A UK REGULATORY PERSPECTIVE ON COMPUTATIONAL FLUID DYNAMICS FOR NUCLEAR SAFETY ANALYSIS

JONATHAN DOWNING, JOHN JONES, ALI TEHRANI, ROBERT MOSCROP

Office for Nuclear Regulation

St James House, St James Square, Cheltenham, GL50 3PR, United Kingdom

ABSTRACT

Nuclear safety analysis typically involves the implementation of a thermal hydraulic system code which has been validated against test data. Computational Fluid Dynamics (CFD) has achieved relatively little penetration into nuclear safety cases for licensing purposes; principally due to the need to demonstrate that uncertainties in the analysis have been accounted for to a high level of confidence. This paper provides a UK regulatory perspective on a number of key CFD uncertainties within the context of nuclear safety analysis.

CFD can sometimes provide a useful role in generalising the lessons learned from tests. CFD can also provide visualisation of phenomena and hence aid in understanding and explaining physical concepts and problems. That being said, a step increase in the level of confidence is required in moving from these qualitative, illustrative benefits of CFD to nuclear safety analysis where a comparison to an assessment criterion is made with nuclear safety significance.

1. Introduction

Single phase CFD is becoming a more mature technology, with some impressive benchmark studies, but these set-piece demonstrations often use more advanced modelling methods than the Reynolds averaged analysis more typically presented in safety cases. The computational demand of CFD generally restricts implementation to the component or sub-assembly scale and the fluid dynamic equations that are solved in an industrial CFD calculation are not the exact governing equations. The implications of some of the key simplifications are illustrated in this paper, with reference provided towards guidance on the production of quality CFD analysis.

Both Eulerian and Lagrangian approaches to multiphase CFD remain primarily in the research sphere with limited technology readiness for industrial licensing. This paper therefore does not focus on multiphase CFD, but concentrates on several key areas of single phase CFD which require special attention within a nuclear safety analysis submission.

It is generally impractical to conduct Direct Numerical Simulation (see Section 3) for problems of industrial interest, and simplifications are necessary with respect to turbulence and near wall treatment. Simplified sub-models are employed in industrial CFD which substitute fundamental solution with empiricism and the validity and applicability of the approach needs to be demonstrated for each application. Demonstrably relevant experimental evidence remains essential to validate CFD results.

2. UK REGULATORY FRAMEWORK

The Energy Act 2013 created the Office for Nuclear Regulation (ONR). ONR is the regulator for nuclear sites in Great Britain. The Health and Safety at Work Act 1974 requires that employers ensure the health and safety of employees and members of the public So Far As Is Reasonably Practicable (SFAIRP). Ensuring health and safety SFAIRP is the legal basis behind reducing risks As Low As Reasonably Practicable (ALARP). The legal requirement of SFAIRP drives a goal setting regulatory environment within the UK where a key requirement is to reduce risks ALARP.

Guidance has developed over time which describes what is considered SFAIRP in particular circumstances. This guidance is known as Relevant Good Practice (RGP). RGP includes Approved Codes of Practice (ACOPs); ONR Safety Assessment Principles (SAPs, Reference 1); ONR Technical Assessment Guides (TAGs); ONR Technical Inspection Guides (TIGs); and publications of the British Standards Institute (BSI), International Atomic Energy Agency (IAEA), and Western European Nuclear Regulators' Association (WENRA). ONR SAPs, TAGs and TIGs are guidance documents for Inspectors when conducting assessments and inspections. RGP applicable to CFD for nuclear safety analysis is described in Section 6.

The Nuclear Installations Act 1965 requires the ONR to attach conditions to a nuclear license. A standard set of 36 license conditions has become established. Within the license conditions are a set of primary powers (Direct, Approve, Notify, Specify, Agree, and Consent). Additional derived powers may be arranged with a licensee if this is a convenient working arrangement. The primary and derived powers are used to specify permissioning milestones such that the licensee requires permission from ONR to start, continue or cease key activities.

3. TURBULENCE MODEL SELECTION

Approaches to modelling turbulence can be grouped into three broad categories in order of decreasing fidelity: Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and Reynolds Averaged Navier Stokes (RANS). That being said, there are a wide range of intermediate and hybrid approaches that lie in between these three broad categories, as illustrated in Figure 1 (Reference 2).

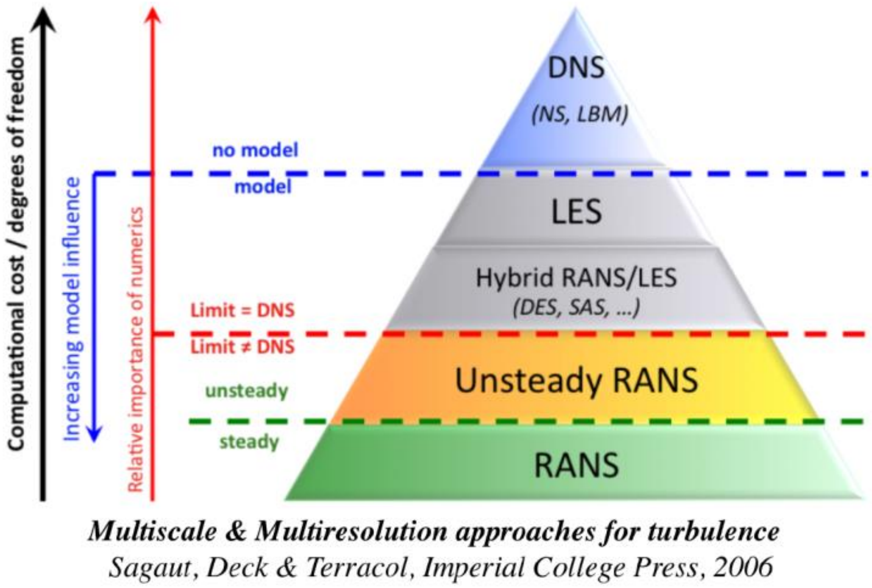

Figure 1 Approaches to Turbulence Modelling

Lewis Richardson wrote in 1922 (Reference 3) that "big whirls have little whirls which feed on their velocity; and little whirls have lesser whirls, and so on to viscosity in the molecular sense". This reflects the range of eddies that need to be represented from the largest integral scale, through the Taylor micro scale, to the Kolmogorov dissipation scale (Reference 4).

In DNS the spatial and temporal discretisation is sufficiently fine that all scales of turbulence are resolved by virtue of the solution of the Navier Stokes equations. DNS is extremely computationally expensive and therefore limited to simple geometries at low Reynolds number with currently available technical computing capability (Reference 5). It is therefore impractical to utilise DNS for the majority of problems of industrial interest (Reference 6).

In LES the larger eddies are directly resolved via the Instantaneous Navier Stokes (INS) equations, whereas the smaller eddies are approximated by a Sub-Grid Scale (SGS) model. The majority of the turbulent energy is contained within the larger eddies and hence it is often acceptable to filter the smaller eddies for a simplified representation. The SGS results in a significant reduction in computational cost compared to DNS. Small eddies are less dependent on the geometry than large eddies with greater predisposition to representation by a universal turbulence model (Reference 7). The combination of viability and reasonable accuracy make LES a promising tool for the simulation of nuclear industry turbulent flow fields.

In RANS the solution variables in the INS equations are decomposed into ensemble averaged and fluctuating components. The RANS equations have the same general form as the INS equations with the solution variables representing ensemble averaged values and Reynolds stress terms representing turbulence. The Reynolds stress terms are often calculated with approximate closure models. The RANS approach to turbulence is the least computationally expensive because all scales of turbulence are represented by a simplification.

A RANS simulation may appear to provide a converged solution, however the result may not be found to be representative of all aspects of flow behaviour when test comparisons are made. RANS CFD may not provide a high confidence representation, to nuclear safety expectations, for applications where turbulent mixing is a dominant phenomenon.

The Boussinesq hypothesis is commonly employed in RANS modelling (with the notable exception of the Reynolds Stress Model). The Boussinesq hypothesis is also known as the eddy viscosity assumption. A turbulent viscosity term is introduced to the Navier Stokes equations in order to simplify the Reynolds stress terms and relate them to the mean velocity gradients. The disadvantage of the Boussinesq hypothesis is that it falsely assumes that turbulent viscosity is an isotropic scalar quantity (Reference 7).

Figure 2 shows a plot of Particle Image Velocimetry (PIV) measurements and LES results (Reference 8). The red versus green points show that the normal and transverse stresses are significantly different in this situation. The anisotropy is well captured by the LES approach. Application of the Boussinesq approximation within a RANS simulation would lead to a failure to predict this anisotropy.

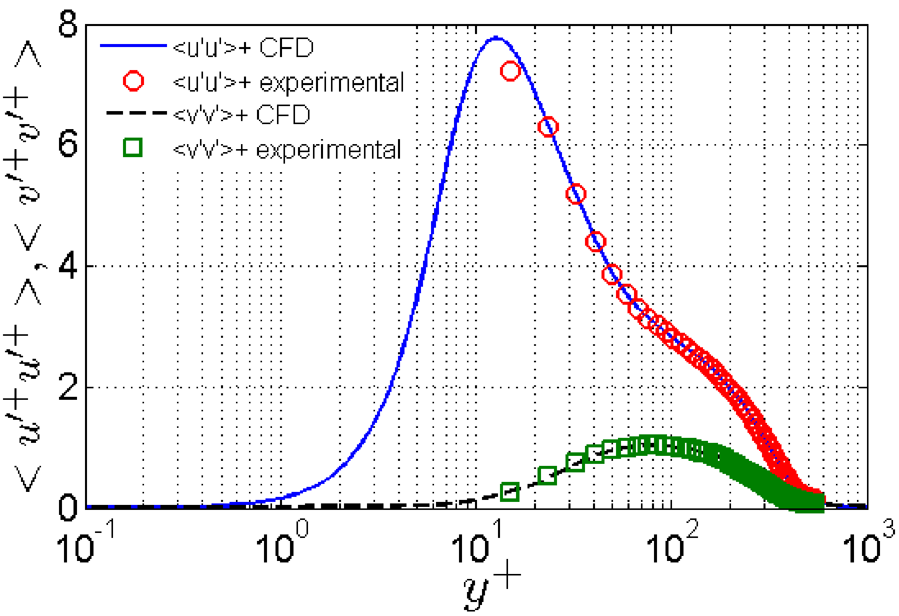

Figure 2 LES Predictions of Reynolds Stresses against Particle Image Velocimetry (PIV) Measurements

In the case of the Spalart-Allmaras turbulent model a single transport equation representing turbulent viscosity is solved. The k-ε model is a well-known and well documented turbulence model. In the k-ε turbulence model two transport equations are solved (one for k and the other for ε) and the turbulent viscosity is calculated as a function of the turbulent kinetic energy (k) and the turbulent dissipation rate (ε).

RANS modelling with the Boussinesq approximation may not provide accurate representation in the following anisotropic scenarios (Reference 5, Reference 8) and the use of more advanced turbulence modelling should be considered:

- Flow separation.
- Reattachment regions.

- Impinging jets.
- Swirling flows.
- High curvature streamlines.
- Secondary flows.
- Near wall region.
- A thermal plume.
- Buoyancy driven flows.
- Laminar or transitional flows.
- Round jets.

A wide range of RANS turbulence models have been developed. The ensemble average limitation applies to all RANS models, however different models have varying computational demands and suitability of application. Table 1 provides a summary of a selection of available RANS turbulence models (Reference 9).

Table 1 RANS Turbulence Model Examples

Model	Description
Spalart-Allmaras	A single transport equation model solving directly for a modified turbulent viscosity. Designed for aerospace applications involving wall-bounded flows on a fine near-wall mesh. Economical but performs poorly for 3D flows, free shear flows, flows with strong separation.
Standard k–ε	The baseline two-transport-equation model solving for k and ε. Coefficients are empirically derived; valid for fully turbulent flows only. Widely used despite the known limitations of the model. Performs poorly for complex flows involving severe pressure gradient, separation, strong streamline curvature. May be suitable for initial iterations.
RNG k–ε	Re-Normalisation Group (RNG) is a variant of the standard k–ε model. Equations and coefficients are analytically derived. Significant changes in the ε equation improve the ability to model shear, moderate swirl, and low Reynolds number flows.
Standard k–ω	A two-transport-equation model developed by Wilcox and solving for k and ω. Where ω is the specific dissipation rate (ε / k). Demonstrates superior performance for wall-bounded and low Reynolds number flows. Can be used for transitional flows (though tends to predict early transition). Separation is typically predicted to be excessive and early. Sensitive to inlet turbulence parameter assumptions.
SST k–ω	The Shear Stress Transport (SST) model combines the k–ω model near walls and the k–ε model away from walls using a blending function. Can be used for low Reynolds number with less sensitivity to inlet turbulence assumptions than standard k–ω, however the dependency on wall distance makes SST less suitable for free shear flows.
Reynolds Stress Model	Reynolds stresses are solved directly using transport equations, however modelling is still required for many terms in the transport equations. Physically the most sound RANS model. Avoids isotropic eddy viscosity assumption. More CPU time and memory required. Tougher to converge due to close coupling of equations. More suitable than other RANS models for complex 3D flows with strong streamline curvature and swirl.

Figure 3 provides an illustration of the approximate relative computer resource requirements of the three categories of turbulence models. Budget constraints and project time pressures can make RANS modelling appear to be an attractive option despite accuracy concerns.

Figure 4 provides an indication of the level of CFD fidelity that is achievable relative to past and future predicted high performance computing capability (Reference 10). This plot indicates that although the computational expense of LES remains a challenge, it should be considered as reasonably practicable when required, given the status of current day high performance computing capability.

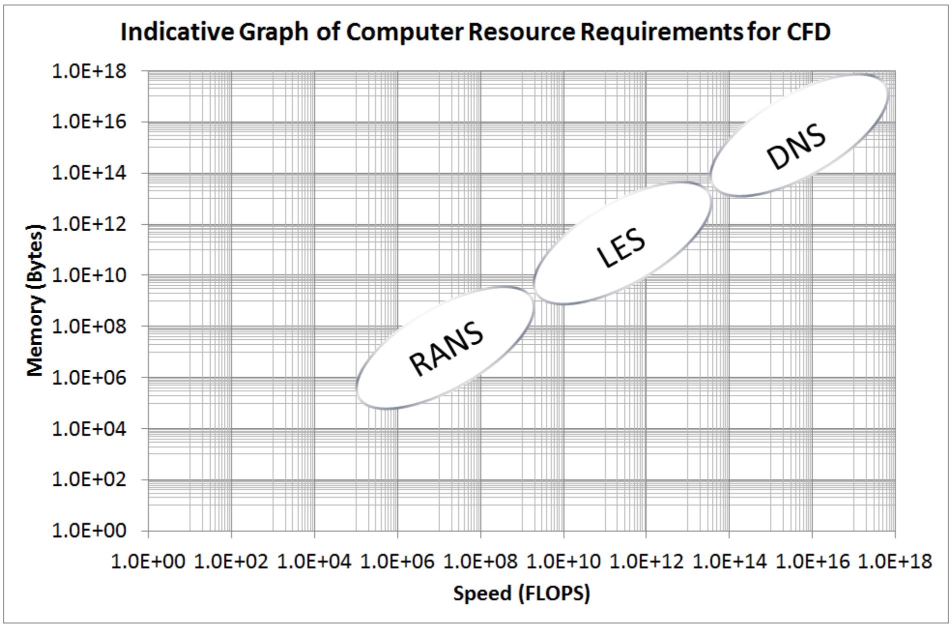

Figure 3 Indicative Graph of Computer Resource Requirements for CFD

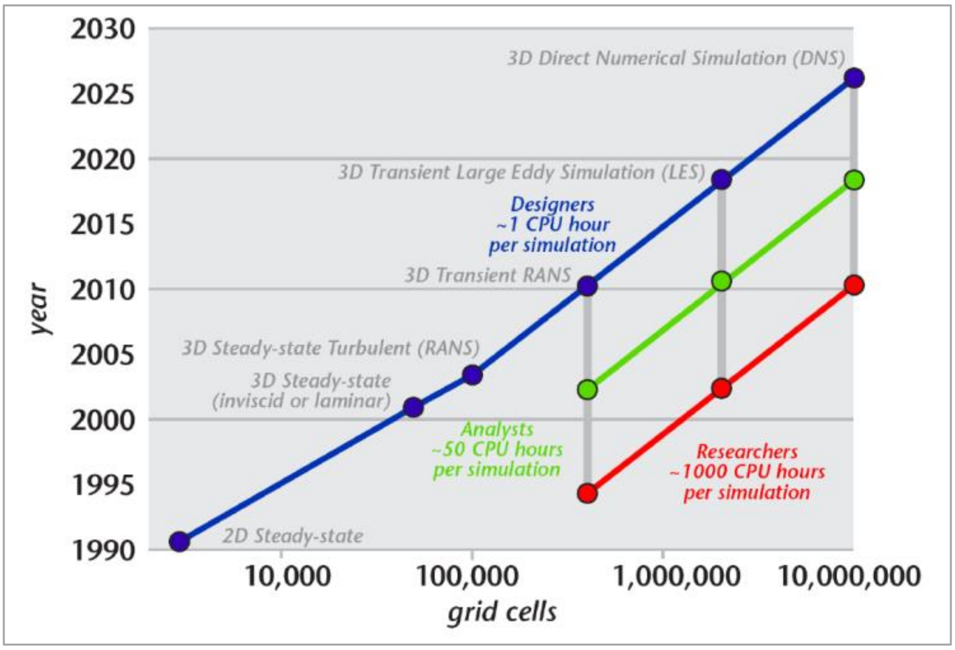

Figure 4 Estimation of Achievable CFD Fidelity Through Time

4. STEADY STATE VERSUS TRANSIENT SIMULATION

A further temptation under time and resource constraints is to apply the simplifying assumption of steady state. All turbulent flows are time varying and the different approaches to turbulence modelling have already been discussed. A flow field may be significantly time varying due to internally induced fluctuations even if the external boundary conditions are constant.

A common example of the incorrect application of the steady state assumption is the flow around a symmetrical bluff body. A vortex will often be shed to one side of the body and then the other. A steady state CFD simulation will not be able to capture this temporal feature of the flow field. The boundary conditions at the inlet and outlet to the domain may be constant and therefore it is not clear that the scenario is transient unless this is tested.

An Unsteady RANS (URANS) prediction of the transient flow around a square cylinder with vortex shedding and a periodically oscillating wake is presented in Reference 11. Pressure isobars at four snapshots corresponding to a full period of wake oscillation are shown in Figure 5. Vortices are shed alternatively from the two sides of the square followed by convection downstream. Reference 11 identifies that steady state RANS will not produce a good match to experiment for this scenario because of the erroneous implied assumption that the flow field is stationary. Transient CFD may successfully predict periodic vortex shedding, and lead to much better concurrence with available experimental data.

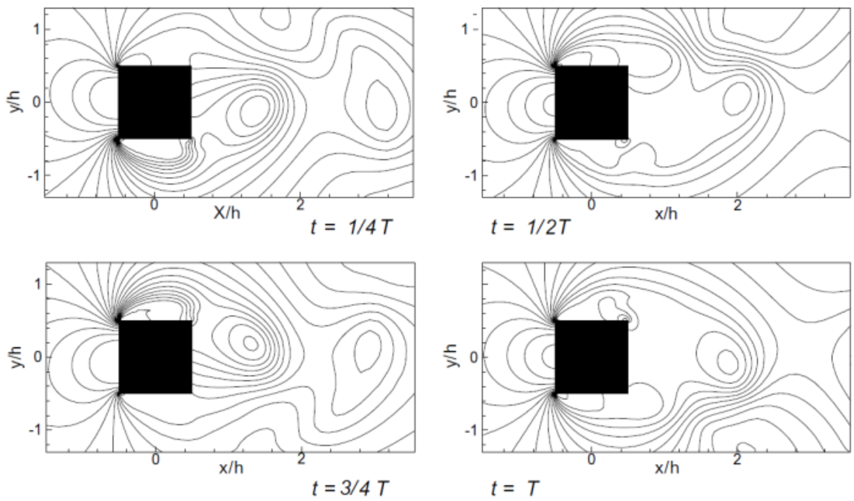

Figure 5 Time History of Pressure Isobars in the Wake of a Square Cylinder

Reference 12 describes the simulation of pollutant dispersion within a canyon. Two steady state RANS models (the standard k-ε model and the Reynolds Stress Model); an Unsteady RANS model (based on Unsteady Reynolds Stress Model); and an LES model of a wind tunnel were produced. Wind tunnel measurements of pollutant concentration against predictions are shown in Figure 6. Transient LES profiles are compared against steady state RANS in Figure 7. URANS predictions against transient LES are presented in Figure 8. The work concluded that steady state RANS poorly predicted the pollutant concentrations due to a failure to capture the turbulent mixing of the flow field. URANS was unable to fully account for the internally induced fluctuations of the flow field and hence pollutant concentration profiles were of limited accuracy. LES produced the most accurate solution of the approaches investigated because the analysis was able to resolve eddies which formed an integral part of the flow field development.

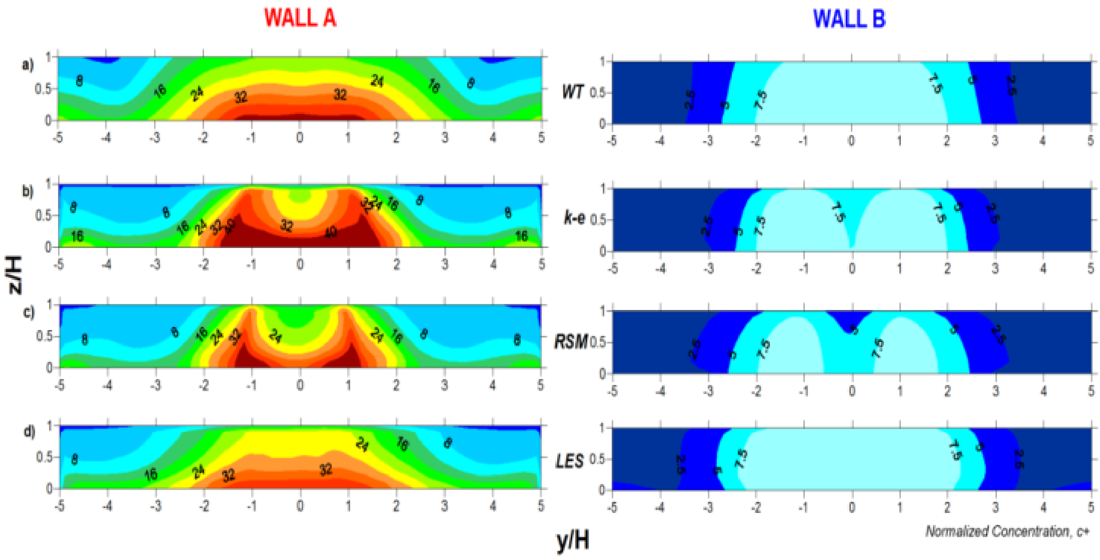

Figure 6 Wind Tunnel (WT) Test Results Against CFD Predictions

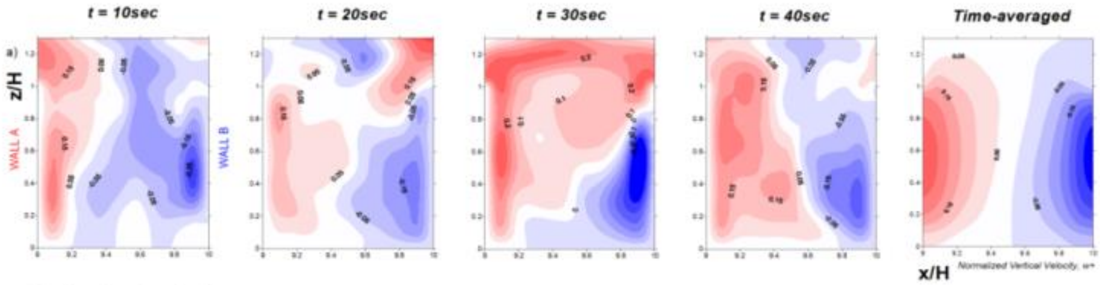

Figure 7 Transient versus Time Averaged Velocity Predictions

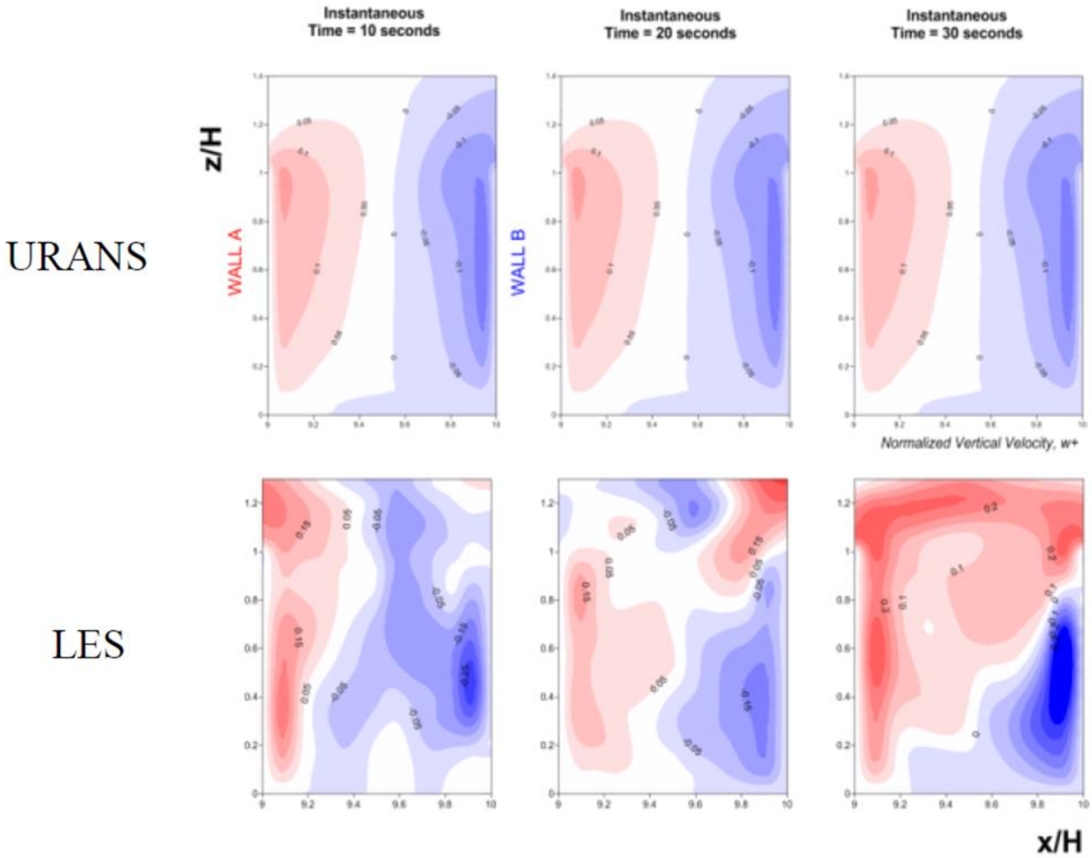

Figure 8 Unsteady RANS versus LES Velocity Predictions

Turbulent mixing of streams of fluid at different temperatures at a T-junction, especially downstream of a bend, can lead to oscillating thermal stresses and high cycle thermal fatigue (Reference 13). Ultimately this can result in pipe failure. This thermal striping phenomenon is intrinsically unsteady and hence steady state RANS modelling is not a suitable approach. It is necessary to adopt a form of transient analysis for this application. An LES simulation of a T-junction temperature distribution is shown in Figure 9 from Reference 14. The Nuclear Energy Agency has published the results of a T-junction benchmark study in Reference 15. LES provided a better agreement to experiment for velocity, temperature and flow oscillation frequency than Detached Eddy Simulation (DES); Scale-Adaptive Simulation (SAS) Shear Stress Transport (SST); and RANS modelling.

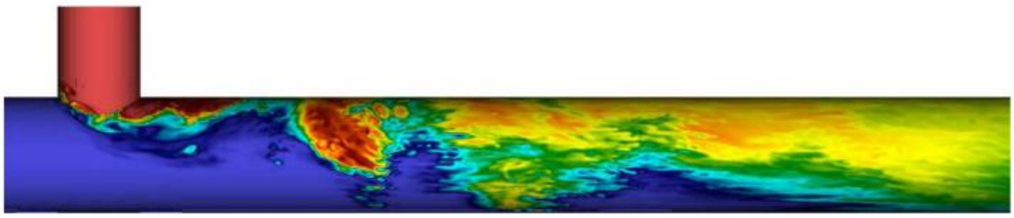

Figure 9 Wall Temperature Distribution from an LES T-junction Simulation

5. GRID DEPENDENCY

Reference 16 describes a DNS grid convergence study of flow around a square cylinder. Figure 10 provides a schematic of the simple geometry studied. Figure 11 shows predicted lift and drag coefficient values as a function of cell size, normalised by the extrapolated result at zero cell size. It can be seen that the chosen cell size can have a significant effect on the output. In order to have high confidence in the output of a CFD analysis it is therefore necessary to establish that the numerical error due to finite discretisation has been reduced to an adequate level. This is often achieved by way of a grid independence study. This involves repeating the simulation with a range of grid sizes (for example coarse, medium and fine) in order to demonstrate that the solution is insensitive to the cell size chosen for the submission.

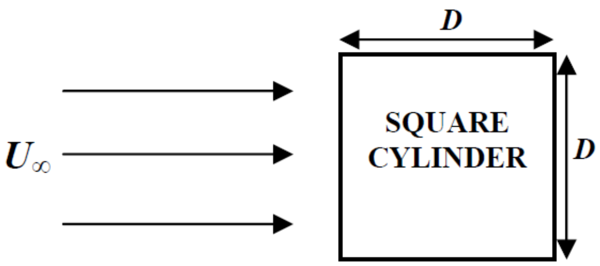

Figure 10 Flow Geometry for Grid Convergence Study

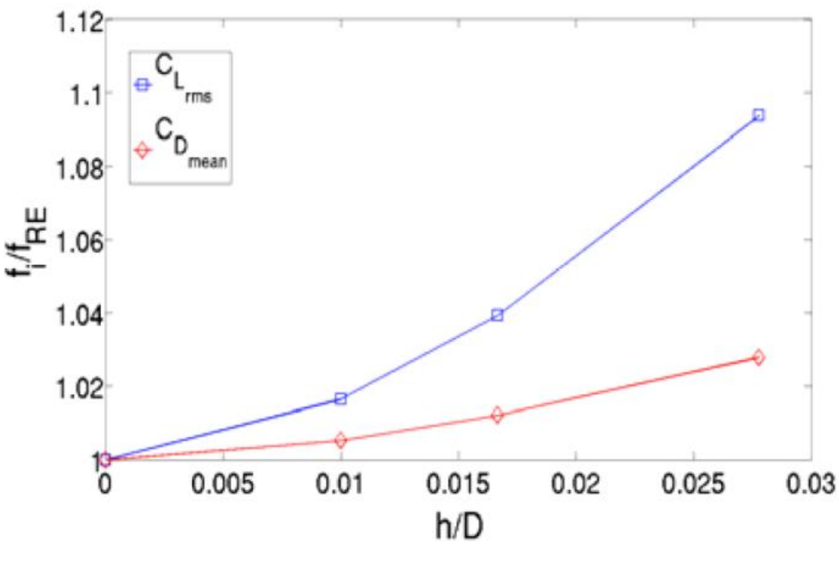

Figure 11 Grid Convergence Study for Lift and Drag Coefficient

Ultimately the validity of the mesh must be established by the validation of the analysis against test data. ONR Safety Assessment Principles AV.1 to AV.8 provide guidance for assessing the verification and validation of models and their data (Reference 1). These principles are provided in Table 2.

The grid convergence study shown in Figure 11 is an example of a sensitivity study to assumptions as described in AV.6. Where significant numerical error occurs in relation to an output of importance then a shortfall to AV.2 is observed because physical processes are not adequately represented.

Table 2 Safety Assessment Principles Pertaining to the Assurance of Validity of Data and Models

SAP	Description
AV.1	Theoretical models should adequately represent the facility and site.
AV.2	Calculation methods used for the analyses should adequately represent the physical and chemical processes taking place.
AV.3	The data used in the analysis of aspects of plant performance with safety significance should be shown to be valid for the circumstances by reference to established physical data, experiment or other appropriate means.
AV.4	Computer models and datasets used in support of the safety analysis should be developed, maintained and applied in accordance with quality management procedures.
AV.5	Documentation should be provided to facilitate review of the adequacy of the analytical models and data.
AV.6	Studies should be carried out to determine the sensitivity of the analysis (and the conclusions drawn from it) to the assumptions made, the data used and the methods of calculation.
AV.7	Data should be collected throughout the operating life of the facility to check or update the safety analysis.
AV.8	The safety analysis should be updated where necessary, and reviewed periodically.

Verification and validation are essential elements of any nuclear safety analysis including CFD submissions. ONR define the term validation in Reference 1. Validation is defined as "the process of confirming, eg by use of objective evidence, that the outputs from an activity will meet the objectives and requirements set for that activity". Reference 17 is the IAEA glossary of terminology used in nuclear safety. 'Model validation' is defined as "the process of determining whether a model is an adequate representation of the real system being modelled, by comparing the predictions of the model with observations of the real system".

ONR define the term verification in Reference 1 as "the process of confirming, eg by use of objective evidence, that an activity was carried out as intended, specified or stated". In terms of grid quality, examples of verification checks may include ensuring that y+ values (non-dimensional distance to the wall) are appropriate to the wall functions; checks on cell aspect ratio, negative volume, extreme grid angles; and examination of important geometry features to ensure that the grid is a realistic representation (Reference 18).

The discretisation methods used to translate the mathematical model into a numerical method for solution by a computer include approximations which result in numerical errors. Relative to reality, CFD can exhibit increased rates of diffusion of heat, mass and momentum; leading to an over-prediction of mixing in some cases (Reference 19). Grid refinement coupled with a higher-order interpolation scheme will minimize false diffusion (Reference 20).

Reference 21 describes regulatory requirements in the United States (US) for analysis methods. The requirements described are directly applicable to thermal hydraulic system code applications in the US, rather than CFD applications in the UK, however the principles of the Evaluation Model Development and Assessment Process (EMDAP) are of interest to analysis methods for nuclear safety in general. An important principle within EMDAP is that the nodalisation and option selection should be consistent between the experimental facility used for validation and the plant analysis. This stands to reason. If 100,000 cells are required to gain good agreement with the experimental facility then a plant model with 10,000 cells will be unconvincing.

The requirement for a consistent grid between experimental facility and plant analysis may be more complicated with Adaptive Mesh Refinement (AMR). AMR is a strategy where the mesh is made finer or coarser during the solution of the problem based on defined refinement criteria. The aim is often to refine the grid in areas where flow gradients are large. AMR can be beneficial in making efficient use of finite computer resource within time constrained projects. AMR is particularly useful for transient problems with moving discontinuities (Reference 22). That being said, the requirement to validate the simulation remains, and a CFD submission would need to justify any deviations between the assumption set for the validation comparison and the plant analysis.

6. FURTHER GUIDANCE

This paper has focussed on a number of uncertainties that are worthy of attention for a single phase CFD submission regarding nuclear safety. CFD is a large subject and this paper does not attempt to be all encompassing. International guidance on the use of CFD for nuclear reactor safety applications can be found in Reference 18. UK Relevant Good Practice relating to CFD for nuclear safety analysis includes the SAPs (Reference 1) and the methods validation TAG (Reference 23). Appendix 1 of Reference 23 provides guidance which is specific to CFD.

7. CONCLUSIONS

For licensing purposes, uncertainties within analysis results have to be accounted for to a high level of confidence.

Steady state RANS CFD can provide an ensemble average approximation, however key aspects of the flow field may be inaccurately represented such as flow separation, turbulent mixing, and vortex shedding.

LES can provide significantly improved predictions relative to RANS by directly resolving large eddies.

LES is computationally expensive but reasonably practicable with current day high performance computing capability.

It is impractical to conduct DNS for the majority of problems of industrial interest.

Applications with internally induced fluctuations in the flow field may require transient simulation even if the boundary conditions are constant.

Adequacy of the grid is an important component of a CFD submission for nuclear safety.

CFD submissions for nuclear safety must be validated against relevant and appropriate test data.

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