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COMPUTATIONAL FLUID DYNAMICS (CFD) MODELLING OF ATMOSPHERIC DISPERSION FOR LAND-USE PLANNING (LUP) AROUND MAJOR HAZARDS SITES IN THE UK

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Abstract: This work discusses the challenges facing the use of CFD models to simulate the atmospheric dispersion of toxic and flammable substances around major hazards sites and major accident hazard pipelines in the UK, for the purpose of providing public safety advice to planning authorities on the risks associated with proposed new developments (e.g. housing, schools, hospitals). Currently, the Health and Safety Executive (HSE) uses the integral dispersion model DRIFT for this purpose, but it has recently faced pressure from developers to accept results from CFD models, despite several unresolved issues. The perceived benefit of CFD is principally that it 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. This work summarises the regulatory context of Land-Use Planning (LUP) in the UK and identifies various unresolved issues with CFD, with the aim of prioritising future research activities.

Key words: *CFD, land-use planning, major accident hazards, UK, model validation*

INTRODUCTION

There have been a number of significant incidents over the last fifty years that have reinforced the need for effective planning controls on population growth around industrial sites where there is the potential for major fires, explosions or toxic releases (e.g. Flixborough, Seveso, Bhopal, Enschede, Toulouse and Buncefield). 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 surrounding area overlaid with contours showing HSE's "consultation distances", which usually comprise three zones that are graded in terms of risks or hazards. Developers and planning authorities can 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 associated population, HSE may advise against a development going ahead.

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 and its relevant statutory provisions, including the Control of Major Accident Hazards (COMAH) Regulations 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 account of the risk, by factoring in the likelihood of an accident. This lengthy process of creating the three-zone maps is undertaken by HSE for around 2000 major hazard installations and approximately 28,000 km of pipelines.

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[1] http://www.hse.gov.uk/landuseplanning/developers.htm, accessed 5 July 2017

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 is used for this purpose, but HSE has recently faced pressure to take into account results from CFD models. However, CFD models have a number of issues that need to be addressed in order for HSE to have confidence in their results. The purpose of this paper is to discuss these issues with the aim of prioritising future research efforts. A brief introduction is first provided to the UK regulatory context.

UK REGULATORY CONTEXT

In the UK, the Seveso III Directive has been implemented through the COMAH 2015 regulations with the LUP requirements implemented through separate planning regulations. 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 a subtly different approach to modelling in the different contexts 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[2]. 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 scenarios considered in HSE's risk assessments are therefore based on the maximum inventory of hazardous substances that an operator is permitted to have onsite. From day to day, the inventory of hazardous substances onsite 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. 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 to 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. 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 providing a solution for a particular configuration at a specific point in time.

The modelling approach required for COMAH is often different from that in LUP because 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 site as it operates currently. One of the reasons for taking this different approach relates to the need to have measures in place to respond to an on-site emergency, which may well 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[3]. 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. This could involve factoring in the effect of terrain or obstructions.

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[2] http://www.hse.gov.uk/landuseplanning/index.htm, accessed 11 July 2017.

[3] http://www.nbcnews.com/news/other/fukushima-evacuation-has-killed-more-earthquake-tsunami-survey-says-f8C11120007, accessed 7 July 2017.

CHALLENGES FOR CFD IN ASSESSING MAJOR ACCIDENT HAZARDS FOR LUP PURPOSES

There are a number of issues with CFD that need to be addressed to have confidence in the use of CFD for the assessment of public safety risk in the context of LUP. These include:

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 fairly standard 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 at some distance downwind the profiles no longer represent the correct atmospheric stability or wind speed. 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 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 hazard scenarios. Further research in this area would be beneficial.

2. Treatment of wind meandering

CFD models that are used for hazard analysis usually do not 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 match experimental data better 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. It is important to use the same modelling approach in both validation studies and hazard analysis. Otherwise, it could be interpreted as validating one model, and then using another model in practice.

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 be undertaken to identify the extent to which the CFD model and any other source models used in the analysis have been validated for these types of flow physics. If there are significant gaps in the model validation then suitable datasets should be identified and a validation exercise carried out. An example of a structured validation procedure for a specific type of major accident hazard is the model evaluation protocol for LNG vapour dispersion models (Ivings *et al*., 2013).

One of the main motivations for the use of 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 (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[4], although there are issues in scaling these results to full scale. Without adequate validation, the accuracy of model predictions is unknown.

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[4] http://www.ffi.no/no/Forskningen/Avdeling-Beskyttelse/MODITIC/Sider/moditic.aspx, accessed 11 July 2017.

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 and evaporation of aerosol droplets and pools following catastrophic failures of vessels storing pressure-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. Whatever approach is taken needs to be well validated. Similar source modelling issues apply to integral models and, over the years, significant research efforts have been directed at addressing these issues (e.g. Webber *et al*., 1992).

5. Verification and grid resolution issues

In CFD modelling, the verification process can be split into two activities. "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 underlying 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 solution 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.

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).

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

In many different studies, CFD models have been demonstrated to produce very different results for the same scenario. For example, the French Working Group on Atmospheric Dispersion Modelling[5] ran a joint modelling exercise in 2010 where a number of professional CFD modelling teams from various companies performed simulations of the same major accident scenarios and then compared their results. The predicted hazardous effect distances 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 7 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 large degree of flexibility in how they can be configured. 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 and 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.

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[5] http://www.ineris.fr/aida/liste_documents/1/86007/0, accessed 11 July 2017

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.

8. 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.

DISCUSSION

To be able to compare risks on an equal basis, it is important to adopt a consistent modelling approach in UK LUP advice for around 2000 major hazard sites and 28,000 km of major accident hazard pipelines. A single site, such as a medium sized chemicals facility, currently requires around 700 separate DRIFT simulations. To use a CFD model with terrain would require an order-of-magnitude increase in the number of simulations, since it would involve a dozen or more separate model runs for dispersion in different wind directions around the 360 degree compass (which only requires one DRIFT run currently). Given that each CFD simulation would require an hour or more of computing time, to compute thousands of CFD runs for every major hazard site is impracticable, even given foreseen advances in parallel computer processing. 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 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. A solution to this consistency problem could be to conduct a detailed benchmarking study between the CFD model and DRIFT, to ensure that they gave the same results for flat sites. However, experience has shown 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. It would still not overcome the significant problem of the lack of experimental data and the challenges faced in validating CFD dispersion models, particularly for dense-gas dispersion over complex terrain.

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 and calculation verification for there to be confidence in the 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. Progress is to be strongly encouraged in all of these areas.

Finally, there is a question of modelling philosophy. Intricate and costly models like CFD are well suited to incident investigations, exploratory studies and certain types of risk assessment, where the input conditions are fairly well-defined, or where the model physics needs to be adapted to study complex flow behaviour, or where there is extensive experimental field-trial data (such as for fire and explosion models for offshore applications). For LUP advice in the UK, 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. Whilst there are clearly challenges to the use of CFD in LUP, its use may be appropriate in other contexts, where particular hazards may need to be studied in more detail.

CONCLUSIONS

The use of dispersion models for LUP within the UK regulatory regime has been briefly outlined and some issues have been raised with the use of CFD for the assessment of public safety risk in this context.

By understanding the limitations and challenges, this paper aims to help to inform the decision to employ CFD. 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 the UK, it is still a valuable tool for use in other contexts such as incident investigations, exploratory studies and certain types of risk assessment.

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REFERENCES

Batt, R., Gant, S.E., Lacome, J.-M., Truchot, B. and Tucker, H., 2016: CFD modelling of dispersion in neutral and stable atmospheric boundary layers: Results for Prairie Grass and Thorney Island, *17th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (Harmo-17)*, Budapest, Hungary.

Blocken, B., Stathopoulos, T. and Carmeliet, J., 2007: CFD simulation of the atmospheric boundary layer: wall function problems, *Atmos. Environ.* **41**, 238-252.

Casey, M. and Wintergerste, T. (Eds.), 2000: Best Practice Guidelines, *ERCOFTAC Special Interest Group on Quality and Trust in Industrial CFD*, European Research Community on Flow, Turbulence and Combustion, http://www.ercoftac.org (accessed 11 July 2017).

Franke, J., Hellsten, A., Schlünzen, H. and Carissimo, B. (Eds.), 2007: Best practice guideline for the CFD simulation of flows in the urban environment, COST Action 732 on Quality assurance and improvement of microscale meteorological models.

Hanna, S.R. and Chang, J.C., 2013: Chlorine and anhydrous ammonia concentrations observed and simulated in the Jack Rabbit field experiment, for releases of 1 or 2 tons in a 30 to 60 second period, *15th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (Harmo-15)*, Madrid, Spain.

Hanna, S.R., Hansen, O.R. and Dharmavaram, S., 2004: FLACS CFD air quality model performance evaluation with Kit Fox, MUST, Prairie Grass , and EMU observations, *Atmos. Environ.*, **38**, 4675-4687.

Ivings, M.J., Lea, C.J., Webber, D.M., Jagger, S.F. and Coldrick, S., 2013: A protocol for the evaluation of LNG vapour dispersion models, *J. Loss Prev. Proc. Ind.*, **26**(1), 153-163.

Koopman, R.P., Cederwall, R.T., Ermak, D.L., Goldwire, H.C.Jr., Hogan, W.J., McClure, J.W., McCrae, T.G., Morgan, D.L., Rodean, H.C. and Shinn, J.H., 1982: Analysis of Burro series 40 m^3 LNG spill experiments, *J. Haz. Mat.*, **6**, 43-83.

Lacome, J.-M. and Truchot, B., 2013: Harmonization of practices for atmospheric dispersion modelling within the framework of risk assessment", *15th Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (Harmo-15)*, Madrid, Spain.

Ketzel, M., Louka, P., Sahm, P., Guilloteau, E., Sini, J.-F. and Moussiopoulos, N., 2002: Intercomparison of numerical urban dispersion models – Part II: Street canyon in Hannover, Germany, *Water, Air and Soil Pollution: Focus*, **2**, 603-613.

Parente A., Gorle C., van Beeck J., Benocci C., 2011: Improved k-ε model and wall function formulation for the RANS simulation of ABL flows, *J. Wind Eng. Ind. Aerodyn*., **99**, 267-278.

Picknett, R.G., 1981: Dispersion of dense gas puffs released in the atmosphere at ground level., *Atmos. Environ.*, **15**, 509-525.

Schatzmann, M., Marotzke, K. and Donat, J., 1991: Research on continuous and instantaneous heavy gas clouds, Contribution of sub-project EV 4T-0021-D to the final report of the joint CEC-project, University of Hamburg, February 1991.

Webber, D. M., Tickle, G. A., Wren, T and Kukkonen, J., 1992: Mathematical modelling of two-phase release phenomena in hazard analysis, AEA Technology report SRD/HSE R584.