expertise, CFD models of turbulence, the "technological singularity" point may be close, driven by abundant computational power.

The opportunities offered by modern methods that exploit large-scale computing enables a change in philosophy when analysing nuclear power plants. Operating and accident conditions can now be re-evaluated and placed in more realistic scenarios with "best estimate plus uncertainty methods", compared to previous methods that used pessimistic conditions to cover the uncertainties left by low-fidelity models.

In 2012, US DoE director Steven Chu stated that "Supercomputing Will Change Our Energy Future"[43]. The reality of this can be seen in recent outputs of the US NEAMS projects where "first principles" simulations can replace experiments and surpass them with finer details.

It is perhaps uncomfortable to acknowledge that the development and tuning of thermal hydraulics models, in the way that has taken place over the last few decades, will be more effectively and rapidly accomplished by Machine Learning algorithms. As these revolutionary developments occur, however, there will need to be a corresponding response in the rate of acceptance of these novel models and methods. This will still require subject matter experts in academia and industry, with expertise in thermal hydraulics to train the new generation of researchers and engineers to harness these tools, as well in the management of complexity and uncertainty.

A summary of the thoughts of the authors in the form of the UK strengths, weaknesses, opportunities and threats has been used to present the concluding comments.

9.1 Strengths and Weaknesses

- The UK is strong in modelling and at the origin of engineering CFD, major commercial codes and RANS. While modelling activities are not as extensive as in earlier decades, there is still a research base which can be strengthened and expanded.
- Nuclear naval propulsion and high temperature gas cooled reactors (AGR experience, which is relevant to VHTRs) are areas in which the UK has maintained research activities, and as a result retains strong expertise.
- The UK is strong in high performance computing for science and engineering as well as in areas such as AI. This provides a strong base for the development of modelling capabilities in compute-intensive aspects of nuclear thermal hydraulics simulation.

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[43] https://www.forbes.com/sites/joshwolfe/2012/05/08/why-the-doe-thinks-supercomputing-will-change-our-energy-future

- The UK has limited experience in the system and subchannel analysis codes that are used for thermal-hydraulics analysis in the majority of international reactor design and safety engineering organisations.
- There is a rapidly diminishing pool of expertise and experience of historical UK NPP design capability; in this area the UK has fallen behind the leading international players.

9.2 Opportunities and Threats

- More benefit can be obtained by choosing to collaborate rather than reinvent or compete in thermal hydraulics research by identifying gaps in international research capabilities and addressing questions currently not considered. However, international activities are extensive and the UK's research funding is limited by comparison.
- New advanced designs being considered (such as liquid metal or molten salt cooled reactors) provide the opportunity for the UK to develop expertise in alternative reactor designs.
- Nuclear thermal hydraulics is potentially on the brink of radical change ("Supercomputing Will Change Our Energy Future"). This is an opportunity that plays to the strengths of the UK research community. One way to gain the benefits of these developments would be for the UK to engage with the US's NEAMS program (Nuclear Energy Advanced Modelling and Simulation). Such involvement could enable the UK thermal hydraulics community to become a contributor in the development of this cutting-edge research, but extensive involvement is likely beyond the scope (and budget) of this project.
- Thermal Hydraulics also serves Nuclear Fusion, where the UK is active. This is a topic in which the UK has the opportunity to develop a strong position.

10 Abbreviations

Acronym	Definition
AI	Artificial Intelligence
ASCI	Accelerated Strategic Computing Initiative
ABND	Average Bubble Number Density Model
ALE	Arbitrary Lagrangian-Eulerian
AMR	Adaptive Mesh Refinement
ATWS	Anticipated transient without SCRAM
ATHLET	Analysis of Thermal-hydraulics of LEaks and Transients
AWF	Analytical Wall Function
BEPU	Best Estimate Plus Uncertainty
BPG	Best Practice Guidelines
BWR	Boiling Water Reactor
CANDU	Canada Deuterium Uranium
CATHARE	Code for Analysis of THermalhydraulics during an Accident of Reactor and safety Evaluation
CCFL	Counter Current Flow Limitation
CFD	Computational Fluid Dynamic
CHF	Critical Heat Flux
CHT	Conjugate Heat Transfer
CRGT	Control Rod Guide Tubes
CRP	IAEA Coordinated Research Projects
CRA	IAEA Coordinated Research Activities
CSAU	Code Scaling Applicability and Uncertainty
CSV	Comma Separated Variable
DES	Detached Eddy Simulation
DMD	Dynamic Mode Decomposition
DNB	Departure from Nucleate Boiling
DNS	Direct Numerical Simulation
DQMOM	Direct Quadrature Method of Moments
DSS	Dynamic System Scaling
ECC(S)	Emergency Core Cooling (Systems)
EPR	European Pressurised Reactor
EVM	Eddy-viscosity Model
FAC	Flow accelerated corrosion
FCT	Flux-Corrected Transport
FE(M)	Finite Element (Method)
FIV	Flow Induced Vibration
FLAIR	Flux Line-Segment Model for Advection and Interface Reconstruction
FOM	Figure of Merit
FSA	Fractional Scaling Analysis
FSI	Fluid-Structure Interaction
FV(M)	Finite Volume (Method)

Acronym	**Definition**
GEN-IV	Generation IV
GMRES	Generalised Minimal Residual Method
HGCR	Heterogeneous Gas Core Reactor
HPC	High performance Computing
HTGR	High-Temperature Gas-cooled Reactor
HTTR	High-Temperature Test Reactor
HVAC	Heating, Ventilation and Air-Conditioning
IATE	Interfacial Area Transport Equation
IBM	Immersed Boundary Method
IET	Integral Effect Test
ITF	Integrated Test Facility
INES	International Nuclear and Radiological Event Scale
JHTDB	John Hopkins Turbulence Database
KOFA	Korean Optimised Fuel Assembly
LBE	Lead Bismuth Eutectic
LBLOCA	Large Break Loss of Coolant Accident
LBM	Lattice Boltzmann Methods
LDV	Laser Doppler Velocimetry
LES	Large Eddy Simulation
LIF	Laser Induced Fluorescence
LFR	Lead-cooled Fast Reactor
LM	Liquid Metal
LMFR	Liquid Metal Fast Reactor
LSTF	See ROSA/LSTF
LOCA	Loss-of-Coolant Accident
LS	Level-Set
LWR	Light Water Reactor
LTE	Local Thermal Equilibrium
LTNE	Local Thermal Non-Equilibrium
MASLWR	Multi-Application Small Light Water Reactor
MSLB	Main Steam Line Break
MSR	Molten Salt Reactor
MSFR	Molten Salt Fast Reactor
MYRTE	MYRRHA Research and Transmutation Endeavour
MYRRHA	Multi-purpose hYbrid Research Reactor for High-tech Applications
MUSIG	MUltiple SIze Group Model
NAPRO	Sodium Properties and Safe Operation of Experimental Facilities in Support of the Development and Deployment of Sodium-cooled Fast Reactors
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NESTOR	New Experimental Studies of Thermal-Hydraulics of Rod Bundles
NURISP	Nuclear Reactor Integrated Simulation Project
NURESAFE	NUclear Reactor SAFEty Simulation Platform
NPP	Nuclear Power Plant

Acronym	Definition
NTH	Nuclear Thermal-hydraulics
NS	Navier-Stokes
NVD	Normalised Variable Diagram
PBM	Population Balance Model
PCCS	Passive Containment Cooling System
PCT	Peak Cladding Temperature
PFBR	Prototype Fast Breeder Reactor
PGSFR	Prototype Gen IV Sodium cooled Fast Reactor
PHWR	Pressurised Heavy Water Reactor
PIRT	Phenomena Identification and Ranking Table
PIV	Particle Image Velocimetry
PLIC	Piecewise Linear Interface Construction
POD	Proper Orthogonal Decomposition
PTS	Pressurised Thermal Shock
PV	Pressure Vessel
PIV	Particle Image Velocimetry
PWR	Pressurised Water Reactor
QMU	Quantifications of Margins and Uncertainty
R&D	Research and Development
RANS	Reynolds-averaged Navier-Stokes
RELAP	Reactor Excursion and Leak Analysis Program
ROSA/LSTF	Japan Atomic Energy Agency Rig of Safety/Large Scale Test Facility
RBMK	Reaktor Bolshoy Moshchnosti Kanalnyy (High Power Channel-type Reactor)
RMS	Root Mean Square
RPV	Reactor Pressure Vessel
RSM	Reynolds Stress Model
SAMOFAR	Safety Assessment of the MOlten salt FAst Reactor
SAR	Safety Analysis Reports
SESAME	Simulations and Experiments for the Safety Assessment of MEtal cooled reactors
SMAP	Safety Margins Action Plan
SBLOCA	Small-Break Loss of Coolant Accident
SCWR	SuperCritical Water-cooled Reactor
SET(F)	Separate Effect Test (Facility)
SHARP	Simulation-based High-efficiency Advanced Reactor Prototyping suite
SFR	Sodium-cooled Fast Reactor
SIG	Special Interest Group
SLIC	Simple Line Interface Construction
SOFIA	Simulateur d’Observation du Fonctionnement Incidentel et Accidentel
SMR	Small Modular Reactor
SST	Shear Stress Transport
SG	Steam Generator
SPH	Smoothed-Particle Hydrodynamics
STRESA	Storage of Thermal REactor Safety Analysis

Acronym	Definition
TBL	Turbulent Boundary Layer
TCL	Two-Component Limit
TH	Thermal Hydraulics
THINS	Thermal Hydraulics of Innovative Nuclear Systems
TVD	Total Variation Diminishing
UQ	Uncertainty quantification
URANS	Unsteady Reynolds-averaged Navier-Stokes
VHTR	Very High-Temperature Reactor
VOF	Volume of Fluid
VVER	Water-Water Energetic Reactor
VERA-CS	Virtual Environment for Reactor Applications, Core Simulator
WCR	Water Cooled Reactor
WMS	Wire Mesh Sensor

11 Organisations

Acronym	**Definition**
AEA	See UKAEA
AIAA	American Institute of Aeronautics and Astronautics (USA)
AEDC	US Air Force Arnold Engineering Development Center (USA)
ANL	Argonne National Laboratory (USA)
ANSYS	Commercial engineering code provider (USA)
AREVA	Nuclear company (France)
AWE	Atomic Weapons Establishment (UK)
AGARD	Advisory Group for Aerospace Research and Development – NATO Agency
BEIS	Department for Business, Energy and Industrial Strategy (UK)
BNFL	British Nuclear Fuels Ltd (UK)
CASL	Consortium for Advanced Simulation of Light Water Reactors (USA)
CEA	Commissariat à l'Energie Atomique et aux Energies Alternatives (France)
CEBG	Central Electricity Generating Board (UK)
CESAR	Centre for Exascale Simulation for Advanced Reactor (USA)
CHAM	Concentration, Heat and Momentum Limited (UK)
CNL	Canadian Nuclear Laboratories (Canada)
Columbia	Columbia University (USA)
CSNI	NEA Committee on the Safety of Nuclear Installations
DoE	Department of Energy (USA)
ECMWF	European Centre for Medium-Range Weather Forecasts (EU)
EDF	Électricité de France (France)
EPRI	Electric Power Research Institute (USA)
EPSRC	Engineering and Physical Sciences Research Council (UK)
ERCOFTAC	European Research Community on Flow, Turbulence and Combustion (EU)
ETH Zurich	Swiss Federal Institute of Technology in Zurich
EU	European Union
EURATOM	European Atomic Energy Community (EU)
GIF	Generation IV International Forum
GRC	NASA Glenn Research Center (USA)
GNU	Free-software and mass-collaboration project (USA)
IAEA	International Atomic Energy Agency
I-NERI	International Nuclear Energy Research Initiative (USA)
INL	Idaho National Laboratory (USA)
IRSN	Institute for Radiological Protection and Nuclear Safety (France)
JAEA	Japan Atomic Energy Agency (Japan)
JAXA	Japan Aerospace Exploration Agency (Japan)
JRC	Ispra Joint Research Centre of the European Commission (Italy)
KAERI	Korean Atomic Energy Institute (Korea)
MIT	Massachusetts Institute of Technology (USA)

Acronym	**Definition**
NASA	National Aeronautics and Space Administration (USA)
NATO	North Atlantic Treaty Organisation
NEA	Nuclear Energy Agency of the OECD
NERAC	Nuclear Energy Research Advisory Committee (USA)
NIRAB	Nuclear Innovation and Research Advisory Board (UK)
NRC	See USNRC
NRG	Nuclear Research and Consultancy Group (Netherlands)
NPARC	National Project for Applications-Oriented Research in CFD (USA)
NRSA	Nuclear Reactor Safety Assessment Unit of the JRC
NSF	National Science Foundation (USA)
NUPEC	NUclear Power Engineering Corporation (now JNES, Japan)
OECD	Organisation for Economic Co-operation and Development
SCK-CEN	Belgian Nuclear Research Centre (Belgium)
Stanford CTR	Stanford Center for Turbulence Research (USA)
STFC	Science and Technology Facilities Council (UK)
UGent	Ghent University (Belgium)
UKAEA	UK Atomic Energy Authority (UK)
USNRC	United States Nuclear Regulatory Commission (USA)

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Originating Office: FRAZER-NASH CONSULTANCY LIMITED
The Cube, 1 Lower Lamb Street, Bristol, BS1 5UD
T: +44 (0)117 9226242 F: +44 (0)117 9468924 W: www.fnc.co.uk

Frazer-Nash Consultancy Ltd
The Cube
1 Lower Lamb Street
Bristol
BS1 5UD

T +44 (0)117 9226242
F +44 (0)117 9468924

www.fnc.co.uk

Offices at:
Bristol, Burton-on-Trent, Dorchester,
Dorking, Glasgow, Plymouth, Warrington
and Adelaide