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

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Abstract. At present there are two main approaches to modelling gas dispersion within the process safety risk assessment arena. Historically the Gaussian approach has dominated, however, with the improvement of computing power available in relatively low-cost platforms, Computational Fluid Dynamics (CFD) has begun to challenge that dominance. Both approaches rely on a mathematical description of transport with advection-diffusion equations. However, there are a number of simplifications that are needed for analytical Gaussian solutions to be derived which are not needed for CFD solutions. The Gaussian approach often applies simplified flows over flat terrain, whereas CFD accounts for flow velocities and turbulence and their effects on mixing and can be applied in more complex three-dimensional environments. The questions this paper asks are: Is CFD modelling more mathematically correct than the Gaussian approach? And, Does the emergence of CFD into the mainstream pose an opportunity or threat? To answer these questions this paper will explore the previously mentioned differences between approaches.

1. 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. 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.

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.

2. Gaussian vs 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 dispersion models 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:

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

This partial derivative 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 differences in Gaussian vs CFD approaches for solving this equation are the simplification vs solution for $\boldsymbol{U}$ and D_m in the above equation.

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 industrial 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 exists on industrial sites.

A CFD approach on the other hand solves the full advection diffusion equation (1) along with the relevant fluid mechanic equations (Navier-Stokes 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 equations

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

Total mass conservation equation

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

Energy Conservation equations

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

These equations are universal fundamental (derived from 1st and 2nd principles) equations for the atmospheric flows and so can be applied to any industrial site with various terrain features (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 dispersion equations (ADE).

In the above PDE, the thermodynamic state for the gas mixture is enforced with perfect gas laws $f(P, \rho, T, y_m)$. For the CFD solution to be performed, it needs then to perform a series of steps:

- Design a numerical domain of simulation 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 (numerical discretisation on a mesh) of the above continuous set of equations.
- 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 complex 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 for the account of turbulence enhancement/dissipation via mechanical (shear) or thermal production. The diffusivity scalar D_m in the 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 computations, the Semi-Implicit Method for Pressure Linked Equations-Consistent (SIMPLEC or SIMPLE-Consistent) algorithm (Van Doormaal and Raithby, 1984) is utilized. The buoyancy model is used to parameterize 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.

3. Gaussian vs CFD – Case study for dispersion of accidental releases

To demonstrate the difference between the Gaussian and CFD approach for cloud dispersion and subsequent consequence modelling, a case study for an accidental release of chlorine (heavy gas) is described below. The CFD Solution is modelled in fluidyn™-PANACHE dedicated software for atmospheric flows and dispersion at local meteorological scale (domains order of 10km size) and time scales of the order of minutes to hours.

The case study is for a major hazards site storing and handling chlorine. The study considered the scenario of 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.

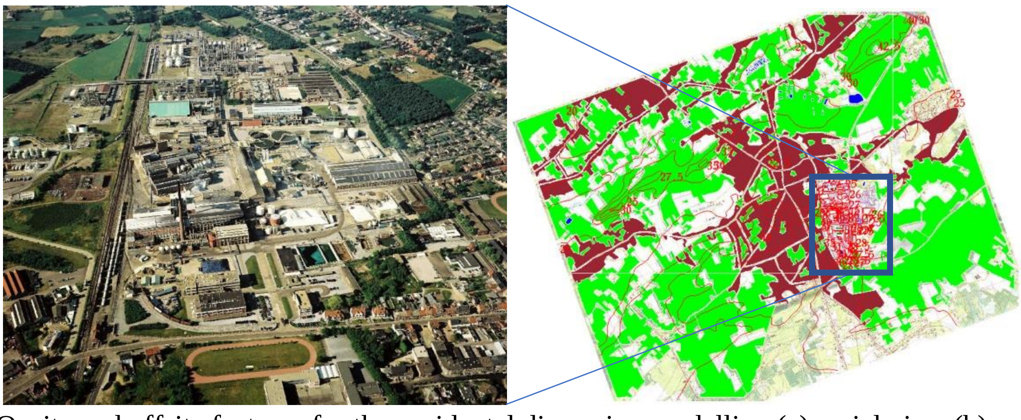

Figure 1: Onsite and offsite features for the accidental dispersion modelling (a) aerial view (b) environment and 3D set-up for CFD Solution.

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.

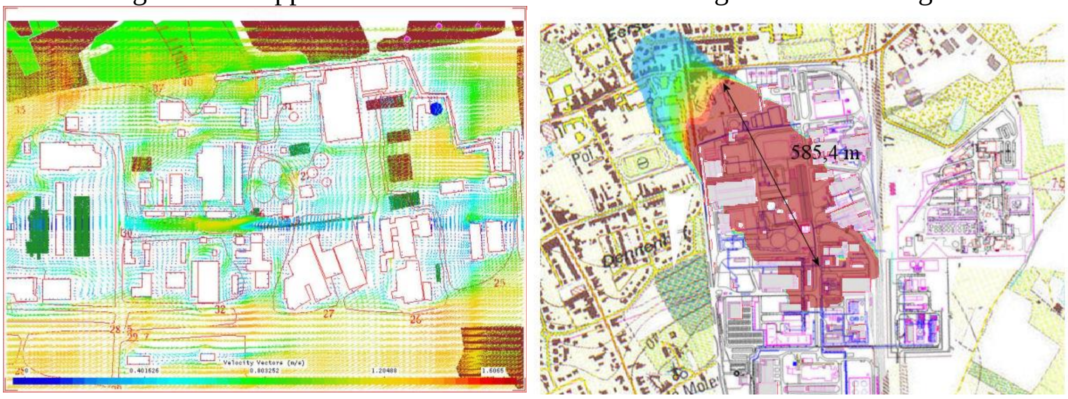

Figure 2: CFD Application for flow (left) velocities vectors and for toxicity map (both at ground level) for a consequence/risk analysis.

By comparison, 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.

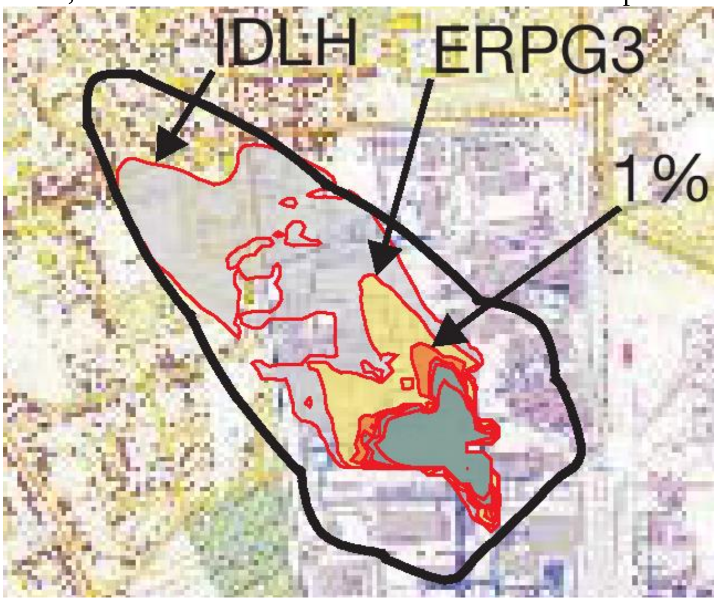

Figure 3: Comparison case between Gaussian model (black thick contour for Lethal effect 1%) and CFD model (red curves for varied thresholds).

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.

4. 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?

In the UK, the 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. As HSL has reported in some recent papers on the subject, the differences can be of an order of magnitude. 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.

The following table looks to consider each of these concerns for both Gaussian models and CFD to compare their relevance.

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

Area of Concern	**Relevant to Gaussian models**	**Relevant to CFD**
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.

5. Looking for a better way

1.1. 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 where a number of guidelines for CFD modelling are in place. Notable amongst these is an 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.

In the UK the HSE endorses the production of such guidelines, in order to improve conformity in CFD modelling outcomes. 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 us to apply in the UK.

1.2. 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 NAFEMS (National Agency for Finite Element Methods & Standards) 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. They also lack input from regulators.

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 &LUIS PEREZ, 2013). There have been a number of other working group studies relating to CFD, but few in relation to atmospheric dispersion and in 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.

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.

6. **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 worries 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. And then when we use more sophisticated models, to lock down the variables that don't need to change. 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.

To enable repeatability and comparability between people using these models, we 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.

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