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Computational Fluid Dynamics (CFD) modelling of atmospheric dispersion for land-use planning around major hazards sites in Great Britain☆

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ABSTRACT

The Health and Safety Executive (HSE) is the statutory authority in Great Britain responsible for providing public safety advice to planning authorities on the risks associated with proposed new developments (e.g. housing, schools, hospitals) near major hazards sites and major accident hazard pipelines. For those sites where there is the potential for an atmospheric release of toxic or flammable substances, HSE currently uses the integral dispersion model DRIFT to quantify the potential hazard. However, HSE has recently faced pressure from developers to accept results from Computational Fluid Dynamics (CFD) models. A benefit of CFD models is principally that they can take into account the presence of terrain and complex obstructions, whereas integral models such as DRIFT assume flat terrain and account for obstacles as a uniform roughness. However, there are a number of unresolved problems with CFD models that need to be addressed in order for HSE to have confidence in their results for use in Land-Use Planning (LUP) assessments. The purpose of this paper is to discuss the challenges associated with using CFD in this specific regulatory context. The aim is to inform the decision on whether or not to accept the use of CFD modelling and to help prioritise future research activities.

1. Introduction

Over the last fifty years, there have been a number of significant incidents that have reinforced the need for effective planning controls on population growth around industrial sites where there is the potential for major fires, explosions and toxic releases, including Flixborough (Kletz, 2001), Seveso (Fabiano and Reniers, 2017), Bhopal (Havens et al., 2012), Toulouse (Dechy et al., 2004) and Buncefield (Atkinson et al., 2015). As part of the overall framework to manage major accident hazard risks, the Health and Safety Executive (HSE) provides public safety advice to developers and planning authorities on the risks posed by major hazard installations and major accident hazard pipelines. A key part of HSE's public safety advice takes the form of a map of the industrial facility and the surrounding area overlaid with contours showing HSE's "consultation zones", which are usually three in number (inner, middle and outer), graded in terms of hazard or risk (see Fig. 1). Developers and planning authorities are currently able to obtain HSE's public safety advice for proposed new developments which fall within these consultation zones via the HSE web app.[1] Depending on the nature of the proposed development and associated population within these zones, HSE may advise against a development going ahead. The decision to grant planning approval still rests with the planning authority, who take into account many other factors. However, in cases where the planning authority goes against HSE's advice and grants approval, but HSE deems there to be a significant risk to public safety, HSE can request the Secretary of State to call-in the application for their own determination.

The process of developing HSE's three-zone maps involves a number of modelling steps and assumptions. HSE bases its advice on the so-called "residual" risk that unavoidably remains after all reasonably practicable measures have been taken by a major accident hazard operator to comply with the Health and Safety at Work Act 1974 and its relevant statutory provisions, including the Control of Major Accident Hazards (COMAH) Regulations 2015 (HSE, 2015). HSE then makes predictions of the consequences of foreseeable and credible release scenarios from the major hazard site or pipeline. For a typical major hazard installation, such as a medium-sized chemicals facility, this process involves around 700 consequence modelling runs. Where it is beneficial to do so, the calculations take into account the risk, by factoring in the likelihood of an accident. This lengthy process of creating

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[1] http://www.hse.gov.uk/landuseplanning/developers.htm, Accessed 24 November 2017.

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Fig. 1. Illustration of three zone map associated with a major hazards site with coloured inner, middle and outer zones, indicating regions of higher risk, medium risk and lower risk, respectively.

the three-zone maps is undertaken by HSE for around 2000 major hazard installations and approximately 28,000 km of pipelines.

An important part of HSE's calculation process involves using a model to predict the atmospheric dispersion of toxic and/or flammable gas. Currently, the integral model DRIFT (Tickle and Carlisle, 2013; Cruse et al., 2016; Coldrick and Webber, 2017) is used for this purpose, but HSE has recently faced pressure to accept the results from CFD modelling carried out to inform Land-Use Planning (LUP) cases. However, CFD models have a number of unresolved problems that need to be addressed in order for HSE to have confidence in their results. The purpose of this paper is to discuss the problems associated with using CFD in this context. A brief introduction is first provided to the regulatory context in Great Britain.

2. Regulatory context

In Great Britain, the Seveso III Directive[2] has been implemented through the COMAH 2015 regulations (HSE, 2015) with the Land-Use Planning (LUP) requirements implemented through separate planning regulations (HSE, 2017; DCLG, 2015, 2017; SG, 2015; NAW, 2015). To comply with or meet the aims of these regulations, dispersion modelling may be used to inform decision making. However, it may be necessary to adopt different modelling approaches to meet the different requirements of LUP (hazardous substances consent), COMAH safety reports and emergency plans.

HSE's role in the LUP process is to provide independent advice on the risks from major accidents to proposed new developments (e.g. housing, schools, hospitals) in order to enable LUP decision-makers (local planning authorities) to manage population growth around major hazard sites, to mitigate the consequences of a major accident, and comply with Article 13 of the EU Seveso III Directive. Since new developments can take years to be realized, it is important for HSE's advice to be based on a methodology that is consistent in the long term.

The dispersion modelling scenarios considered in HSE's risk assessments for LUP are based on the maximum inventory of hazardous substances that an operator is permitted to have onsite by virtue of their hazardous substances consent. These substances are listed in Schedule 1 of the Planning (Hazardous Substances) Regulations (DCLG, 2015, 2017; SG, 2015; NAW, 2015), and can consist of a combination of both Part 1 generic classes of hazardous substances (i.e. H1 Acute Toxic – Category 1, P2 Flammable Gases, etc.) and Part 2 named hazardous substances (i.e. 10. chlorine, 27. carbonyl dichloride, 29. phosphine, etc.). From day to day, the inventory of hazardous substances on site may change, but by basing the risk assessment on consented maximum quantities, the company has the flexibility to operate within these limits without having to continually seek re-approval from the Hazardous Substances Authority (HSA) or planning authority. This provides a degree of certainty so that the developer can also make plans without having new areas restricted for development part-way through the planning process. Provided that a site operator does not apply to vary the consent, or new science leads to an improved understanding of the hazards or risks, public safety consultation distances defined by HSE will typically remain the same for the duration of the operations on the major hazards site, which can be 20–30 years.

In HSE's dispersion modelling for LUP consultation distances, obstructions such as buildings, fences and hedgerows are factored into the model in a generic way (as a roughness length) rather than by resolving each obstruction individually. Over time, the obstructions may change as buildings are constructed and demolished and seasons change the vegetation, but the generic roughness length should remain broadly the same. One of the reasons for taking this approach is that, from a long term LUP perspective, it is not practicable to monitor all obstructions around all major hazards sites and repeat risk assessments as they change over time. Applying a generic roughness length is straightforward with integral dispersion models, but more complicated with CFD models, which are better suited to resolving individual obstructions and to providing a solution for a particular configuration at a specific point in time.

In dispersion model predictions for LUP, HSE also simplifies the range of weather conditions into four categories. These are based on particular combinations of wind speed and atmospheric stability: D2.4, D4.3, D6.7 and F2.4 (where the letter signifies the Pasquill class and the number signifies the wind speed in metres per second at a reference height of 10 m). The probabilities assigned to each of these categories, and to the wind directions, are determined from analysis of data from weather stations near to the major hazards site, which are provided by the UK Met Office, based on observations over a ten year period. Tests have been undertaken to demonstrate that the risks determined from these four categories are in close agreement with the risks calculated from a full set of weather data, for a range of different release scenarios and locations (Turner et al., 2006). However, in keeping with the need for HSE to provide advice that is consistent in the long term, the weather data used to calculate the public safety consultation distances may remain the same for the period of operations on the major hazards site.

The modelling approach required in COMAH reports is often different from that required for LUP because in the former case the assessment is repeated on a five-year cycle (or sooner if there are significant changes) and it is important that the COMAH assessment represents the most accurate picture of the site as it operates currently. One of the reasons for taking this different approach with COMAH relates to the need to have measures in place to respond to an on-site emergency, which may involve the evacuation of local populations. There can be high costs and risks associated with needlessly evacuating too many people when an incident takes place. Rather than base dispersion modelling on consented maximum quantities, the COMAH safety report and emergency plan should consider credible release scenarios for the *current* scale of operations. The modelling could also take into account the effects of terrain or obstructions, and the best current knowledge of the weather conditions at the particular site, which could involve using data from an on-site weather station.

To summarize, dispersion model predictions for LUP, COMAH safety reports and emergency plans may need to use different approaches, since the decision-making objectives of the modelling in each case is

[2] http://ec.europa.eu/environment/seveso/, Accessed 15 December 2017.

quite different. The remaining part of this paper focuses specifically on dispersion modelling issues related to LUP.

3. Challenges for CFD in assessing major accident hazards for LUP purposes

There are a number of problems with atmospheric dispersion models based on CFD that need to be addressed in order for HSE to have confidence in their use for the assessment of public safety risk in the context of LUP. Some of these issues, such as verification, are common to integral models, but there are specific significant challenges for CFD, which are described below:

3.1. Problems in sustaining realistic atmospheric boundary layers

The popular commercial CFD software packages for assessing major accident hazards (e.g. FLACS, KFX, Fluidyn-Panache) use Reynolds-Averaged Navier-Stokes (RANS) turbulence models and wall functions which are known to have problems in sustaining realistic Atmospheric Boundary Layers (ABLs) along the length of computational domains of 1 km or more (Blocken et al., 2007). Although realistic ABL profiles may be imposed at the inlet to the CFD domain, the turbulence model progressively modifies these profiles until they no longer represent the correct atmospheric stability or wind speed. The problem usually becomes progressively worse with distance downwind. Batt et al. (2016) showed that this could affect the hazard range of dispersing flammable or toxic clouds.

This issue has been recognized for more than a decade and specially tuned RANS models have been developed for ABLs to solve these problems (e.g. Parente et al., 2011). However, there is a compatibility problem because these tuned RANS models were not designed to predict other important phenomena in major accident hazard scenarios, such as jets, wakes and gravity-driven flows. The standard RANS models were originally tuned to produce reasonably good predictions in a range of engineering flows (Pope, 2000) and there are concerns that tuning a model to give better predictions solely in ABLs may worsen the model's performance for other important flows relevant to major accident hazards. Further research in this area would be beneficial.

3.2. Treatment of wind meander

Meander in this context refers to the natural, low frequency, lateral back-and-forth motion of the wind that causes plumes to move from side to side over time. Most integral dispersion models (including DRIFT) take into account the effects of wind meander by making the lateral plume spreading rate a function of the averaging time (Draxler, 1976; Nielsen et al., 2002; TNO, 2005; Tickle and Carlisle, 2013). In contrast, RANS-based CFD models that are used for hazard analysis do not usually account for wind meandering effects, but instead assume that the wind direction and speed remains constant over time. Some CFD studies in the literature have used fluctuating wind conditions to improve the agreement with experimental data in validation studies (Hanna et al., 2004), but there appears to be no widely-accepted generic method for applying these fluctuations in predictive modelling, nor are such methods widely used in practice. However, wind meandering may be important for widening the area affected by the hazardous cloud.

It is important that any approach used to account for meandering effects in a CFD model is used consistently in both validation studies and hazard analysis. Otherwise, it could be interpreted as validating one model, and then using another model in practice.

3.3. Model validation

Validation is critical to demonstrate that a model is fit for purpose. In order to consider model validation fully, the principal flow physics that are likely to influence the release and dispersion behaviour in a major accident hazard should be identified and a literature review should be undertaken to identify the extent to which the model has been validated. This includes consideration of any source models used in the analysis. If there are significant gaps in the model validation then suitable datasets should be identified and a validation exercise be carried out. An example of a structured validation procedure for a specific type of major accident hazard is the model evaluation protocol for Liquefied Natural Gas (LNG) vapour dispersion models developed by Ivings et al. (2013). Ideally, validation should be considered at an early stage in a project, to avoid spending time on a very detailed modelling study only to find that the model is poorly validated.

The judgement as to whether an atmospheric dispersion model is validated is usually made on a statistical basis. There are various different Statistical Performance Measures (SPMs) that assess the scatter and the model bias (i.e. under- or over-prediction). Information on the quantitative acceptance criteria for different SPMs can be found in, for example, Chang and Hanna (2004) and Ivings et al. (2013).

One of the main motivations for using CFD in LUP is to take into account the effect of terrain, which cannot easily be simulated using integral dispersion models. In particular, there is an interest in major accident hazard scenarios involving flows of dense gas over hills. However, the data available to validate models for such scenarios is very limited. Field-scale data comprise the Burro (Koopman et al., 1982), Porton Down (Picknett, 1981) and Jack Rabbit I (Fox and Storwold, 2011; Hanna and Chang, 2013) trials, although each of these has significant limitations (e.g. uncertain source conditions, lack of adequate sensors and availability of the data). There have been useful wind tunnel trials with terrain, including those at Hamburg University for zero wind and neutral stability (Schatzmann et al., 1991) and at Surrey University for a two-dimensional hill (Robins et al., 2016), although there are issues in scaling these results to full scale. Without adequate validation, the accuracy of model predictions is unknown.

3.4. Uncertainty in source models for complex release scenarios

Some of the release scenarios considered in major accident hazards involve complex physics, such as flash-boiling, evaporation of aerosol droplets, and evaporation from pools produced by catastrophic failures of vessels storing pressure- or temperature-liquefied gases. There are various ways in which these sources can be simulated in a CFD model and it remains an open research topic in some areas (Hanna and Chang, 2008; Dixon et al., 2012; Gant et al., 2014; Fiates et al., 2016). Whatever approach is taken needs to be well validated. Similar source modelling issues apply to integral models and generally this is a more mature field of research, with significant efforts having been directed at addressing these issues (e.g. Webber et al., 1992).

3.5. Verification and grid resolution issues

Verification is the process of determining that a computational model accurately represents the underlying mathematical model and its solution (NAFEMS, 2014). For CFD models, verification can be split into two activities (Roache, 1998). “Code verification” is the process of ensuring the CFD software algorithms have been coded correctly, which is largely the responsibility of CFD software vendors. “Calculation verification” is the responsibility of the CFD software user and it involves checking that the model equations are solved accurately in each CFD calculation, which usually requires sensitivity tests to be performed on numerical model input parameters, such as the choice of grid resolution, time-step and (in some cases) particle count.

The computing effort required for a CFD simulation increases with the number of computational grid cells, time-steps and particles. Therefore, there is often a conflict between the need to produce a well-resolved CFD simulation and the need to keep computing times down and costs low. This is particularly an issue for simulating major accident hazards involving complex sources which produce large clouds, where the grid needs to be fine enough to resolve the strong gradients in concentration and velocity near the source, yet the computational domain also needs to extend several kilometres. Grid sensitivity studies are rarely reported when CFD model predictions are presented to HSE, and therefore it is frequently unclear whether or not a grid-independent solution has been achieved.

For certain major accident hazard scenarios involving flows of dense gas over rough surfaces, there are also difficulties in conducting verification tests, due to the treatment of rough walls within RANS models, which places limits on the cell sizes near walls (Batt et al., 2016).

3.6. Variability in model results due to user-effects, model complexity and issues with best practice and regulatory oversight

In a number of studies, dispersion models have been demonstrated to produce very different results for the same scenario. This has been particularly an issue for CFD-based dispersion models. For example, the French Working Group on Atmospheric Dispersion Modelling (Lacome and Truchot, 2013, 2015) ran a joint modelling exercise in 2010 where a number of professional CFD modelling teams from various companies simulated the same major accident scenarios and then compared their results. The predicted hazardous effect distances for a large carbon monoxide release were found to vary by up to an order-of-magnitude for the same scenario (between 100 m and 1 km). Similar overall findings were obtained by Ketzel et al. (2002) who compared five different CFD models for pollutant dispersion within street canyons. Predicted concentrations were found to vary by up to a factor of seven between the different models, despite them all using identical computational grids, inflow profiles, surface roughness and boundary conditions.

The main reason for this significant variability in CFD results is that the models are complex and there is a larger degree of flexibility in how they can be configured, as compared to integral models. CFD models use many different sub-models to account for various effects (turbulence, wall friction, buoyancy etc.) and each sub-model involves various input parameters. Without running a validation exercise, it is often unclear which sub-model or input parameter value is the best one to use. Different CFD modellers may therefore decide to use different options and produce very different results. In addition, care must be taken to avoid errors being produced by the numerical solution method.

It is also possible to take a well-validated model and then use it inappropriately to obtain erroneous predictions. Validation is a necessary step, but on its own it is not sufficient to demonstrate that a CFD model will produce reliable predictions when it is used in practice. To help address this issue, the CFD modelling community has published various best practice guidelines, which cover both general topics and specific applications (Casey and Wintergerste, 2000; Franke et al., 2007; Lacome and Truchot, 2013). It is important to continue support for these efforts.

The high degree of model complexity and its strong influence on CFD results means that it may be necessary to have in-depth regulatory oversight of CFD when it is used to support safety-critical decisions. The regulator could be seen as failing in its duties to ensure public safety if it did not examine the modelling work in detail, which could require access to the CFD software and the input/output files.

3.7. High costs and long computing times

CFD is costly in terms of software licensing fees, computing resources and employment of suitably trained and qualified staff. This can lead to tension between the need to conduct a cost effective CFD modelling study and one that applies the level of rigor appropriate for making safety-critical decisions. The amount of effort required to conduct a rigorous CFD modelling study should not be under-estimated.

3.8. Other sources of uncertainty

In addition to the items mentioned above, there are several other sources of uncertainty in modelling atmospheric dispersion of toxic and flammable gases. A potentially significant issue, raised by Hanna and Chang (2008), is chemical removal processes, such as gravitational settling of droplets and particles, dry deposition of gases, wet deposition through the action of precipitation, chemical reactions and photolysis. These effects have previously been studied for application to air quality models (due to their importance in acid rain, for example) but there have been relatively few studies with sufficiently high concentrations to be relevant for major accident hazards. Significant work is ongoing currently on this topic as a result of the recent Jack Rabbit programme of large-scale chlorine releases (Fox and Storwold, 2011; Fox et al., 2016, 2017). Several experimental studies have recently been published (Hearn et al., 2012, 2014) and laboratory tests are underway at Arkansas University (Spicer et al., 2017). The work is important because modelling studies have suggested that deposition could lead to a significant reduction in the predicted dispersion distances (Hanna and Chang, 2008; McKenna et al., 2017). However, these modelling studies did not account for saturation effects, which could have a significant influence on the hazardous cloud size. In order to account for deposition properly, it may be necessary to consider land-use type, the season, time of day and weather conditions, which are all likely to affect deposition rates. These issues will affect both integral models and CFD. Work is ongoing at HSE to investigate these matters.

3.9. Balancing CFD's drive to highly detailed modelling against uncertainties and variability in the context of LUP

The final problem for CFD models in the context of LUP relates to CFD's drive towards highly detailed modelling balanced against the LUP imperative to accommodate inherent uncertainties and variability. As stated previously in Section 2, in the context of LUP in Great Britain, there is a requirement for HSE to represent the LUP major accident hazard risks over the long term. The representation of this risk is extremely complex. For a site such as a chemical plant, the LUP assessment needs to consider a range of events which represent all potential hazards or risks associated with the storage and processing of both named hazardous substances and generic classes of hazardous substances, along with appropriate event frequencies. The assessment also needs to take into account all possible weather conditions and remain representative over perhaps a 20–30 year period, during which time the plant will age and the surrounding environment will change. Significant assumptions need to be made in calculating the risk to render the problem amenable to analysis. In the LUP context, there will always necessarily remain inherent uncertainties and variability. Within this whole framework, the atmospheric dispersion model sits as just one part of the analysis process.

When it comes to choosing that atmospheric dispersion model, there are a range of different options available, from simple empirical correlations to integral models and CFD. Even within the field of CFD, there are many different options available, from the common RANS models, which typically take a few hours to run, to state-of-the-art Large Eddy Simulation (LES) models that simulate the time-varying motion of turbulent eddies in the atmosphere, which may require days or even weeks of computing time. Progressing through this list of models from empirical to integral to CFD and LES, the complexity and level of input detail required increases. However, in the context of LUP this detail is inherently not available and so the choice of modelling assumptions for the more complex CFD and LES models becomes highly problematic. To compensate for this, considerable additional effort would be needed to investigate the sensitivity of the CFD and LES model predictions to their input conditions. At some point, it is necessary to take a step back and balance the need for highly detailed predictions against the need to accommodate inherent uncertainties and variability in the analysis.

4. Discussion

HSE has to provide LUP advice for around 2000 major hazard sites and 28,000 km of major accident hazard pipelines. To be able to compare risks on an equal basis, it is important to adopt a consistent modelling approach. A single site, such as a medium sized chemicals facility, currently requires around 700 separate DRIFT simulations. To use a CFD model that takes into account the effects of terrain would require an order-of-magnitude increase in the number of simulations, since it would involve a dozen or more separate model runs to simulate dispersion in different wind directions around the 360° compass (which currently only requires one DRIFT run, since DRIFT does not factor in the terrain). Given that each CFD simulation would require an hour or more of computing time, it would be impracticable to compute thousands of CFD runs for every major hazard site, even given foreseen advances in parallel computing. The effort required to collect data, construct models and post-process results would also be disproportionate.

To reduce the number of CFD simulations, it could be possible to identify those sites with significant terrain effects and only simulate just those with CFD, whilst retaining the existing DRIFT model results for “flat” sites. However, this would go against the need for a consistent modelling approach to be used for all sites, and it could lead to challenges from developers, planning authorities and public interest groups to use one or other model that gave them the most favourable outcome. To address this issue and have confidence in the CFD model predictions for LUP, it would be necessary to establish a level of equivalency between the CFD model and DRIFT model predictions. However, experience from model benchmarking studies (Lacome and Truchot, 2013, 2015; Ketzel et al., 2002) suggests that the two models would probably not agree, which could lead to complex ad-hoc adjustments of model results in order to achieve consistency, which would be both scientifically dubious and difficult to implement in practice.

The need for a consistent modelling approach also brings in the CFD issues identified in the previous section. There are research questions that need to be addressed on issues such as correct treatment of ABLs for there to be confidence in using CFD results for LUP applications. Although there has been progress with good practice guides, the problem of different users producing different CFD results for the same scenario has yet to be resolved. A critical issue is the lack of experimental data and the challenges faced in validating CFD dispersion models, particularly for dense-gas dispersion over complex terrain. Progress is to be strongly encouraged in all of these areas.

Whilst HSE currently considers that the integral model DRIFT provides the appropriate and proportionate approach for assessing public safety risk in the context of LUP, HSE recognizes that there is a role for CFD in other areas, such as incident investigations, exploratory studies and certain types of risk assessment. These are all applications where the input conditions are fairly well-defined, where the model physics needs to be adapted to study complex flow behaviour, and/or where there is extensive experimental data available to calibrate or validate the CFD models. These applications differ fundamentally from LUP, where it is necessary to consider the full spectrum of credible accident scenarios across all weather conditions, the scope of the modelling effort is very wide and not tightly focussed, and the modelling methodology must be applied consistently across all sites in the long term.

The above discussion has sought to highlight some of the issues affecting HSE's views on dispersion modelling in LUP, and the issues facing CFD in this context. It is hoped that this will help inform the decision on whether or not to accept the use of CFD modelling and to help prioritise future research activities. HSE is committed to ensuring that its use of models is fit for purpose and based on the best available scientific evidence. It will continue to keep abreast of developments in the field of dispersion modelling, in particular on practical models that can account for the effects of terrain/obstructions and deposition, and the experimental evidence base for validating these models.

5. Conclusions

The use of dispersion models for LUP within the regulatory regime in Great Britain has been briefly described. Problems with using CFD for the assessment of public safety risk in this context have been identified. By understanding the challenges facing the use of CFD, this paper aims to help to inform the decision on whether or not to employ these models. Although the issues raised here are not comprehensive and the work has focused on problems rather than solutions, it is hoped that the discussion will help to shape the direction of future research efforts to address these issues and lead to greater confidence in the use of CFD. Whilst there are clearly challenges to the use of CFD for LUP in Great Britain, it is still regarded as a valuable tool for use in other contexts, such as incident investigations, exploratory studies and certain types of risk assessment.

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