



Back to basics: What you need to know about dispersion modelling

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Abercus is an independent consultancy specialising in advanced engineering simulation within the energy sector – computational fluid dynamics (CFD), finite element analysis (FEA), the development of bespoke software tools and teaching/training.





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Abercus' goal is the **democratisation** of advanced engineering simulation. **Abercus enables its clients to build expertise and develop their own engineering simulation capabilities**.





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Agenda

- Why carry out dispersion modelling?
- Modelling approaches for dispersion
- Computational fluid dynamics (CFD)
- Parameters affecting dispersion
- Application of CFD for dispersion
- Verification and validation
- Interpretation of results
- What is fit for purpose?
- Consistency across the industry
- Summary.



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Plume dispersion impacting neighbouring helideck



Offshore helideck design guidelines, HSE.



Buncefield dense gas dispersion followed by an explosion





- Flammable releases (accidental and planned):
 - Flammable releases may lead to explosive atmospheres
 - Explosion strength depends on cloud characteristics
 - · "Not all explosions are created equal"
 - · Accurate risk studies require evaluation of ventilation, release, and dispersion
 - Mitigation measures usually more efficient if applied to gas dispersion than to explosion
- Toxic releases (accidental and planned):
 - Toxic releases can impair occupied areas such as living quarters and control rooms



Dispersion modelling

Intentional

Unintentional

Dispersion distances Stand-alone assessment Volume of accumulation Part of an explosion risk assessment



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- Integral models (PHAST, FRED, ADMS3, AERMOD...)
- Computational fluid dynamics (CFD)



Integral models







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Computational fluid dynamics





Computational fluid dynamics





Effects of obstructions



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Effects of obstructions

- In practice there is usually an obstruction associated with the release source
- So, to model realistic dispersion behaviour, it is necessary to use a modelling approach that can capture the effects of obstructions.







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- CFD is an acronym for the term computational fluid dynamics
- Computational using computers to solve a set of equations
- Fluid (typically) liquid or a gas
- Dynamics motion
- Computational fluid dynamics is an approach for solving the governing equations of fluid flow using computational methods.





• CFD is often described as a numerical wind tunnel or wave tank



RJ Mitchell wind tunnel, University of Southampton

Reference required



- CFD is an approach for solving the governing equations of fluid flow using computational methods, but why don't we just solve these equations analytically?
- The governing equations are complex, non-linear partial differential equations

$$\frac{\partial(\rho u_i)}{\partial t}\mathbf{e}_i + \frac{\partial(\rho u_i u_j)}{\partial x_j}\mathbf{e}_i = \mu \frac{\partial^2 u_i}{\partial x_j^2}\mathbf{e}_i + (\rho - \rho_0)g_i\mathbf{e}_i - \frac{\partial \tilde{\rho}}{\partial x_i}\mathbf{e}_i$$

- They have been solved for a few simple geometries, but no general solution is known
- Generally, whenever an analytical solution is not possible, numerical methods offer an alternative approach.



Realistic dispersion modelling

 Accurate prediction of release and dispersion is a pre-requisite for determining explosion loads

 Integral models cannot account for geometry/terrain effect









Toxic Gas release in Urban Areas







 Chlorine release, D =10 cm hole, 225 kg/s for 300s (total release 67.5 ton)

Scenario I: Wind from South (190 degrees, towards downtown)

Scenario 2: Wind from East (80 degrees, from Lake Michigan)



Application specific CFD codes – FLACS (Gexcon)

• A commercial CFD tool for modelling dispersion, explosion and fire effects, widely used in the offshore oil and gas sector





Application specific CFD codes – KFX (DNV GL)

- A commercial CFD tool for modelling dispersion and fire effects
- EXSIM (explosion CFD code) now integrated





Application specific CFD codes



FLACS model for the 2600m³ full-scale rig at Spadeadam (Courtesy of Gexcon)

- Based on the porosity distributed . resistance (PDR) approach
- Current state of the art fixed mesh, . cannot adapt to the dispersing plume
- FLACS/KFX models can look impressive, but always remember they are simplified.





General purpose CFD codes

- There are a number of general purpose CFD codes available, for example: (FLUENT, STAR-CCM+, OpenFOAM, CFX...)
- General purpose codes can model a wide variety of problems, not just dispersion/safety application, but must be customised.





General purpose CFD codes

- Capture the geometry in a body-fitted mesh
- Adaptive meshing, so the CFD mesh can be adapted to the path of the dispersing jet/plume
- General purpose codes need to be customised
 - To implement the atmospheric boundary layer
 - Additional models such as the ACE method for capturing congestion





Subsea releases



https://www.youtube.com/watch?v=yRD5QYAkOoA



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Computational fluid dynamics (CFD)

Subsea releases




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- Ventilation
 - Environment (wind, temperature)
 - Geometry (walls, obstacles)
- Release
 - Process stream (material, phase)
 - Geometry (size, shape, location)
- Mitigation
 - Deluge, etc.



Ventilation

- Natural ventilation
 - Wind speed
 - Wind direction
- Forced ventilation
 - HVAC
- Geometry effects
 - Eddies, recirculation zones
 - spatial variations
- Other effects
 - Flow set up by strong fin fans/heat sources or exhaust releases
 - Atmospheric stability conditions

Parameters affecting dispersion

Ventilation (example - natural ventilation)



- Illustration: spatial variation in flow inside process module
- Location of leak of major importance



Parameters affecting dispersion

Ventilation (example – forced ventilation)



• Example of flow pattern established within a ventilated closed module



Ventilation

- Removal of gas
- Dilution
- The flow fields set up by wind are complex:
 - Varying flow speeds
 - Varying flow directions
 - Dead zones caused by obstructions
- Local flow condition at the leak location can have very large impact on cloud





Wind measurements at Nelson Platform

Parameters affecting dispersion

Release – process stream effects

- Material and temperature
 - Lighter-than-air (e.g., natural gas)
 - Neutrally buoyant
 - Heavier-than-air (e.g., propane)
- Storage conditions
 - Pressurized / atmospheric
 - Superheated / saturated / sub-cooled



eec

Parameters affecting dispersion



Effect of wind speed and buoyancy



Job-200165, Var-ER (-) firme- 0.000 (s) X= 38 : 72, Y= 78, 78, Z= 0.8 : 23 m



Job-200125. Var-EH (-) Time- 0.000 (s) X= 38: 72, Y= 73 - 78, Z= 0.8: 23 m 8 m/s wind - Shorter dispersion distance

- Larger flammable volume

I.5 m/s wind

- Longer dispersion distance
- Smaller flammable volume



Dense gas – propane release, 7 kg/s





Dense gas dispersion

Buoyancy

- Vapour evolving from liquid denser than air
- Also due to low temperature following a cryogenic spill
- Vapour cloud slumps with gravity effects
- Spreads at low level; affected by ground topography

Atmospheric effects

- Strongly influenced by ambient weather
- In stable conditions, may get stratification
- Inhibits mixing with air





Parameters affecting dispersion

Release – geometry effects

- Size and shape of the breach
 - Crack vs. full-bore vs. flange, etc.
 - High / low momentum
 - Jet atomization (droplet size distribution)
- Breach elevation and orientation
- Nearby obstacles
- Bunding



Effect of breach shape



Release – momentum effects

• Turbulent jet: entrainment leads to enhanced mixing of released



Diffusive releases: only shear layer mixing (dense releases)



Parameters affecting dispersion

Release – free jet





Release – impinging jet





Effect of release direction





Effect of wind/release direction





Effect of release rate



Addition of obstacles or confinement

Small obstructions:

- Local increase in mixing and speed
- Reduction in momentum of jet (allowing buoyancy more chance to act)

Large obstructions:

- Confining walls or roof may lead to recirculation, reentrainment and increasing gas concentrations
- Do not need a fully enclosed space







Releases in confined and congested volumes

- Releases into confined and congested volumes can produce flammable clouds with significantly smaller release rates than in the open
- Need to understand how mixtures accumulate and the parameters that affect this accumulation
- Ventilation is a key factor





Gas accumulation

- Need to understand how much flammable mixture is produced by a release
- Can vary significantly depending on the nature of the release and the enclosure





Releases in obstructed volumes

- Full scale experiments at Spadeadam test site (UK)
 - Dispersion and explosion studied
- Medium scale experiments in Gexcon test site (NO)







Experiments with realistic releases





Effect of release rate on overpressure



All other conditions (confinement, release and ignition locations) unchanged



Parameters affecting dispersion

Effect of release rate on overpressure



Several other conditions varied among tests







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Application of CFD for dispersion

Explosion risk analysis



- Spatial congestion

Many conceivable cases!



Application of CFD for dispersion

Explosion risk analysis (realistic worst case)

- Approach:
 - Dispersion simulations to identify biggest cloud size
 - Variation in leak direction
 - Leak rate
 - Wind/ventilation condition
 - Limited set of explosion simulations based on the dispersion simulations
 - Variation in ignition points
 - Cloud variation
 - Typically 30-40 simulations





Application of CFD for dispersion

Explosion risk analysis (realistic worst case)





Application of CFD for dispersion

Explosion risk analysis (realistic worst case)

- Dispersion
 - Challenge to identify worst conditions





Effect of release direction

Effect of release rate

LEL

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UEL > UEL

Application of CFD for dispersion

Cloud representation

- Dispersion simulation:
 - Inhomogeneous gas cloud
- Explosion simulation:
 - Equivalent stoichiometric cloud
 - Scaling of the inhomogeneous gas cloud to a smaller stoichiometric gas cloud giving similar explosion loads as the original cloud
- Options:
 - Combustible volume
 - Volume above LFL
 - Q9 (equivalent stoichiometric volume)







Application of CFD for dispersion

Effect of cloud size on overpressure





Application of CFD for dispersion

Worst case analysis

• Simplified representation of largest gas cloud from dispersion simulations



Application of CFD for dispersion

Case study - LNG terminal (realistic worst case load)




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Verification and validation

"All models are wrong but some are useful"

Robustness in the strategy of scientific model building, Box GEP, in Robustness in Statistics, Launer RL and Wilkinson GN, Academic Press, pp 201–236, 1979.

In order to gain confidence in our models and ensure that they are useful and fit for purpose, verification and validation is essential.



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Verification and validation

- Verification: the process of determining that a computational model accurately represents the underlying mathematical model and its solution
- Validation: the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model
- Verification is the domain of mathematics and validation is the domain of physics.



Verification and validation

- One of the major benefits of CFD is that it is a *first principles* approach, which enables a large degree of flexibility on the applications to which it can be applied
- However... with this flexibility come great responsibility
- Who is responsible for verification and validation?

Verification and validation

Who is responsible for V&V?

Code verification

Does the code correctly solve the underlying equations, as intended? **Responsibility: code vendor/developer? Ultimately the user**.

Calculation verification

Is the CFD prediction independent of the mesh/time-step used? **Responsibility:The user.**

Uncertainty quantification

How does the CFD prediction vary with the simulation inputs? Is the prediction sensitive to the inputs? **Responsibility:The user.**

Validation

Quantitative comparison with experiment. Is the prediction within the required bounds? **Responsibility:The user.**



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- Even if we have a perfectly validated CFD model, we still need to take care to properly interpret the prediction
 - The aim of the analysis ought to come from the client, and the output of the analysis should address their question in their terms
 - In our experience, the output is often driven by what is easily derived from commercial CFD software, which may be different from what the client really needs.
- The interpretation of predictive information can have a significant bearing upon the engineering decisions drawn from simulation and this is not always well communicated.



Atmospheric dispersion

- It is well known that the flow structure within a jet or plume in cross flow comprises a pair of counter rotating vortices*
- As a consequence, the highest concentration within the plume, at the centre of each of the vortices, may not lie on the centreline of the dispersing plume.



Jet in a cross flow, Ercoftac Wiki UFR 1-05, http://www.kbwiki.ercoftac.org/w/index.php/Abstr:Jet_in_a_Cross_Flow

* This is true for steady crossflow and is often observed in experimental wind tunnel studies. For real releases in the atmospheric wind environment, the plume is often observed to be more unsteady, which raises the question about the validity of the wind tunnel approach and RANS CFD approaches for this application. Maybe the LES CFD approach with a mechanism to capture the unsteadiness of the oncoming wind profile will become more widely adopted in future, but for now that remains a separate discussion.



Atmospheric dispersion

 In Abercus' experience, one common method for conveying CFD predictions for atmospheric dispersion is to present contours of plume concentration/temperature on a plane through the plume source and aligned with the wind direction.



Projection plot – plan view



Atmospheric dispersion

• For this example, the contour plot along the centreline of the plume provides a good indication of the plume behaviour, in terms of the concentration within the plume and the distance over which the plume extends.



Contour plot – centreline of plume



Atmospheric dispersion

- For lower wind speeds, however, the counter rotating vortices may be more apparent, as in the example opposite
- In this case, a contour plot on the centreline will not pick up the true extent of the plume
- A projection plot, however, does properly capture this behaviour.



Projection plot – plan view



Atmospheric dispersion

- For lower wind speeds, however, the counter rotating vortices may be more apparent, as in the example opposite
- In this case, a contour plot on the centreline will not pick up the true extent of the plume





Contour plot – centreline of plume



Atmospheric dispersion

- Essentially, what Abercus calls a projection plot is the superposition of the sequence of envelope plots
- The benefit of this kind of plot is that it always shows the true extent of the plume (projected in the direction of the view)
 - start off with a blue background, which is representative of the background concentration
 - then superimpose each envelope plot, starting with the lower concentrations.

Atmospheric dispersion





Atmospheric dispersion

- The projection plot shows the plume extending further and lower than is apparent from the contour plot along the plume centreline
- This is the same CFD prediction, but it just demonstrates that due consideration ought to be given to the interpretation of the CFD data
- The projection plot properly captures the plume extent and behaviour on a single image, whereas the contour plot on the plane along the nominal centre of the plume may be misleading (and non-conservative).



- Analysis of accidental ignition events (GP3 FPSO) bring forth inherent limitation of a few deterministic scenarios
- 'Conservative' method to account for uncertainties in important parameters (proposed by UK HSE)





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Atmospheric dispersion

- It is well known that the flow structure within a jet or plume in cross flow comprises a pair of counter rotating vortices
 - This is true for steady crossflow and is often observed in experimental wind tunnel studies
 - For real releases in the atmospheric wind environment, the plume is often observed to be more unsteady
 - Abstraction validation!



Jet in a cross flow, Ercoftac Wiki UFR 1-05, http://www.kbwiki.ercoftac.org/w/index.php/Abstr:Jet_in_a_Cross_Flow



Atmospheric dispersion







NAFEMS What is verification and validation?, https://www.nafems.org/publications/resource_center/wt09/ Jet in a cross flow, Ercoftac Wiki UFR 1-05, http://www.kbwiki.ercoftac.org/w/index.php/Abstr:Jet_in_a Cross Flow

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What is fit for purpose?

Atmospheric dispersion – stablility class

Stability Class Table

Wind Speed			Day: Incoming Solar Radiation			Night: Cloud Cover	
Miles per Hour	Knots	Meters per Second	Strong	Moderate	Slight	More than 50%	Less than 50%
Less than 4.5	Less than 3.9	Less than 2	A	A-B	В	E	F
4.5 - 6.7	3.9 - 5.8	2 - 3	A-B	В	С	E	F
6.7 - 11.2	5.8 - 9.7	3 - 5	В	B-C	С	D	E
11.2 - 13.4	9.7 - 11.7	5 - 6	С	C-D	D	D	D
More than 13.4	More than 11.7	More than 6	С	D	D	D	D

Notes:

- For completely overcast conditions during day or night, the stability class is D.
- This table is for releases over land. If the release occurs over water, the stability class will be either D or E.
- Wind speed is measured from a wind reference height of 10 meters.
- Strona incomina solar radiation corresponds to clear skies with the sun high in the sky (solar angle greater than 60



Atmospheric dispersion

 Are the wind tunnel approach and RANS CFD approaches commonly used for this application fit for purpose?



Borex plume experiments, Aarhus University, Denmark, http://envs.au.dk/en/knowledge/air/models/background/borex/

Jet Ç Vortex systems I. Vortex pair 2. Horseshoe vortex 3. Wake vortex street Vortex curve Separation line

Jet in a cross flow, Ercoftac Wiki UFR 1-05, http://www.kbwiki.ercoftac.org/w/index.php/Abstr:Jet in a Cross Flow



Atmospheric dispersion

- Are the wind tunnel approach and RANS CFD approaches commonly used for this application fit for purpose?
 - For stable atmospheres, the wind tunnel and RANS approaches may be realistic
 - For unstable atmospheres, the wind tunnel and RANS approaches cannot capture the unsteadiness and meandering of the plume
 - Maybe the LES CFD approach with a mechanism to capture the unsteadiness of the oncoming wind profile will become more widely adopted in future.





Jet in a cross flow, Ercoftac Wiki UFR 1-05, http://www.kbwiki.ercoftac.org/w/index.php/Abstr:Jet_in_a_Cross_Flow



Atmospheric dispersion

- Are the wind tunnel approach and RANS CFD approaches commonly used for this application fit for purpose?
- Wind tunnel and RANS CFD maybe:
 - Conservative in terms of dispersion distance*
 - Non-conservative for dispersion spread, which presents a risk for flammable releases



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* Wind tunnel and RANS approaches are likely to be conservative in terms of dispersion distance since plume meandering promotes mixing and, therefore, dilution. This would be true for a plume that remains entirely turbulent and becomes diluted though turbulent mixing. However, watch the Borex plume video for the unsteady atmosphere and you'll notice that the turbulent region of the plume is limited in it's extent. As the plume moves downstream, the plume-scale turbulence dissipates and the plume is gently carried along under the influence of the larger scale atmospheric turbulence, such that pockets of plume drift along in an almost laminar manner without further mixing. Therefore, it is not unequivocally clear whether the wind tunnel and RANS approaches are conservative in terms of dispersion distance.



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Consistency across the industry

- CFD is becoming increasingly used in the oil and gas sector as the benefits of the approach in terms of improved insight and better understanding of flow phenomena are realized
- Whilst there might be high-level agreement within industry regarding the general approach for many routine applications, the devil is in the detail – inevitably there must be inconsistency
- User variation and inconsistencies is a potential issue wherever engineering simulation methods are used, and this is bad for the confidence in the simulation methods
- An approach that is considered to be routine for one industry may not be appropriate for another industry.



Consistency across the industry

Atmospheric dispersion – examples of poor practice





Consistency across the industry

Atmospheric dispersion – blind benchmark exercise





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Summary

- CFD is a powerful tool that is increasingly used:
 - to deliver valuable insight at the design stage
 - to provide improved understanding of installation and operational issues
 - to demonstrate technology readiness for novel products and approaches
- Not using CFD can result in numerous poor design choices or implemented safety measures
- Just be mindful that CFD may not always be appropriate if simpler methods are fit for purpose, use them!



Summary

- Even if the underlying simulations are identical, their interpretation by different parties and the engineering decisions based upon the simulation output may be significantly different
- Simulation output should be driven by what the engineering needs, rather than what is easily derived from commercial simulation software simulation software
- Confidence is achieved through verification and validation without robust validation, CFD will always remain, for some, simply colourful fluid dynamics
- More blind-benchmarking should be pursued to improve confidence in CFD for dispersion applications.





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