Reliability Issues of LES-Related Approaches in an Industrial Context

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Large-Eddy Simulation (LES), Detached-Eddy Simulation (DES) and Scale-Adaptive Simulation (SAS) are increasingly being used as engineering tools to predict the behaviour of complex industrial flows. Often the flows studied have not been examined previously and the required grid resolution is unknown. Industrial users studying these flows tend to be using commercial CFD codes and do not usually have access to high-performance computing facilities. Due to the significant computing times required, it is difficult to undertake systematic grid-dependence studies. There is therefore a risk that LES, DES and SAS will be performed using overly coarse grids which may lead to unreliable predictions.

The present work surveys a number of practical techniques that provide a means of assessing the quality of the grid resolution in large-eddy simulations and related approaches. To examine the usefulness of these techniques, a gas release in a ventilated room is examined using DES and SAS. The grid resolution measures indicate that overall the grids used are relatively coarse. Both DES and SAS model predictions are found to be in poor agreement with experimental data compared to steady and unsteady Reynolds-Averaged Navier-Stokes (RANS) results using the SST model. The SAS model also shows the greatest grid sensitivity of the four models tested. The work highlights the need for grid-dependence studies and the potential problems of using coarse grids.

Keywords: *Quality, grid resolution, large-eddy simulation, gas dispersion*

Introduction

There has been a steady increase in the use of LES for safety related studies in recent years, e.g. [1, 2]. This has particularly been the case in the fire-safety industry, largely due to the increasing popularity of the Fire Dynamics Simulator freeware [3]. A recent report by the Organisation for Economic Co-operation and Development (OECD) [4] has also recommended that LES, DES and SAS models be used in assessing nuclear reactor safety.

In view of the current and expected future use of LES-related models in safety critical applications there is a need for practical advice for CFD users on quality and trust issues, similar to that produced a number of years ago by ERCOFTAC for RANS models [5]. The main issues that distinguish the quality of LES-related models from steady RANS include: grid dependence, subgrid-scale (SGS) modelling, wall treatments, turbulent inflow conditions and numerical schemes. The present work concentrates on the first of these issues, namely grid resolution. This is a critical issue for LES, DES and SAS models.

In many engineering studies, the flows considered have never been studied previously and reference data from Direct Numerical Simulation (DNS) or experiments are not available. In such cases, CFD is being used as a truly predictive tool. In a best practice study, since the required grid resolution is unknown, simulations should be performed using a number of different meshes to establish a grid-independent result, whereby increasing the grid resolution further does not significantly affect the statistical parameter of interest (e.g. mean heat transfer coefficient). This is a key requirement in order for the predictions to be repeatable. In theory, a different engineer using a different code should be able to produce matching CFD results without having to tune the grid resolution.

Due to the significant computing times involved in performing LES, DES or SAS, very few grid-dependency tests are usually performed in industrial studies. Often the grid is designed using the finest resolution possible given the available computing resources. It is a pragmatic approach driven by the assumption that a coarse grid could produce poor predictions but a grid can never be too fine. However, the maximum grid resolution that can be afforded may still be inadequate and the CFD results consequently unreliable. A further limitation of such an approach is that it may not be affordable to run multiple simulations to examine the sensitivity of the results to changes in the boundary conditions, within the range of the uncertainty in the physical flow conditions. Tests to examine the sensitivity of the results to the choice of LES model or the numerical treatment are also rarely performed.

A further complication with turbulence models like LES and DES, where the model itself is a function of the grid cell size, is that the discretisation and model errors can interact dynamically. Various studies have tried to obtain a grid-independent LES by refining the grid (i.e. decreasing the cell size, h) whilst keeping constant the filter width, Δ, used in the SGS model [6, 7, 8, 9]. Geurts [6, 7] refers to the ratio between the filter width and the mesh size (Δ/h) as the "SGS resolution". Increasing the SGS resolution increases the number of grid nodes spanning the filter width and correspondingly decreases the spatial discretization error. Geurts [10] found that between 4 and 6 nodes are required to produce a grid-independent solution, although the number of cells depends upon the numerical differencing scheme employed. In practice, most commercial CFD codes assume instead that $\Delta = h$, a choice that is largely driven by the high computational cost of increasing the SGS resolution: every doubling of the SGS resolution leads to a factor of 16 increase in the computational cost [11]. Moreover, it has been shown that decreasing the discretisation error does not necessarily improve the accuracy of the results [10].

The aim of the present work is to survey measures that have been proposed in the literature to assess the grid resolution of LES. A number of these measures are then used to assess the grid resolution in CFD simulations of a gas release in a ventilated room. The flow is typical of a practical scenario investigated as part of an industrial safety study.

Grid Resolution Measures

A number of grid resolution indices have been proposed in the literature. Following Celik et al. [12], these can be classified into four groups: rules of thumb, techniques based on prior RANS simulations, single-grid estimators and multi-grid estimators. The first two of these approaches can be used before running any LES calculations and are therefore cost effective in terms of computing time. Single-grid estimators require one LES calculation, whereas multi-grid estimators require a number of LES calculations and usually some form of Richardson extrapolation.

LES grid resolution has been assessed using prior RANS simulations by Addad et al. [13] for a buoyancy-opposed wall-jet and by Van Maele & Merci [14] for a tunnel fire. In both cases, they examined the ratio of the integral turbulence length scale $l_I = k^{3/2} / \varepsilon$ (determined from the RANS simulation) to the filter width Δ, and found that l_I / Δ needed to be greater than around 12 for the LES to be well resolved. This criteria does not apply in the viscous sub-layer near walls or where the flow relaminarises. These regions can be detected by the magnitude of the turbulence Reynolds number or the ratio of the integral to the Kolmogorov length scales, as suggested by Van Maele & Merci [14].

Results from prior RANS simulations can also be used to assess near-wall cell sizes, where it is typically advised to maintain (x^+, y^+, z^+) < (100, 2, 20) in the (streamwise, wall-normal, spanwise) directions when wall-friction effects need to be predicted accurately [15, 16]. Guidance on the design of near-wall grids for DES is provided by Spalart [17] and in the notes from the recent ERCOFTAC workshop [18].

Another possible resolution indicator based on prior RANS simulations is the ratio of the filter width to the Kolmogorov length scale, $\eta = \left(\nu^3 / \varepsilon\right)^{1/4}$. In free-shear flows the LES grid resolution should be insensitive to this ratio, but in boundary layers the size of the near-wall eddies scale with viscous length scale, ν / u_τ. Celik et al. [19] found that for sufficient LES grid resolution the ratio Δ / η should be less than around 25, although they noted that the value should be a function of the turbulence Reynolds number, Re_t. The ratio Δ / η was also examined in recent LES of impinging jets by Hadžiabdić & Hanjalić [20].

The simplest single-grid estimator is the ratio of the SGS to the molecular viscosity, ν_t / ν. Celik et al. [19] proposed a slight modification, using the effective viscosity ratio, ν_{eff} / ν, where the effective viscosity comprises the sum of the SGS and numerical viscosity, which as a first approximation is taken as twice the SGS viscosity. They recommended that for a high Re_t of 1200 the ratio ν_{eff}/ν should be approximately 20, while for a low Re_t of 300 it should be around 5. Celik et al. [12] also proposed a functional form of ν_{eff}/ν which they called the Relative Effective Viscosity Index.

Another single-grid estimator is the Subgrid Activity Parameter, s, devised by Geurts & Fröhlich [6], which is calculated from the ratio of the turbulent dissipation to the total dissipation. A value of zero indicates that the modelled component is negligible, whilst a value of one indicates that the simulation is a high Reynolds number LES. For an example of its application to channel flow, see Brandt [8].

The ratio of the resolved to the total turbulent kinetic energy, k_{res}/k_{tot}, has also been used as a single-grid estimator. The total turbulent kinetic energy can be considered to comprise the sum of the modelled (k_{mod}), resolved (k_{res}) and numerical (k_{num}) components, although commonly the numerical component is ignored. The modelled component is difficult to calculate if standard or dynamic Smagorinsky SGS models are used, but trivial if an SGS model solves a transport equation for k. Well-resolved LES should aim to resolve 80% of the turbulence energy [21]. An example of this approach applied to study a non-premixed flame is given by Kempf et al. [22]. A similar index called the "Measure of Turbulence Resolution", calculated from the ratio k_{mod}/k_{tot}, has also recently been proposed for use with the Fire Dynamics Simulator CFD code [3], where for well-resolved LES it is recommended to maintain the ratio below 20%.

A fourth single-grid estimator involves plotting the power spectrum and examining the profile to see whether the -5/3 slope characteristic of turbulence in the inertial subrange is obtained. This approach was used for example by Zhou et al. [23, 24] to study forced plumes.

A further single-grid estimator is the ratio of the filter width to the Taylor microscale. This was explored in the recent work on LES of turbulent mixing in a T-junction by Kuczaj & Komen [25].

There are two multi-grid estimators that have previously been proposed to examine grid resolution issues with LES: the Index of Quality, LES_IQ_k, of Celik et al. [19] and the systematic grid and model variation approach of Klein [26]. The former is based on Richardson extrapolation on the resolved turbulent kinetic energy. Celik et al. [19] obtained good LES predictions when LES_IQ_k was of the order 80 – 95%. The grid and model variation approach of Klein [26] involves running three LES calculations: a standard LES, a coarse-grid LES and an LES with the SGS model constant modified. Recently, Celik et al. [27] proposed further refinements to the LES_IQ_k measure, incorporating empirically-derived corrections for low and high Reynolds number flows.

Each of the above grid resolution measures has advantages and limitations. The RANS-based techniques are reliant upon the accuracy of the RANS model, which may be a limiting factor in massively separated flows for example. If the flow involves regions that are nearly laminar, the turbulent length scale ratios from RANS simulations also become meaningless indicators. In most applied LES studies the turbulent viscosity is significantly larger than the molecular viscosity and the subgrid resolution parameter will therefore nearly always be close to unity. The fundamental problem with methods involving the resolved turbulent kinetic energy is that k_{res} can be higher in an LES solution than the total turbulent kinetic energy from DNS. Whereas one might expect k_{res} to increase as the grid is refined, it has been shown in mixing layers, jets, wakes and channel flows that k_{res} can actually decrease [19, 26]. This implies that the resolved turbulent kinetic energy is not always a reliable indicator of grid resolution. With the exception of the approaches using Richardson extrapolation [19, 26], most grid resolution indices do not account for numerical dissipation which in many situations is of the same order or even larger than the modelled dissipation. Equally, it is not possible to evaluate parameters such as k_{res}/k_{tot} or the subgrid activity parameter for MILES or "no-model" approaches. Turbulence spectra cannot easily be plotted over the entire flow field to produce, for example, contours of grid resolution quality. Furthermore, the slope of the concentration or temperature spectra is modified in buoyant flows and difficulties can be encountered in low Reynolds number flows where a distinct inertial subrange may not exist. Finally, Brandt [9] has shown that multi-grid approaches based on Richardson extrapolation can produce misleading results due to the grid resolution not being within the asymptotic range.

Example Application of Grid Resolution Measures

The flow investigated in this work involves a continuous jet of methane gas released into a ventilated small room. The configuration was previously examined to assess the implications of new hazardous area classification legislation [28]. The main interest in studying this flow is to predict the size of the flammable gas cloud. The room has internal dimensions 4 × 4 × 2.9 m high with two ventilation inlets and two outlets, positioned on opposite walls. A box with dimensions 2 × 1 × 1 m is placed against one wall. The room ventilation rate is 12 air-changes-per-hour and the gas is released in one corner of the room at a rate of 0.86 g/s through a circular nozzle with an open cross-sectional area of 2.5 mm^2.

Four different turbulence treatments are tested: steady RANS, unsteady RANS, SAS and DES. Due to the nature of the high-speed jet flow, LES calculations could not be performed. The steady and unsteady RANS simulations used the SST model [29] combined with a wall treatment that switches smoothly from a low-Reynolds-number model to a wall function near solid surfaces. The DES model was the SST-based version of Strelets [30] without the more recent "delayed-DES" modifications. In the DES calculations, the RANS model was found to be active in the high-speed jet region, in a thin layer immediately adjacent to walls and in a predominantly laminar region on the opposite side of the room from the jet, but the remainder of the room was modelled in LES mode. Both the SAS and DES models used a spatial discretisation scheme that switches from upwind-biased second-order to central differencing in regions where flow unsteadiness is resolved, using a blending function described in Strelets [30]. The filter width in the DES model was equal to the cube-root of the cell volume (i.e. an SGS resolution equal to one). For the steady and unsteady RANS, an upwind-biased second-order convection scheme was used throughout. All calculations were performed using the commercial code ANSYS-CFX11 [31].

To achieve a Courant number of unity or less in the majority of the region modelled by LES, a time-step of 0.1 seconds was used. Time-averaged parameters were typically calculated over a period of 700 seconds. Three computational grids were used: coarse, medium and fine, with 224,000, 412,000 and 660,000 nodes respectively. The grids comprised a mix of tetrahedral cells with prism layers on walls and refinement in regions where there were significant gradients in flow parameters. Further details of the model setup can be found in Gant [32].

To provide an overview of the main flow features, Figure 1 shows the predicted streamlines from a steady RANS simulation. The gas jet is confined within a narrow cavity in one corner of the room where the flow recirculates, giving rise to locally high gas concentrations. The buoyant gas then rises in a plume towards the ceiling.

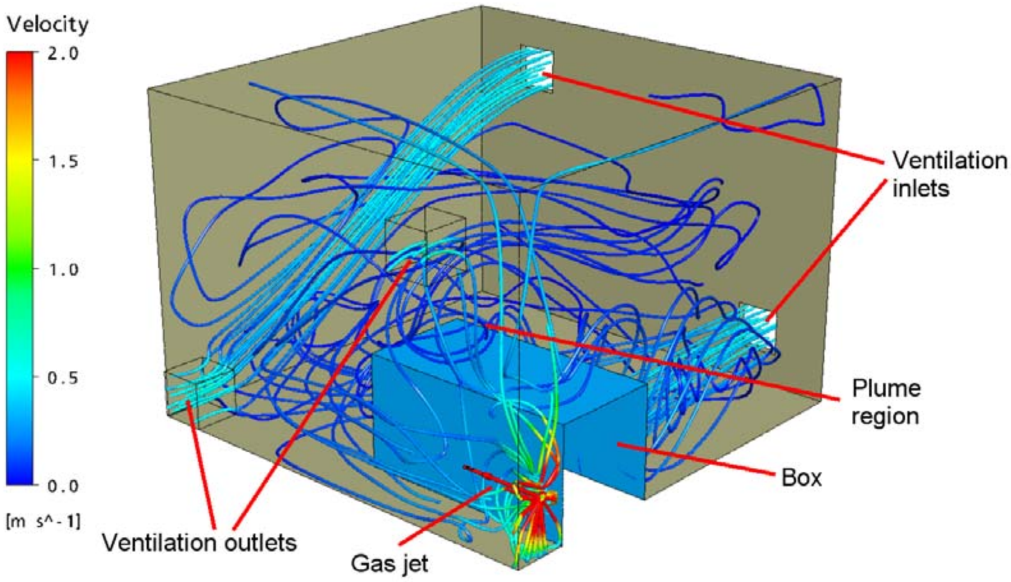

Fig. 1 Streamlines coloured by mean velocity

Figure 2a shows the shows the ratio of the integral turbulence length scale to the cell size, l_I/Δ, for the fine mesh. The ratio is highest above the jet, in the plume region, where it has a maximum value of around 10. Elsewhere in the room the ratio falls to around 5 and in the predominantly laminar regions a value of one or less. The ratios are smaller for the medium and coarse grids, which have values in the plume region of around 6 and 4 respectively. Since it is recommended [13, 14] that l_I/Δ exceed 12 for well-resolved LES, this implies that even the fine grid is relatively coarse in the these simulations.

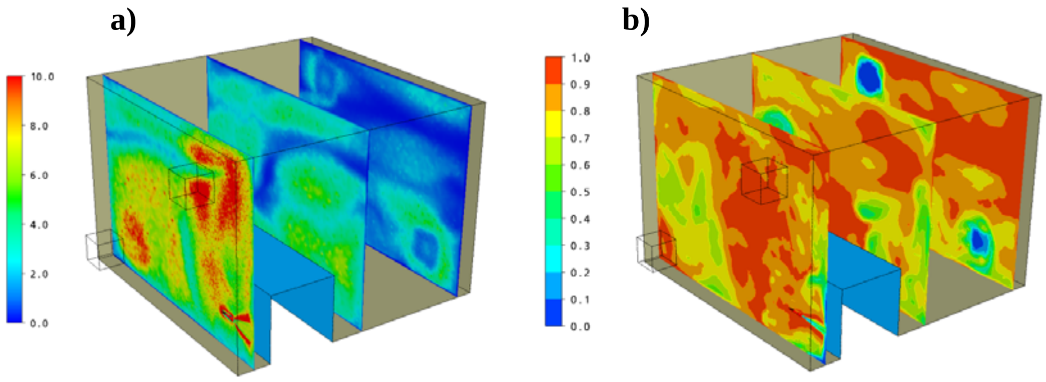

Fig. 2 a) Ratio of the integral length scale to the computational grid cell size calculated using steady RANS on fine grid; **b**) Ratio of resolved to total turbulent kinetic energy for the DES

The ratio of the resolved to the total turbulent kinetic energy is shown for the fine-grid DES in Figure 2b. The total turbulent kinetic energy is calculated from the sum of the resolved and the modelled components. The results show that the DES model resolves 70 – 90 % of the turbulence energy in the majority of the plume region. This might at first be considered to suggest that the grid resolution is reasonable. However, it takes no account of any numerical dissipation. Broadly similar results were obtained for the SAS model.

The ratio of the SGS to the laminar viscosity for the DES model on the fine grid was around 15 – 40 in the plume region above the jet. Given that the turbulent Reynolds number here was around 2000, these values were high compared to the target value of around 20 suggested by Celik et al. [19], indicating the grid is too coarse. In the same region, the viscosity ratio was around 100 – 200 with the SAS model and around 200 – 300 for the URANS and RANS models. Away from the jet and plume regions, in the core of the room, both DES and SAS models had viscosity ratios less than 20.

In the DES calculations, the subgrid activity parameter, s, was close to one throughout most of the room and showed relatively little sensitivity to the grid resolution, which again indicates that all the grids are coarse.

The power spectral density based on the concentration fluctuations in the plume for the DES results showed the spectra decaying at high frequencies faster than the -5/3 power law with no clearly discernible inertial subrange. This appeared to be related to the separation of turbulent length scales being too small for there to be a well-defined inertial range, and the influence of buoyancy effects.

The index of quality, LES_IQ_k, based on Richardson extrapolation of the turbulent kinetic energy between the medium and fine grids produced values generally above 60% in the plume region, although its value fluctuated significantly between neighbouring cells due to the non-smooth distribution of the ratio of cell sizes on the medium and fine grids. Its value was less than the target of at least 80% recommended by Celik et al. [19] for well-resolved LES, indicating that the grids were too coarse. At various points in the flow the LES_IQ_k value either exceeded a value of 100% or became negative. The former problem was linked to the estimated total turbulent kinetic energy becoming negative in certain regions. In other locations, the ratio of the estimated modelled to total turbulent kinetic energy was larger than unity ($k_{mod}/k_{res} > 1$), which gave rise to negative values of LES_IQ_k. The refinements to LES_IQ_k proposed recently by Celik et al. [27] for low and high Reynolds numbers were not tested.

Mean gas concentrations at 14 points in the room were recorded in the experiments [28]. To obtain accurate positioning of the sampling probes, their locations were aligned by laser. Once the flow in the room had reached a steady state, gas samples were pumped into bags over a period of ten minutes and subsequently their concentrations were measured using two photo ionisation detectors, which were checked against a calibrated gas mixture before and after each test. In early experiments using the same room, but with a slightly different gas leak configuration, a repeatability test was undertaken in which the equipment (including all sampling lines and ventilation system) was completely dismantled, then reassembled and the measurements repeated. The average difference between the two sets of measured gas concentrations was 0.05% vol/vol, and the maximum different 0.18 % vol/vol. Other potential sources of experimental error are discussed in the report by Ivings et al. [28].

Figure 3 shows the error between the CFD and the measured values averaged over all the measurement positions. For the fine grid, the DES and SAS results have more than double the error of the URANS or RANS model predictions. The error diminishes as the grid is refined in the RANS results, whereas with the DES and SAS models the reverse trend is produced with the greatest error on the finest grid. For the fine-grid DES model the average error is above 1% vol/vol. This is significant when compared to the lower flammable limit of methane of 4.4 % vol/vol. In relative terms, the error between the CFD and measured values varied from approximately 52% for the medium-grid DES to 35% for the fine-grid steady SST, when averaged over all 14 measurement locations. Further results comparisons are given by Gant [32]. Similarly poor predictions using DES compared to various RANS models for a number of indoor air flows were also recently reported by Zhang et al. [33].

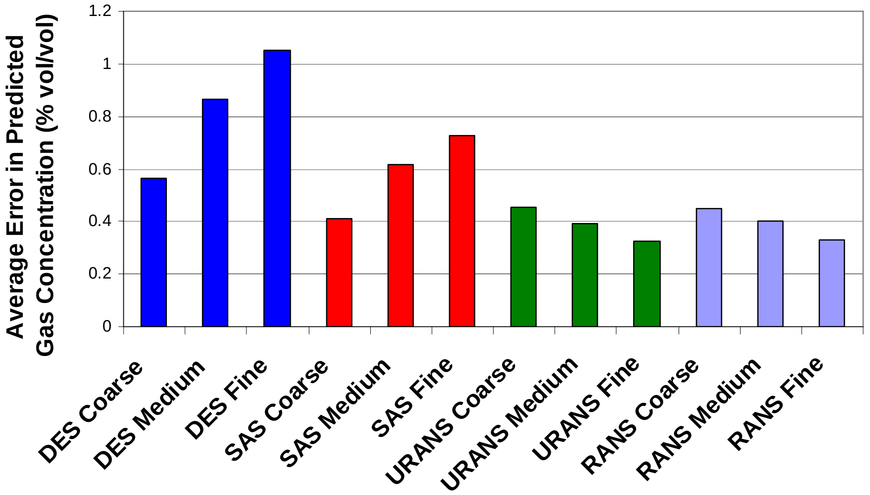

Fig. 3 Average error between the CFD and experimental mean gas concentrations

The predicted gas cloud volumes defined using the Vz criterion [34] are shown in Figure 4. The statistical uncertainty in the predicted mean values is indicated by error bars which show the 95% confidence interval, calculated using a bootstrapping method described by Theunissen et al. [35] with the block length algorithm of Patton et al. [36]. The large temporal fluctuations in the cloud size with the DES and SAS models produce relatively wide confidence intervals, typically around 8%, compared to less than 1% for URANS or RANS.

One of the claimed advantages of the SAS model is that it is less grid-dependent than LES or DES since the model equations do not rely explicitly on the size of the grid cell. However, the results shown in Figure 4 show that the SAS model exhibits the greatest grid sensitivity of the four models tested.

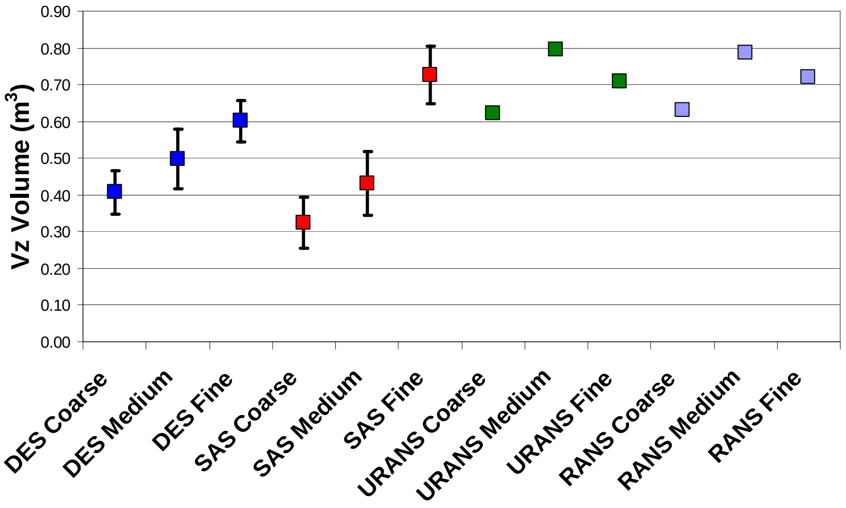

Fig. 4 Mean Vz gas cloud volumes and their 95% confidence intervals

Discussion & Conclusions

A total of ten separate measures to assess the quality of the spatial resolution used in LES have been identified in the literature review. These include approaches based on prior RANS simulations, single-grid estimators involving just one LES calculation, and other approaches involving multiple LES calculations. The advantages and disadvantages of each approach have been documented and references provided for examples of their use.

For the case study involving a gas release in a ventilated room, the various grid quality measures indicated overall that the spatial resolution was marginal for

LES-related models. This perhaps explains why the index of quality, LES_IQ_k, produced inconclusive results in parts of the flow, since the resolution was not in the asymptotic range for Richardson extrapolation. Some of the grid quality measures could not provide useful information in regions of the flow where the turbulence levels were very low or where there was insufficient separation between the large and small turbulence length scales. This was particularly an issue for the RANS-based approaches in laminar regions of the flow and the power spectral density in the plume. The ratio of the modelled to the total turbulent kinetic energy appeared to show that the grid resolution was reasonable, but this was likely to have been overly optimistic, since it did not take account of any numerical dissipation.

The predicted gas concentrations from the DES, SAS, URANS and RANS models were compared to experimental measurements. It was found that the DES and SAS models performed relatively poorly in comparison to RANS and URANS. Contrary to the anticipated behaviour, the DES and SAS predictions deteriorated as the grid was refined. The SAS model also showed the greatest grid sensitivity of the four models tested. The relatively poor behaviour of the DES and SAS models was likely to have been a consequence of using overly coarse grids. To improve the simulations by using finer grids would require significant computing times. The fine-grid DES took 134 CPU-days of computing time whilst the equivalent steady RANS took around 8 CPU-days. The cost of undertaking well-resolved DES or LES should not be underestimated, especially for industrial flows.

Overall, the literature review and case study have indicated that there is currently no universal measure that has been demonstrated to provide wholly reliable estimates of the LES grid quality in complex industrial flows. Although various quality indices provide useful information in some circumstances, none appears to take into account the full range of effects resulting from numerical dissipation, turbulent kinetic energy increasing instead of decreasing with finer grids, grid resolution not being within the asymptotic range for Richardson extrapolation, and regions of the flow that are nearly laminar. Industrial users of LES-related approaches should be aware of the capabilities and limitations of the different resolution indices. Although some measures provide useful information that may assist, for example, in designing LES grids more efficiently, without having to experiment with many different resolutions, confidence that grids are sufficiently well-resolved requires careful assessment of results obtained using different grids, not sole reliance on any single resolution index. A number of promising refinements to the LES Index of Quality (LES_IQ_k) to widen its range of applicability have recently been proposed [27] and these deserve further study. As well as undertaking grid-sensitivity tests, it should also be remembered that additional simulations may be required to assess the sensitivity of the predictions to the turbulence model, the numerical treatment and the boundary conditions to be confident of the quality of the results.

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