Computational Fluid Dynamics or Gaussian – is there a right way to model gas dispersion?

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At present there are two main approaches to modelling gas dispersion within the process safety risk assessment arena; Gaussian and Computational Fluid Dynamics (CFD). Historically the Gaussian approach has dominated due to additional complexity and required computing power for CFD. However, with the improvement of computing power available in relatively low-cost platforms, CFD has begun to challenge that dominance.

Both approaches rely on a mathematical description of the transport of dispersing gases with the use of advection-diffusion equations. However, the Gaussian approach relies on a number of simplifications required for analytical solutions which aren't needed for CFD. For example, the Gaussian approach often applies simplified flows over flat terrain, whereas CFD accounts for flow velocities and turbulence and their effects on mixing, which can be applied in more complex three-dimensional environments.

Due to the extra complexity of CFD, with many more variables to adjust, its use is often viewed with caution by practitioners and the regulator within the UK, preventing it from becoming more mainstream. However, many of the concerns around CFD are equally applicable to Gaussian, and could be addressed if a standardised set of rules was agreed.

This paper considers the differences between the two mathematical approaches, exploring which method may be more mathematically correct. Then, the current areas of concern for CFD modelling are outlined, with their applicability to both approaches discussed. Finally, a way forward is proposed to allow CFD to be used with confidence in a more mainstream environment in the UK.

Keywords: CFD, modelling, Gaussian, dispersion, risk assessment, emergency planning

Introduction

Within the process industries there is a need to understand risk.

When looking to understand the risk due to a release of flammable or toxic gas, models are required to simulate the dispersion. This then allows the hazard footprint and potential consequences to be understood. This in turn informs decisions on safeguards put in place to detect or respond to such an incident, or where it is acceptable or not to locate people. This also influences the emergency response planning for a site. Big decisions are made on the grounds of the results of these models.

A model looks to simulate reality, but there are many constraints that mean simplifications have to be made. Rather than reality, best representations are made, proportionate to the level of risk that needs to be understood, or the level of investment that needs to be made.

For gas dispersion, Gaussian plume models are common place and have been used for many years. They are well known to be idealised and over simplified but have been the best available for most applications. More recently the opportunity to use Computational Fluid Dynamics (CFD) to look at the physics of the dispersing cloud has become available, as the constraints of time and resource are diminishing, with improving computing power. What was once inaccessible for mainstream risk assessment is now within reach.

The use of CFD for explosion modelling is generally accepted as the appropriate approach within the industry, however this is not the case for dispersion modelling. Following the Piper-Alpha explosion in 1988, the need for CFD-based consequence models for offshore facilities was recognised. In the UK, there was a gradual shift towards the use of CFD in the last three decades as models have become more sophisticated and reliable, with CFD being extensively used for offshore safety studies since 1995 (Roald Hansen, 2013). The use of CFD modelling onshore is only a relatively recent development, even then this is largely for explosions rather than for dispersion modelling. Why is CFD not more widely accepted as appropriate for simulating gas dispersion?

This paper explores the differences between Gaussian plume models and those generated within CFD, presenting the main numerical techniques, and comparing the pros and cons of each. It will look to conclude which is the more mathematically correct approach.

The paper goes on to describe the current use of these models within the field of risk assessment for high hazard process industries. It will highlight the challenges faced by industry and the regulator in the use of these models.

Having set out the concerns associated with the use of models, this paper will culminate with a proposed way forward, informed by the progress made in this area by other countries.

Gaussian Versus CFD

Mathematical Framework and Numerical Solution

Dispersion of gases (pure species, then air and compound mixtures) involves their transport with the mean atmospheric flow (including the coherent flow structures) and mixing in ambient air via turbulent and ultimately molecular diffusion. Both Gaussian and CFD dispersion models attempt to describe and solve such physical processes within a distinct mathematical and numerical framework. For the flow regimes at play, the mass conservation equation in Eulerian form for each dispersed species can be applied as a mathematical framework for dispersion. It reads:

$$\frac{\partial(\rho y_m)}{\partial t} + \nabla\cdot(\rho \boldsymbol{U} y_m) = \nabla\cdot D_m \nabla(y_m) + S_m \tag{1}$$

Where:

- ρ is the density of the gas mixture
- y_m is the mass fraction of species m
- $\boldsymbol{U}$ is the velocity vector
- D_m is the turbulent diffusion coefficient applied to species m
- S_m is the mass source term for species m

This partial differential equation (PDE) for the mass fraction y_m of species m expresses from left to right, the local time variation rate of concentration for species m as the result of the advection of mass by velocity (3 component vector $\boldsymbol{U}$) and mixing with surrounding material under diffusive process with intensity D_m and a potential source input S_m (at leak location). In the above equation all variables (y_m, $\boldsymbol{U}$, D_m, S_m) are both time and space varying. The gas mixture density, ρ, depends on the respective molar masses and fractions of the species. The major difference in Gaussian and CFD approaches for solving this equation is the simplification of the solution for $\boldsymbol{U}$ and D_m in equation (1) above.

In standard Gaussian models, $\boldsymbol{U}$ and D_m are assumed to be constant (in time) and uniform (horizontally) with a single vertical (imposed) variation with altitude (related to atmospheric stratification). This simplification reduces the above equation to a diffusion equation (in a moving reference frame with velocity $\boldsymbol{U}$). An analytical solution for a Dirac delta source (in space and time) can be expressed with a Gaussian law function of shifted position ($r + \boldsymbol{U}t$) for the cloud centre, as for a diffusion process in a random motion/Brownian motion. The cloud from such a source is a Gaussian plume with centre line and transverse profiles of concentration showing symmetric Gaussian shapes with spreading size, as determined from turbulent intensity estimates in empirical law. The assumptions made here for $\boldsymbol{U}$ and D_m are not a true reflection of what is observed in real world applications where there are terrain undulations (hills, cliffs) and obstacles (buildings, processes etc.).

Furthermore, many leak-related dynamical processes operate at short range from the source. Examples are the inertia and momentum from the release (high speed jet flow, explosive release), and the density of the release with either heavier (downward buoyancy) or lighter (or hotter) than air (for positive buoyancy). Therefore, the initial time step (and short range) sequences of dispersion for Gaussian models are often modified with other models termed as integral models: analytical jets or creeping behaviour, with empirical air entrainment rates and heat exchanges.

Again, these integral models are unable to account for the presence of obstacles, heat sources, or varied drag and turbulence coupling effects that exist on industrial sites.

A CFD approach on the other hand solves the full advection diffusion equation (ADE) (equation (1)) along with the relevant fluid mechanic equations (Navier-Stokes (N-S) Equations) for the atmospheric flow and the turbulence. The extended set of equations are again conservation equations for momentum, total mass, energy (or enthalpy) and turbulence closure intensities and dissipation rate.

Momentum conservation equation:

$$\frac{\partial(\rho \boldsymbol{U})}{\partial t} + \nabla\cdot(\rho \boldsymbol{U}\boldsymbol{U}) = \nabla\cdot\ \tau - \nabla \mathrm{p} + S_U \tag{2}$$

Total mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho \boldsymbol{U}) = S_\rho \tag{3}$$

Energy Conservation equations:

$$Cp\left[\frac{\partial(\rho T)}{\partial t} + \nabla\cdot(\rho \boldsymbol{U} T)\right] = -\nabla\cdot\ q + \left[\frac{\partial p}{\partial t} + \boldsymbol{U}\cdot\nabla p\right] + \tau\colon \nabla \boldsymbol{U} + S_T \tag{4}$$

Where:

- τ is the viscosity tensor related to molecular then turbulent viscosity

- p is the pressure
- T is the fluid mixture temperature
- S_U, S_ρ, S_T are the local source terms for res. momentum, mass and heat.

These equations are universal fundamental equations (derived from 1st and 2nd principles) for the atmospheric flows and so can be applied to any industrial site with various terrain features such as vegetation cover, hills, buildings, process units, storage tanks. The numerical solutions of the Navier-Stokes PDE equations provide the time and space variations of all necessary scalar and vector fields to be applied to the advection dispersion equation (1).

In the above PDEs (equations (1), (2), (3) and (4)), the thermodynamic state for the gas mixture is enforced with perfect gas laws $f(p, \rho, T, y_m)$. For a CFD solution, a series of steps need to be carried out:

- Design a numerical simulation domain encompassing the environment and the industrial site with a 3D set-up for all above mentioned features that may perturb the flow and produce enhanced turbulence.
- Build a discrete approximate version of the above continuous set of equations (numerical discretisation on a mesh).
- Set-up the boundary conditions on the lateral faces of the domain for the selected meteorological scenario and at the source location of the leak.
- Solve the time and space discrete set of coupled equations for flow (u, v, w, p, T, r) and transport (y_m) for the species.

In the CFD solution, the major physical processes at play that are approximated (empirically) in Gaussian models are explicitly solved in the method, resulting in complex non-homogeneous 3D flows and dispersion patterns. Gravity effects (for heavy/light gases) are explicit in S_U for the external forces in momentum equations, pressure build-up in front of obstacles and pressure drop in the lee of buildings, and flow acceleration (corridors). In the discrete version of the Reynolds Average Navier-Stokes (RANS) equations (the standard method for capturing the large scale energy dominant flow structures in leak dispersion applications), a practical limitation on mesh size is applied, so small scale motions are below the grid scale. In solving for k (the turbulent kinetic energy) and eps (its dissipation rate), two specific PDE equations for turbulent fields are added. Both k and eps are local (time and space varying) scalar fields, explicitly solved to account for turbulence enhancement/dissipation via mechanical (shear) or thermal production. The diffusivity scalar D_m in dispersion equation (1) is estimated from k and eps fields. Thereby, it is neither empirically derived nor uniform in xy-space and time but rather derived from the turbulence fields.

The fluidyn™-PANACHE CFD model includes a dedicated 'NT' solver. The NT solver is a pressure-based fully implicit segregated method on meshes that solves all governing equations separately and uses an iterative method for both steady state and transient cases. To couple the pressure and momentum equations in the numerical computation, the Semi-Implicit Method for Pressure Linked Equations-Consistent (SIMPLEC or SIMPLE-Consistent) algorithm (Van Doormaal, 1984) is utilised. The buoyancy model is used to parameterise the body force term in the N-S equations. Dispersion of the gaseous pollutants is modelled by solving the standard Eulerian advection-diffusion equation in a computational domain. Residuals on each field (and related discrete equations) are used to check the convergence of the solution during the simulation.

Consequence modelling is generally carried out to predict a potential hazard, or to simulate a hazard following a release, so that the potential impact can be understood. The fundamental aim of dispersion modelling is to simulate and understand the behaviour of a gas as it is released into the atmosphere. CFD modelling gives a more realistic representation of real life results of gas dispersion, by taking into account features such as buildings, process plant, terrain, etc.

As shown above, the CFD methodology is more mathematically correct, solving the full advection diffusion equation (1) coupled with momentum, mass and enthalpy equations (2), (3) and (4), thereby with less simplification than the Gaussian approach. However, in the past such methods were not as easily accessible as they are now, due to limitations in technology and available computing power. In the past hand calculations and broad assumptions were needed to simulate dispersion, however advancements in technology and easier access to higher computing power mean that such simplification is no longer required. Moving from hand calculations, to Gaussian style models and on to CFD modelling is a natural progression of methods as technology advances; the use of CFD is an evolution not a revolution.

Case Studies for Dispersion

To demonstrate the results of the different mathematical equations used for the CFD and Gaussian approaches for cloud dispersion, a number of case studies are presented below. For each case, the CFD solution was modelled in fluidyn™-PANACHE dedicated software for atmospheric flows and dispersion at local meteorological scale (domains order of 10 km size) and time scales of the order of minutes to hours. Results for a Gaussian approach were modelled in the DNV GL Phast software (version 7.22), using source terms matching those of the CFD modelling and standard model defaults.

The following case studies are shown and analysed. They have been selected from real sites considering the potential effects of theoretical releases, to span various flow and leak release situations:

- Case Study 1 Chlorine Release from Pipe Manifold: a very large industrial platform in Belgium
- Case Study 2 Chlorine Release from a pipe: complex natural topography in the Alps valley, small industrial site
- Case Study 3 Acrylonitrile loss of containment: quasi flat terrain but very complex, congested industrial site

Case Study 1: Chlorine Release from Pipe Manifold

The first case study is for a major hazards site storing and handling chlorine. The study considered an accidental release from a pipe manifold, in a central position on the plant. Key features included a complex series of obstacles within the site itself and a patchwork of surrounding surface types i.e. open flat vegetation vs residential zones, as shown in Figure 1 below.

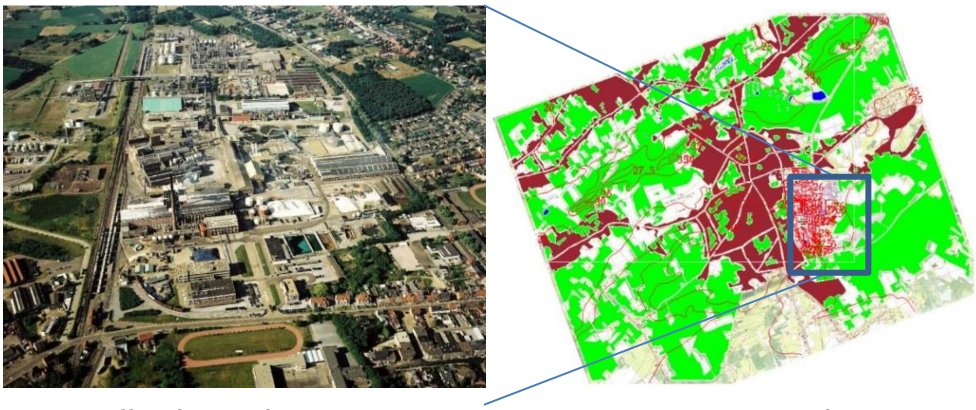

Figure 1: Onsite and offsite features for the accidental dispersion modelling, aerial view (left) and environment and 3D set-up for CFD Solution (right)

A 3D representation was made and the atmospheric flows established. Following this, dispersion modelling was carried out using the CFD approach. The results of this modelling are shown in Figure 2 below.

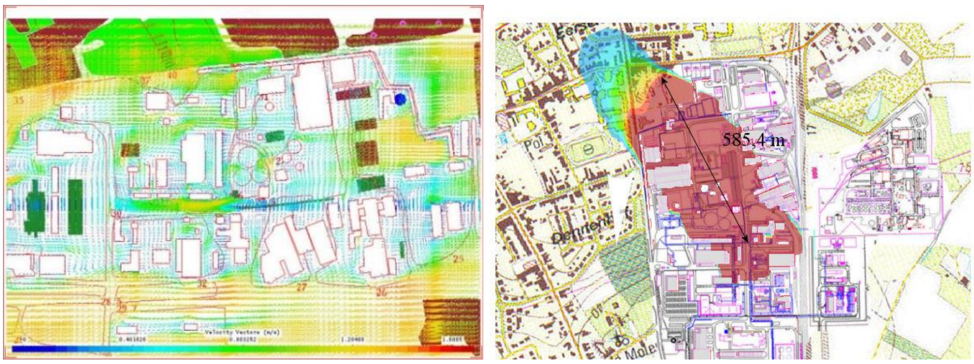

Figure 2: CFD results for a consequence/risk analysis for flow velocities vectors (left) and for toxicity map (right), ground level effects.

For comparison, as described above, the same dispersion was performed in a Gaussian (and integral) model (DNV GL Phast). This was compared against the results of the CFD model by overlaying the two on a map, as shown in Figure 3 below. It shows the results from the Gaussian model in the black contour, this model gives a smooth and idealised plume, compared to the red contours from the CFD model which show patches and pockets due to the complexity in the atmospheric flow. This is due to turbulent diffusion as induced by obstacles, flow shear and cloud splitting. In this case, the 1% lethal effect is shown in orange for the CFD model and the black contour for the Gaussian model, it can be seen that the effects of the lethal footprint are quite different.

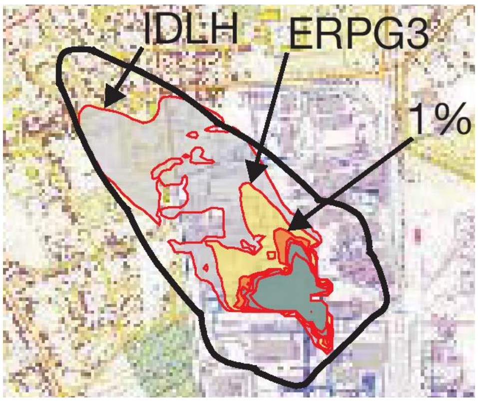

Figure 3: Comparison case between Gaussian model (black thick contour for Lethal effect 1%) and CFD model (red curves for varied thresholds).

The results of the two models, if looked at in isolation, would result in a different understanding of the risk from a toxic release and which would justify different levels of investment to mitigate such an incident. In this particular case study, the hazard footprint is reduced by CFD modelling, but there are many examples where this can result in further reaching hazards.

In this particular case, the release is directed downwards from an elevated pipe, within a fully packed unit. The initial large transverse dimension of the 1% contour from the Integral Gaussian model is produced by the collapsing and creeping flow model for heavy gases. The elongated shape then is the Gaussian dispersion.

On the other hand, the patterns for dispersion is much more complex in the CFD solution due to the detailed flow patterns and the enhanced turbulence as induced by the process units and in buildings wakes.

Both the close range mixing at leak source and the longer range complex paths taken by the fluid and transported chlorine explain the significant differences between results from the models.

Case Study 2: Chlorine Dispersion from Hole in Pipe

The second case study is for a site located in a very complex terrain in the Alps. The atmospheric flow over the domain is strongly impacted by top crest accelerations, changes in direction and low winds in the valleys, but it still shows strong mechanical turbulence in the Atmospheric Boundary Layer (ABL). The study considered an accidental release of chlorine from a hole in a pipe located on a moderately extended industrial site, with tall buildings in the vicinity of the release. Key features included a number of buildings within a close field, as shown in Figure 4 below.

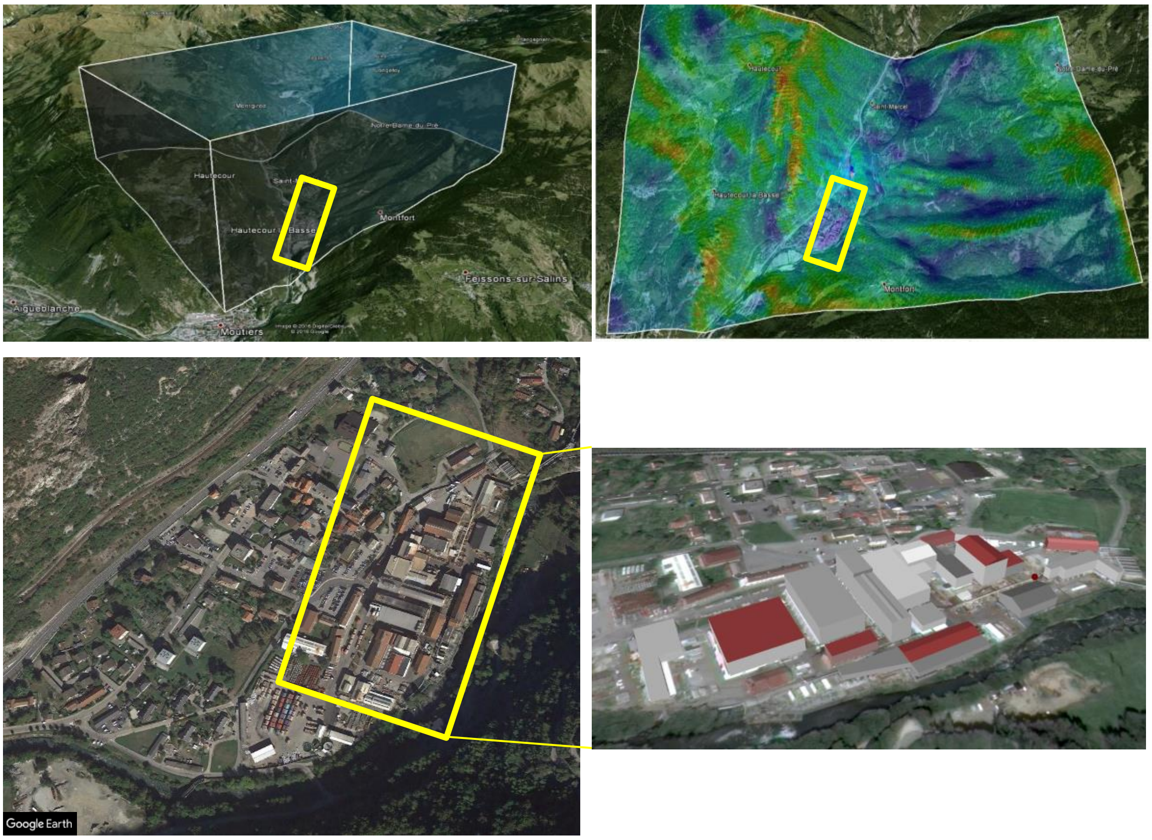

Figure 4: Features for Case 2 dispersion modelling - Terrain (top left) and surface flow from CFD (top right), site aerial view (bottom left) and local 3D set-up for CFD solution (bottom right).

As for case 1 above, a 3D representation was made and dispersion modelling carried out using CFD, with the same case modelled using a Gaussian approach. This was compared against the results of the CFD model by comparing the two footprint maps side by side, as shown in Figure 5 below. The red contours correspond to a toxic dose equivalent to 1% lethality, whilst the yellow contours correspond to the toxic dose threshold of irreversible effects. The release point is shown as a red dot on the CFD images, and a yellow dot on the Gaussian images.

One important point to note is that for each direction considered in CFD, the flow is significantly diverted on the site with strong stagnation areas, due to the surrounding obstacles. Therefore, the CFD contours shown are for multiple directions (135°N, 225 N, 315°N) and both F3 and D5 wind class results combined. For Phast, the results from the worst case weather condition (F3 weather) are shown, in a direction of 225°N.

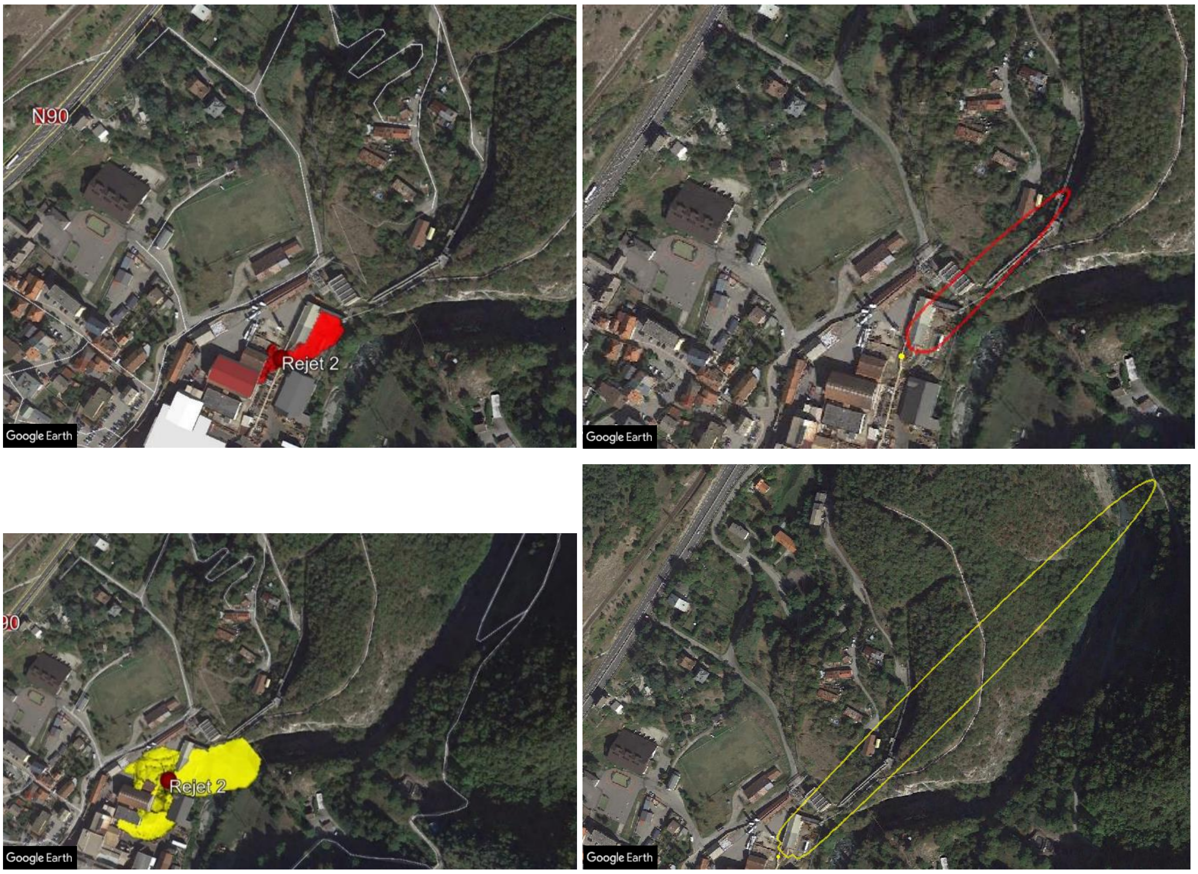

Figure 5: Case 2 dispersion modelling results, CFD multi-direction envelop (left) and Gaussian ground level effects for F3 and 225°N meteorological condition (right).

The results show that the Gaussian model predicts much further reaching hazard contours than the CFD model. This is likely because the Gaussian model assumes a flat terrain with no obstacles: the plume goes through the first building encountered (L shape North East of the leak) and straight up the hill. The CFD model takes into account the local flow deviations caused by the topography and buildings (for all weather conditions and wind directions), along with the enhanced turbulence impact on the dispersion of the gas.

Case Study 3: Acrylonitrile Dispersion from Pool

The third case study is for a large industrial site on a relatively flat terrain. The distances between units and buildings are quite large and the expected behaviour for the plume is long range impact. The study considered the dispersion of acrylonitrile from a pool formed from an accidental release, with a pool area of approx. 670 m^2 and a low dispersion rate from the pool. Key features included a complex series of obstacles within the site itself and a patchwork of surrounding surface types i.e. vegetation vs residential zones, as shown in Figure 6 below.

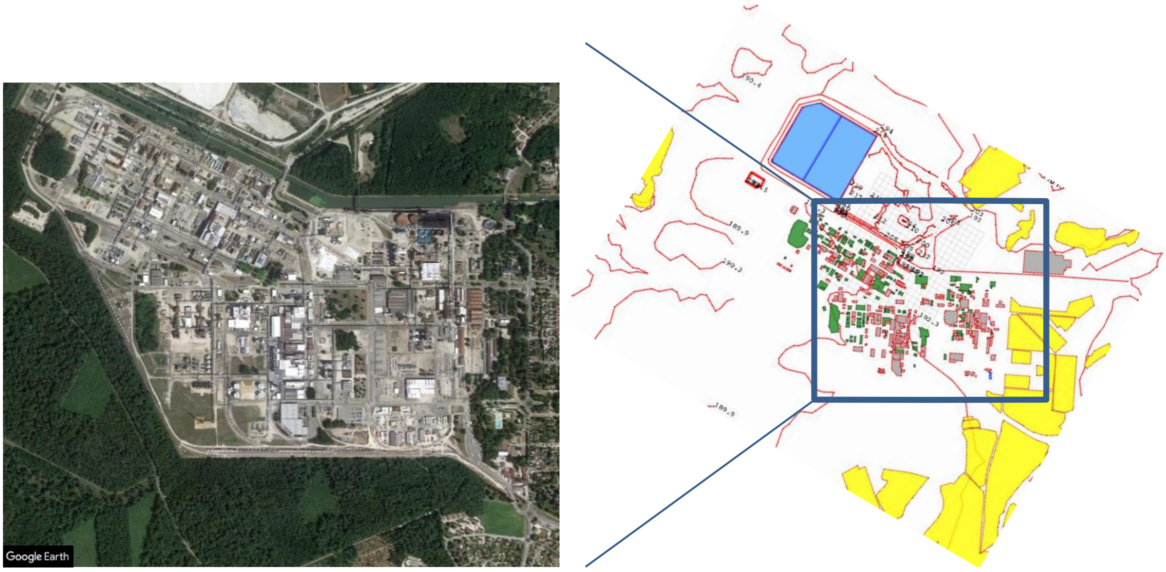

Figure 6: Onsite and offsite features for Case 3 dispersion modelling, aerial view (left) and environment and 3D set-up for CFD Solution (right)

Again, as for case 1 and 2 above, a 3D representation was made and dispersion modelling carried out using CFD, with the same case modelled using a Gaussian approach. This was compared against the results of the CFD model by comparing the two footprint maps side by side, as shown in Figure 7 below. The red contours correspond to a toxic dose equivalent to 1% lethality, whilst the yellow contours correspond to the toxic dose threshold of irreversible effects. The release point is shown as a red dot on the CFD image and a yellow dot on the Gaussian image.

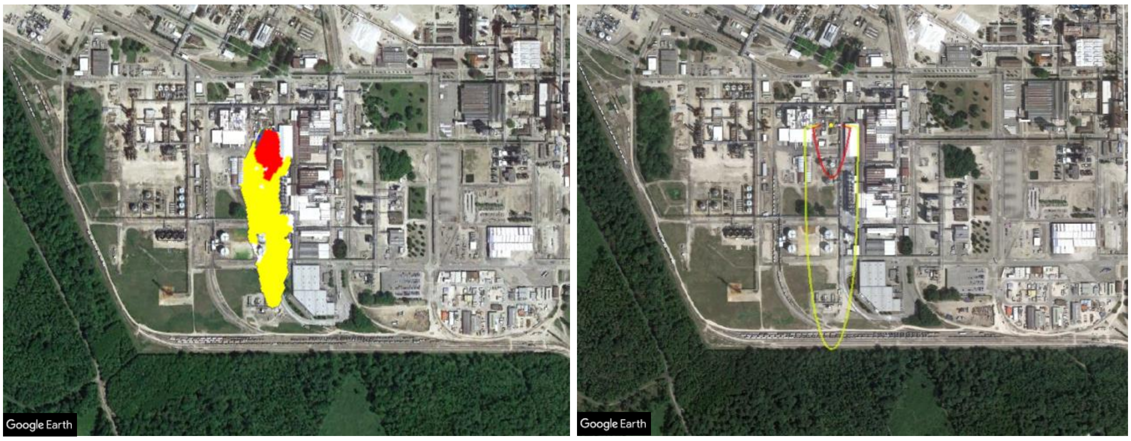

Figure 7: Case 3 dispersion modelling results, CFD (left) and Gaussian (right), ground level effects.

Here, the results from the CFD and Gaussian models are similar, with the red contours akin and the yellow contour travelling slightly further for the Gaussian results. In this case the results are similar because in the wind direction considered the plant is relatively open with sparse obstacles upstream, few blocking obstacles in the near vicinity and downstream and a relatively flat topography. Furthermore, the typical sizes of the obstacles encountered downstream are not disrupting the path nor the spreading of the gas plume, resulting in an initial large dimension for the source and a long plume. In such a situation a Gaussian model can produce a good prediction of real life effects from this scenario.

Current Position

CFD is not currently adopted in the mainstream of risk assessment for high hazard sites. Practitioners have been deterred by the complexity and cost, and the regulator is wary that CFD can open up opportunities for error. There are many more variables that can be manipulated, judged incorrectly, or set in error. But are these concerns real, or are we just more comfortable on the well-trodden path? If we stepped back and looked at the simplified methods as a modern technique today, would we accept them as best practice? – Think about the special effects in an old film, if we looked at them now would they stand up to today's standards given all of the technological advances?

Over the years, practices in all aspects of process safety have moved on and improved, following knowledge and experience gained. Examples include changes around how we manage the risk to occupied buildings following incidents such as Flixborough and Hickson and Welsh, changes in our approach to leadership and safety culture following Buncefield, improved knowledge in chemicals influencing how we handle and store them. In all of these cases, we wouldn't go back to how we did things before given what we know now. Why not make a similar move ahead when it comes to dispersion modelling; as discussed earlier the natural progression of methods is moving from hand calculations, to Gaussian style models and on to CFD modelling.

In the UK, the Health and Safety Executive (HSE) has a number of concerns with the wide spread use of CFD largely due to the variability which often arises between CFD results. CFD is well suited to models of highly complex situations by providing flexibility across a range of parameters, however, this also leads to a greater scope for error with reliance placed upon the competence of the user. Between different CFD models for the same scenario there can be large differences in the results produced. A recent paper on the subject by members of the HSE has reported that the differences can be of an order of magnitude (Gant, 2018). However, there is also a large variation within the field of risk assessment, due to variations in data sources and assumptions, so variation of an order of magnitude from different approaches is not uncommon. Furthermore, separate users of the same model may produce divergent results, due to level of experience with the programme or a lack of understanding of the mathematic principles behind the code.

This section will go on to discuss the following key areas of concern in further detail for both Gaussian and CFD.

Lack of Conformity Between Models

The first area of concern raised for CFD is a lack of conformity between models, in particular the potential for large variations in results between different models for the same case. Numerous literature studies suggest that there is a large inconsistency between results from different models, however this may be impacted by some of the other areas of concern raised for CFD. Further, there is little evidence of this kind of comparison for Gaussian models; there may be a similar level of inconsistency between models, but this is not studied with the same amount of scrutiny as CFD.

Flexibility of Parameters

The second area of concern for CFD modelling is the flexibility in choice of parameters available to the user. Since CFD is a more complex model than Gaussian, there are a larger number of parameters which can be amended by the software user. If users are free to set parameters, without any guidance or rules, this allows a variation in parameter selection for different users, which could lead to a large fluctuation in results.

In the Gaussian approach, simplifications made reduce the number of parameters that are available to be set by the user. Many of these parameters are pre-set in the software as a default, but users may still be able to amend them, which can impact on the output results from the model. Further, representative parameters that are pre-set by software, such as the parameters to represent the Pasquill stability classes, varies across commonly used Gaussian models, which could also cause variation in results from Gaussian models.

Software User Competence

The third area of concern for CFD modelling is software user competence.

For CFD, as the method is complex, software user interfaces are often similarly complex, with a lot of interaction required to set up and run a modelling case. Inputs are a very deliberate action. Therefore, it is unlikely to be used by analysts that do not have an understanding for the development of the model and how it works.

Gaussian models often have more user-friendly interfaces, which means an inexperienced user can feel more at ease and confident in handling the software. However, this means that the software is more susceptible to being misused; this ease of use means a user may amend data without fully understanding the ramifications if these don’t make sense within the mathematics or are outside of the limits of the model.

Competence is fundamental for the use of any modelling software; users should not operate and use results from modelling software unless they are competent to do so. Users should be trained on the software, not allowed to blindly use it without guidance; this may be through the use of user manual, or via facilitated training. Sanity checks on user inputs and outputs should also be carried out. Further, users should understand the limitations and methods of the software they use, as misuse of these could give invalid results. The competence of the user for both modelling approaches is key to ensuring results can be trusted and used within a risk assessment.

Validation and Verification

The fourth area of concern for CFD modelling is the validation and verification of the software.

For CFD models there has been a large amount of effort put into validation and verification. However, the level of effort varies between the software providers and this is not always clear, especially as not all providers are forthcoming with the supporting evidence, preferring to keep this internal.

Similarly, effort is also put into validation and verification for Gaussian methods. Again, showing supporting evidence varies depending on the provider. In addition, validation for these models is often for a narrow area of use. However, the models are often used beyond the limits of this validation, without understanding the implication this may have on the reliability of the results; this is closely linked to the user competence concern raised above.

Experiments for Comparison

The final area of concern for CFD modelling discussed here is the use of experiments for comparison against the model results.

There are few large scale experiments that have been carried out to allow comparison to modelling results for CFD. This is no different to experimental results for comparison to Gaussian models, however this is not generally raised as a concern in regards to using Gaussian models.

Summary

The table below summarises the findings of the exploration of each of the above areas of concern for Gaussian and CFD models, to compare their relevance.

Table 1: Summary of areas of concern and their relevance to Gaussian and CFD models

Area of Concern	Relevant to Gaussian models	Relevant to CFD models
Lack of conformity between models	Little evidence of comparisons	Literature studies suggest large inconsistency
Flexibility of parameters	Simplification may be made to reduce the choice for users, but there are differences between the representative parameters. E.g. representation of Pasquill stability classes varies between commonly used models	Flexibility in choice of parameters, if not set by rules
Software user competence	Often user-friendly interfaces, but can be misused as user can be given false sense of ease of use without understanding limitations or mathematics of the model	Often user interface is complex, so unlikely to be used by analysts that do not appreciate the development of the model
Lack of validation and verification	Validation is often for narrow area of use, however the models are used beyond this	Large amount of effort in validation and verification, however this varies between model providers, in particular in how forthcoming they are with evidence
Few large scale experiments to compare with models	Same experiments available for all models	

As summarised here, many of the challenges facing the use of CFD are not new or specific to its use but are instead universal challenges for any form of modelling. The question is, why is the use of CFD challenged in these areas, but Gaussian methods are accepted in spite of this?

Looking for a better way

Validation and Verification

Efforts have been made to improve the convergence between CFD modelling results from different models. These include the publication of best practice guidelines which assign the validation and verification requirements for CFD models.

A number of best practice guidelines have been produced. In the United States a number of guidelines for CFD modelling are in place. Notable amongst these is an American Society of Mechanical Engineers (ASME) standard for the verification and validation of CFD modelling, though this is heat transfer focused (ASME, 2009). Other examples of international guidelines include the Guidelines for Nuclear Safety Evaluation Defined by the Atomic Energy Society of Japan (AESJ) which were created to utilise CFD models for dispersion calculations for nuclear safety evaluation of radiation dose. The guidelines incorporate a verification and validation scheme using experimental data and dictates that all final calculated results are to be modified using an uncertainty factor as suggested in the ASME code.

Recent efforts have been made in the EU, through projects such as SAPHEDRA to evaluate the way forward for risk consequence modelling, particularly in relation to gas dispersion (HSE, 2017). This highlights the benefits and flexibility that CFD modelling can provide, but also the perceived challenges. Due to the need for consistency between modelling at different sites, or even different users modelling the same scenario, certain parameters must be controlled. The use of CFD is advised for more challenging or complex situations but not as a generic tool, despite the greater accuracy and detail of the modelling.

In the UK the HSE endorses the production of such guidelines, in order to improve conformity in CFD modelling outcomes (Gant, 2018). They have presented on the topic at various conferences, but they have not issued formal guidance. There are a large number of guidelines, but there is currently no single point of reference for what good looks like for anyone to apply in the UK.

Rules for Modelling

As well as seeking to find common ground on the approach to validation and verification, some good practice is emerging on how to use models.

The Atmospheric Dispersion Modelling Liaison Committee (ADMLC) recently updated guidelines for short range dispersion modelling of releases to atmosphere from industrial sources. The original guidelines were introduced in 1995 and ADMLC believed that modelling techniques have evolved sufficiently to require additional advice (ADMLC, 2004). These guidelines are generic, and apply to all forms of dispersion modelling, acting as a universal guide to ensure regulatory conformity.

Notably, the National Agency for Finite Element Methods & Standards (NAFEMS) has a CFD working group, which includes members from industry, academics and consultants. This group has produced 'How to guides' with CFD best practice guidelines, but these are only made available to members.

A French working group, created in 2009 at the request of the French Ministry of Ecology, Energy, Sustainable Development and Spatial Planning, investigated gas dispersion modelling for land use planning near high hazard industries. By first assigning the same modelling task to separate modelling groups the study identified variables between the models and investigated methods of regulating certain parameters. The outcome of this work was a definition of best practice for the use for 3D modelling of atmospheric dispersion. This included guidelines for validation and also specific parameters within the modelling relating to mesh, boundary conditions, the definition of a source term and the modelling of turbulence (San Jose, 2013). There have been a number of other working group studies relating to CFD, but few in relation to atmospheric dispersion and particularly in relation to high hazard industries. Hence, the outcomes of this group were particularly relevant for our consideration. The work of this group is not yet widely adopted and, other than a summary, has not been translated from French.

Clearly there is a common agreement that a set of guidelines for CFD modelling is needed, so that all modelling is based on the same core principles. There are a number of industry standards available for using CFD to model explosions, including NORSOK Z-013 (NORSOK, 2010) and ISO 19901-3:2014 (ISO, 2014), but no equivalent for gas dispersion. There is currently no accepted rule set adopted as best practice within the UK. This leaves too much choice in how to represent situations which will introduce variance in the solutions provided by different modellers and uncertainty with the regulator.

The Way Forward

In order to understand and manage risk from high hazard industries it is important that we continuously improve and embrace new technologies to move us forward in our knowledge and understanding. Now that CFD is more accessible in terms of computing power and affordability, it is only concerns around application that hinders its application.

It is clear that when looking to understand a complex situation, oversimplification will not be helpful. But we should also recognise that trying to simulate everything may be unnecessary. What we need is a middle ground. An agreement of where extra sophistication is needed or not. For simple cases where the terrain is generally flat and surrounding features are minimal, Gaussian and CFD results are likely to be very similar. Here, a Gaussian approach is considered more appropriate as the modelling process would be quicker and more cost effective. For highly complex cases, with complicated features, a CFD approach would clearly be best, as the simplifications in the Gaussian approach would be unable to replicate the real-life dispersion accurately. Here, the Gaussian model could under or over estimate the effects of a major hazard, so further work based on these results, such as emergency response planning, may be incorrect. It is for the area in between simple and complex where the use of the models is not as clear cut. Selection of an appropriate model should be based on a number of factors:

- **What is the purpose of the modelling?**
    - The intended purpose of the modelling may influence which type of model is most appropriate. Modelling may be intended for use in areas such as risk assessment, emergency planning, designing inherently safe plant, land use planning. Each of these may require a different level of detail and accuracy, consideration of which would influence whether a simpler Gaussian model is most appropriate or whether a more complex CFD model should be used.
- **What level of understanding is required?**
    - If a basic or high level of understanding of the behaviour or outcome is required, the more simplistic Gaussian approach may be more applicable.
    - If initial modelling using the Gaussian approach suggests that in fact further understanding is required, then CFD would be the more appropriate approach.
    - The level of risk at a site may influence the level of understanding required; a higher risk site is likely to require a more in depth understanding of the hazards than a low risk site.
- **What is in the vicinity of the release?**
    - If there are a number of vulnerable populations or environmental receptors in the vicinity of the release, the more complex CFD approach may be more appropriate to fully understand the behaviour of the release and the potential impact to people and the environment.
    - If there are obstacles in the vicinity of the release (such as equipment, buildings, vegetation etc) that could impact the behaviour of the dispersion, CFD may be more appropriate. The more obstacles there are, the more applicable CFD is to fully understand the impact these obstacles would have on the release – they could limit or in fact extend the effect of the release.
    - If the topography in the vicinity of the release is generally flat with few undulations, a Gaussian approach may be more appropriate. However, if the topography has complex characteristics with large variations, this may be better suited to the more complex CFD approach as this will account for the impact these variations may have on the dispersion of the gas.

When we do use more sophisticated models, the variables that don't need to change should be locked down. By codifying the aspects that should be common to all, or that are less important, we avoid the issue of there being too many variables, so reduce the chance for inadvertent error.

Based on the best practice guidelines mentioned above (e.g. in AFME in US, JAES in Japan, NAFEMS, or within the French Working Groups GT3D-Dispersion conclusions), suggested key aspects that should be standardised are given below.

Table 2: Suggested key aspects to be standardised

Numerical key aspect	**Equivalent physical key aspect**	**Description and best practice expected**	**Codification**
Computational domain	Dimensions of the numerical model of terrain.	All boundaries should be set so that there is a separation distance of 5 times the height of the buildings, except for the outlet boundary which should be at 10.	
Floor geometry	Topography	The topography is often provided in terms of altitude curves or points with a defined altitude.	Software should be able to build a floor surface out of this data, interpolating between points and curves and smoothing out the result.
Geometry	Obstacles	The obstacles can be defined in 3 ways depending on their location and expected influence on the release: • Actual 3D shape • Equivalent roughness • Equivalent porosity (for congested areas)	Because the number of obstacles can be large (especially on industrial platforms or in urban settings), the possible shapes of obstacles need to be predefined. The roughness and porosity data should also be predefined for each type of element (e.g. pipe racks, urban areas, water bodies, vegetations, etc.)
Boundary conditions	Ground, sky and lateral sides of the domain	The boundary conditions are of two types: a wall boundary condition for the ground, where the roughness parameter and the boundary layer should be described, and an open boundary condition for the lateral ones and the sky which can become inlet and/or outlets depending on the wind direction.	The codifications of the boundary conditions would prevent the redefinition of inlets and outlets of the wind inside the domain, depending on the wind condition. The wall boundary condition can also be made dependent on the roughness parameter (i.e. the land occupancy) without external intervention of the user.
Input condition	Weather condition	The input condition defines the meteorological class chosen. One of the challenges in CFD codes is to describe and maintain the input atmospheric profiles on the domain.	The input conditions must be codified first by its horizontal data: Wind direction and velocity. Then by its vertical definition: The logarithmic law best describing each atmospheric stability. This is the most important aspect and needs to be set directly by the software.
Mesh		Generally, a coarse mesh involves the high numerical diffusion that generates an inaccurate solution, the finer the mesh the more precise the solution. The mesh needs to have the following features: • able to capture as accurately as possible the shapes of the obstacles and source • be as fine as possible in the vertical direction next to the ground	An automatic mesh can make sure that the requirements regarding the vertical distribution of the mesh are satisfied, as well as the refinement needed next to obstacles and sources. However, provision must be given to allow the user to modify the mesh in accordance with their modelling objectives.
Resolution	Dispersion	The turbulence model should be appropriate, as well as the gravity model and the various characteristic numbers.	The resolution can be set by default inside the software without any external user input, except for non-conventional use.
Initial condition	Wind	The initial condition in the framework dictates how the wind field is established in the field and is dependent on the convergence of results.	The convergence criteria can be set inside the solver.
Postprocessing	Result analysis	The results should be integrated in the overall hazard assessment in a way that makes sense.	The calculation of chemical doses and the inclusion of thresholds should be done automatically.

Numerical key aspect	Equivalent physical key aspect	Description and best practice expected	Codification
Validation	Level of confidence	A specific set of validation cases both in wind tunnels and real scale should be undertaken and provided.	Prior to any attempt at modelling, the validation results should show the magnitude of the experimental standard deviations for free field modeling (Prairie grass) as well as in the presence of obstacles or for releases of dense gases (Fox Kit Field, MUST and others). The validation manual provided by the software suppliers should provide these cases.

To enable repeatability and comparability between people using these models, the industry, regulators and modellers need to agree a set of rules. These rule sets need to be developed for specific applications, such as the one discussed here: atmospheric dispersion.

References

ADMLC, 2004, Guidelines for the Preparation of Dispersion Modelling Assessments for Compliance with Regulatory Requirements – an Update to the 1995 Royal Meteorological Society Guidance. Available from: https://admlc.com/model-guidelines/

ASME, 2009, Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer. Available from www.asme.org

Batt, R., Grant, 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, Budapest, Hungary, 9-12 May 2016

Franke, J., Hellsten, A., Schlünzen, H. and Carissimo, B., 2007, Best Practice Guideline for the CFD Simulation of Flows in the Urban Environment Action COST 732 – Quality Assurance and Improvement of Microscale Meterological Models, International Journal of Environment and Pollution. 44 (1-4)

Gant, S.E. and Tucker, H., 2018, Computational fluid dynamics (CFD) modelling of atmospheric dispersion for land-use planning around major hazards sites in Great Britain, Journal of Loss Prevention in the Process Industries

HSE, 2017, RR1099 - Review of consequence model evaluation protocols for major hazards under the EU SAPHEDRA platform. Available from www.hse.gov.uk

ISO, 2014, ISO 19901-3:2014 Petroleum and natural gas industries — Specific requirements for offshore structures — Part 3: Topsides structure, Edition 2. Available from www.iso.org

Meroney, R., Ohba, R., Leitl, B., Kondo, H., Grawe, D. and Tominaga, Y., 2016, Review of CFD Guidelines for Dispersion Modelling, Fluids

NORSOK, 2010, NORSOK Z-013 Risk and Emergency Preparedness Assessment, Edition 3. Available from www.standard.no

Roald Hansen, O., Davies, S., Gavelli, F. and Middha, P., 2013, Onshore Explosion Studies – Benefits of CFD-Modelling, Chemical Engineering Transactions, Vol. 31

San Jose, R. and Luis Perez, J., 2013, Harmonisation of Practices for Atmospheric Dispersion Modelling within the Framework of Risk Assessment. 15th International conference on harmonisation within atmospheric dispersion modelling for regulatory purposes (HARMO 15), May 2013, Madrid, Spain. Technical University of Madrid. Madrid, pp.718-723,

Van Doormaal, J. P. and Raithby, G. D., 1984, Enhancements of the simple method for predicting incompressible fluid flows. Numerical Heat Transfer 7 (2), pp.147-163