CFD modelling of atmospheric dispersion for land-use planning (LUP) around major hazard sites in the UK

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Outline

- Background
- UK regulatory context
- Challenges for the use of CFD in providing public safety land-use planning advice in the UK
- Discussion
- Summary

Background

- Purpose of land-use planning
  - To manage population growth around major hazard sites
  - To help mitigate the consequences of major accidents
- Legislation: EU Seveso III Directive on the control of major-accident hazards involving dangerous substances

Source: https://visitenschede.nl

Enschede, Netherlands (2000)

23 killed, 1000 injured

Source: http://dx.doi.org/10.1016/j.jhazmat.2004.02.039

Toulouse, France (2001)

30 killed, 2242 injured

Cost €1.5 billion

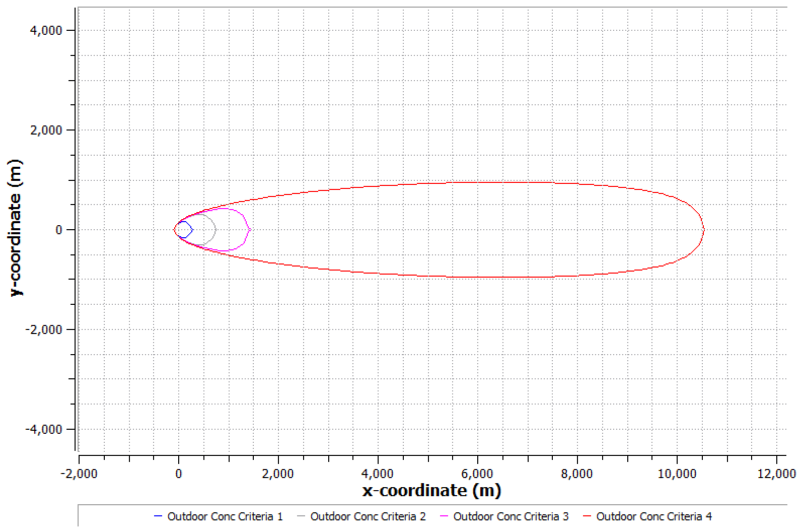
Buncefield, UK (2005)

0 killed, 43 injured

Cost €1.2 billion

Background

- HSE currently uses the integral model DRIFT to simulate atmospheric dispersion of toxic and flammable substances for land-use planning
- Faced pressure to use Computational Fluid Dynamics (CFD) results
- Perceived benefit of CFD: it accounts for terrain and obstructions
- Applications often involve dense gas dispersion e.g. LNG, LPG, Cl_2, SO_2, HF



Sample DRIFT results

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UK Regulatory Context

In the UK, the Seveso III Directive is implemented through:

COMAH 2015 regulations

- Operator's COMAH safety reports and emergency plans

Land-Use Planning regulations

- Hazardous substances consent
- Advice on land-use planning to prospective property developers and planning authorities

COMAH = UK Control of Major Accident Hazard Regulations

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– Advice on land-use planning to prospective property developers and planning authorities

Modelling approach may differ depending upon its use

COMAH = UK Control of Major Accident Hazard Regulations

Dispersion Modelling Approaches

Example of differences in dispersion modelling approach:

Quantity of hazardous substances released in an accident scenario

1. For consent and land use planning advice:

Consented maximum quantities

2. For COMAH and emergency plans:

Scale of current operations

Dispersion Modelling Approaches

Example of differences in dispersion modelling approach:

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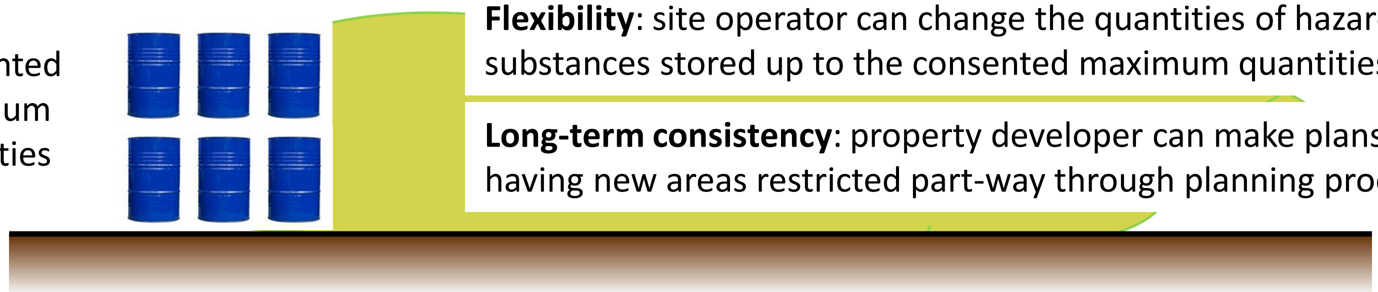
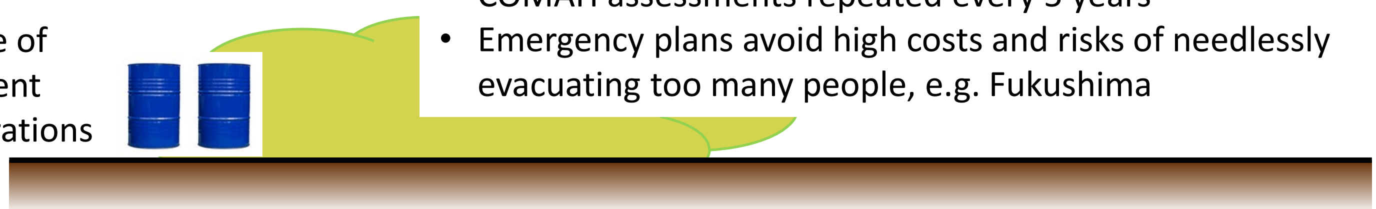


Flexibility: site operator can change the quantities of hazardous substances stored up to the consented maximum quantities

Long-term consistency: property developer can make plans without having new areas restricted part-way through planning process

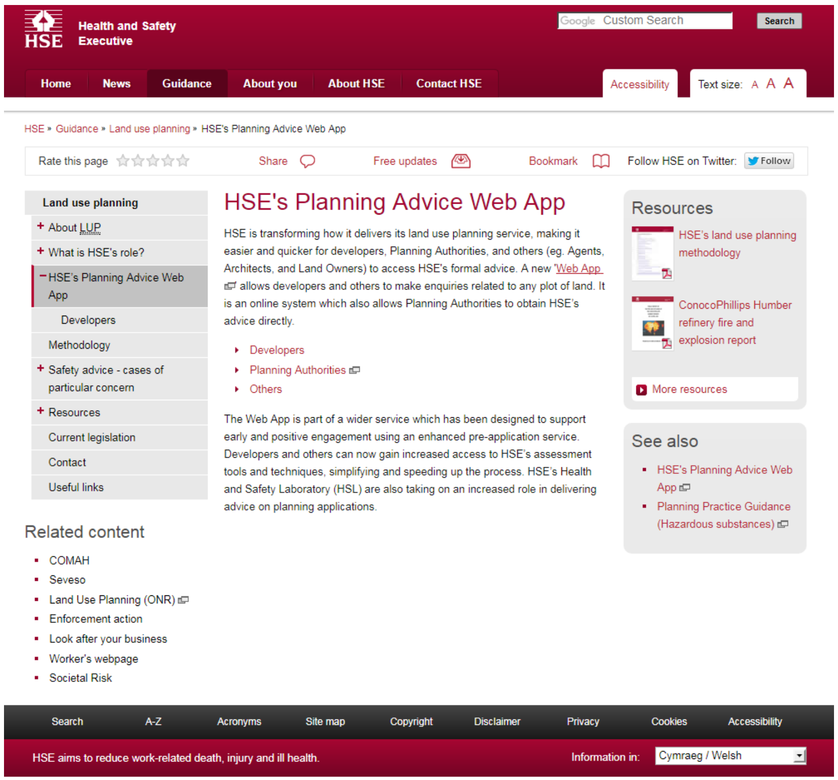
2. For COMAH and emergency plans:

Scale of current operations



- COMAH assessments repeated every 5 years
- Emergency plans avoid high costs and risks of needlessly evacuating too many people, e.g. Fukushima

HSE land-use planning advice



http://www.hse.gov.uk/landuseplanning/planning-advice-web-app.htm

HSE land-use planning advice is based on:

- Three-zone maps of residual risk for:
  - Around 2000 major hazard sites
  - 28,000 km of major accident hazard pipelines
- Type of proposed development
  - Sensitivity, vulnerability of populations and number of people

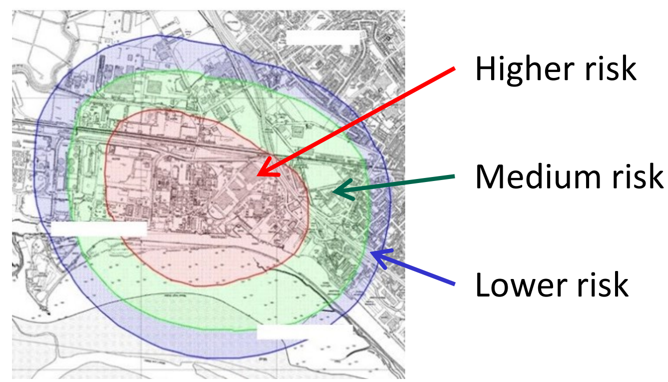


Figure for illustration purposes only

Residual risk = unavoidable risk that remains after all reasonably practicable measures have been taken by a major accident hazard operator to comply with the relevant regulations

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CFD Challenges

1. Problems in sustaining realistic atmospheric boundary layers
2. Treatment of wind meandering and averaging times
3. Uncertainty in source models for complex releases
4. Verification and grid resolution issues
5. Variability from user effects
   - Model complexity
   - Regulatory oversight
   - Best practice
6. High costs and long computing times
7. Lack of model validation

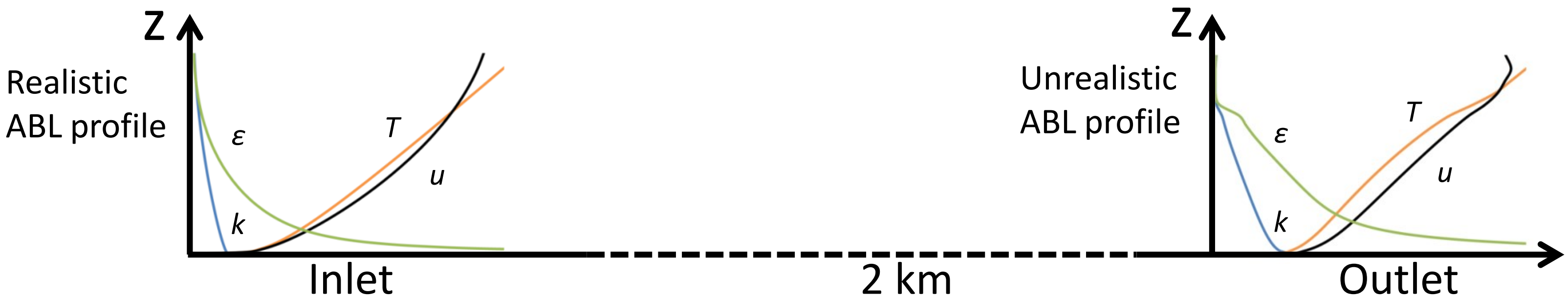
RANS turbulence models, e.g. FLACS, KFX, Fluidyn-Panache

These issues are acknowledged by most CFD experts – they are not new

Some also apply to integral models, but there are specific significant challenges for CFD

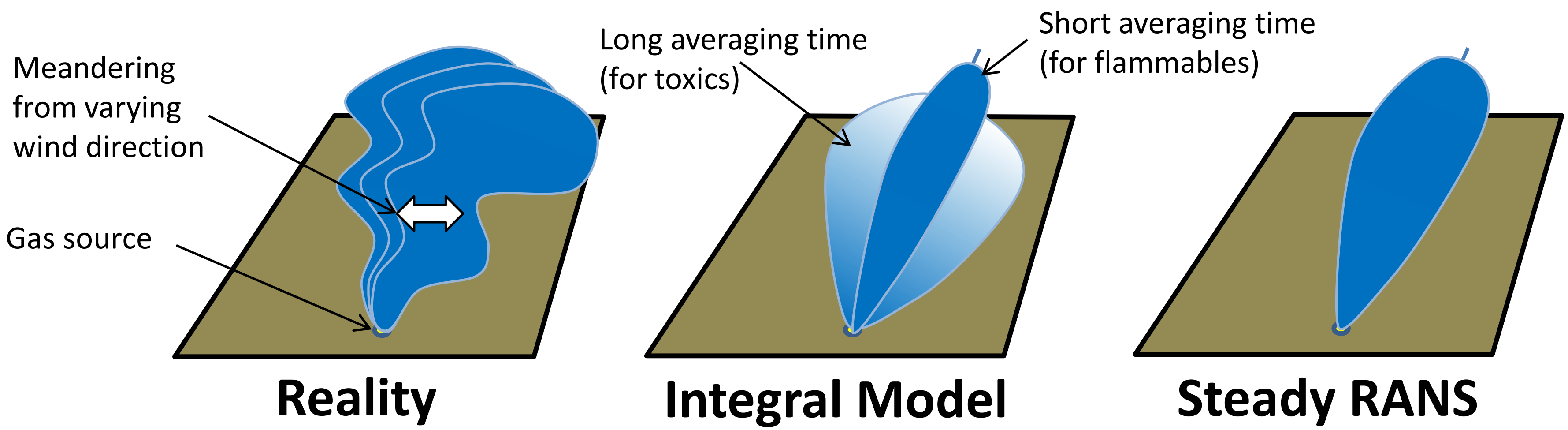
1. Sustaining Realistic ABLs

- **Problem:** Standard *k-ε* based turbulence models change the ABL profiles along the length of the computational domain



- Issues known for more than a decade (e.g. Blocken *et al*., 2007)
- Modification to profiles can affect the predicted hazard range
- Tuned turbulence models have been developed specifically for ABLs (e.g. Parente *et al*., 2011)
  - Incompatible with models needed for accident scenarios with jets and gravity-driven flows
  - Zonal/hybrid approach? ← Further work needed
- Dispersion behaviour may be dominated by local building effects for small releases (e.g. street canyons), but for significant cases the hazard range may extend kilometres
- It is important to have confidence in the prediction of ABLs

2. Wind Meandering and Averaging Time

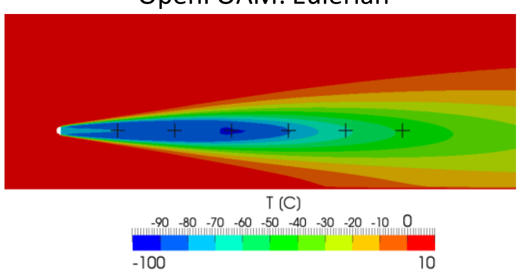


- Problem: steady RANS does not account for wind meandering and influence of averaging time
- Unsteady RANS simulations for hazard analysis often still use steady inflow conditions
  - They focus instead on predicting the behaviour of short duration (puff) releases
- Some meandering wind inflow conditions proposed to match experiments (e.g. Hanna *et al*., 2004 with FLACS) but inputs are often not generic and approaches are not widely used in risk assessment ← Further work needed
- Need to validate the same model that is used in practice

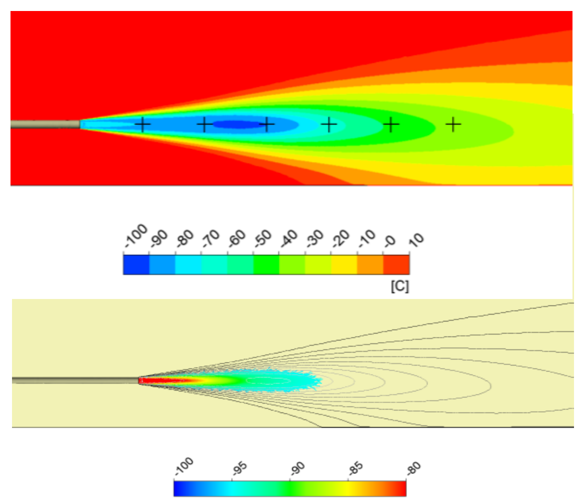
3. Source Models for Complex Releases

- Examples:
  - Catastrophic failure of vessels storing pressure-liquefied gases
  - Flashing two-phase jets from leaks in pipework
- CFD modellers have flexibility in choosing source models
  - E.g. multi-fluid (Eulerian), particle-tracking (Lagrangian), evaporation models etc.
  - Choice is specific to the CFD software and often the modeller
  - Whatever approach is taken needs case-specific validation

OpenFOAM: Eulerian



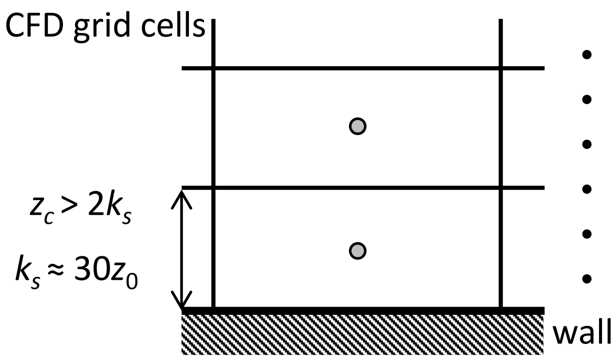
CFX: Lagrangian



Dixon C.M., Gant S.E., Obiorah C. and Bilio M. "Validation of dispersion models for high pressure carbon dioxide releases" IChemE Hazards XXIII Conference, Southport, UK, 12-15 November 2012
http://www.icheme.org/~/media/Documents/Subject%20Groups/Safety_Loss_Prevention/Hazards%20Archive/XXIII/XXIII-Paper-21.pdf

4. Verification and grid resolution

- "Code" verification – primarily the responsibility of CFD software vendor
- "Calculation" verification – responsibility of the CFD user
  - User inputs, including any user-coded functions
  - Grid resolution, time-step, particle count
- Cost of CFD simulation increases with:
  - Finer grid
  - Shorter time-steps
  - More particles
- Potential conflict between need to reduce errors and undertake a cost-effective study
- Grid resolution: particular problems for dense-gas dispersion over rough walls with RANS



- Sand-grain roughness $k_s \approx 30z_0$, where z_0 is the aerodynamic roughness length
- k-ε wall functions have limit on minimum height of near-wall cell of $z_c > 2k_s$
- e.g. Thorney Island, $z_0 = 0.01$ m, $k_s = 0.3$ m, minimum cell height, $z_c > 0.6$ m
- But the dense gas cloud is only about 1 m deep
- Only one grid cell resolving the cloud ← Further work needed
- Solution: smooth wall?

5. Variability from User Effects

- Several studies have found large discrepancies in CFD model results for the same scenario

French Working Group on Atmospheric Dispersion Modelling
Source: http://www.ineris.fr/aida/liste_documents/1/86007/0

3.6 kg/s carbon monoxide release

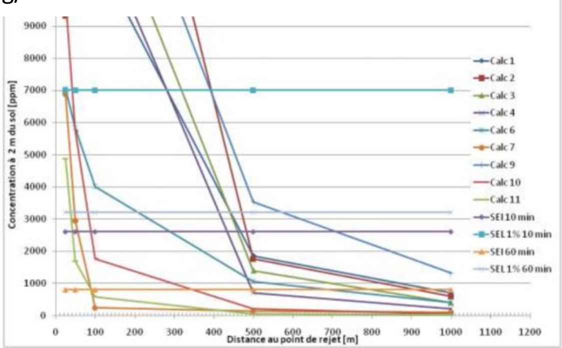


Figure 13 : Distances d'effet obtenues par les différentes modélisations.

Ketzel *et al.* (2002) "Intercomparison of numerical urban dispersion models"
Water, Air, & Soil Pollution, https://doi.org/10.1023/A:1021301316096

"Identical grids, inflow profiles, roughness of buildings and ground as well as boundary conditions were used by all codes"

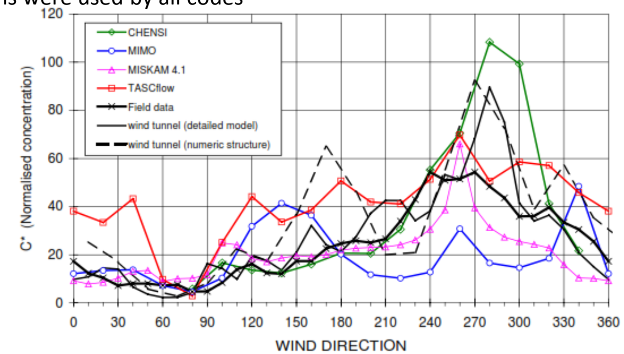


Figure 4 Normalised concentrations versus the wind direction calculated by 4 CFD codes and measured in the full-scale experimental site and in the wind tunnel.

- Complexity: many sub-models, unclear in advance which sub-model is best for the application
- Freedom for users to configure CFD models differently (more so than with integral models)
- Models may be well validated, but still can be used inappropriately
- Best practice initiatives ⟵ Further work needed, e.g. ERCOFTAC BPG is 17 years old
- Need for detailed regulatory oversight, e.g. assessment of input/output files

6. High Costs and Long Computing Times

- CFD is costly
  - Commercial software licencing
  - Computing resources
  - Employment of suitably qualified CFD experts

- Tension between:

Need for rigor appropriate for making safety-critical decisions

↕

Need to conduct a cost effective CFD modelling study

- Resources required for rigorous CFD study should not be under-estimated

7. Model Validation

- Validation is essential to demonstrate a model is fit for purpose
- Steps include:
  - Assessing the important flow physics for application of interest
  - Identifying suitable experimental datasets
  - Examining model performance
- Example: LNG Model Evaluation Protocol published by NFPA
- Land-use planning applications: dense gas dispersion with terrain e.g. LNG, LPG, Cl_2, SO_2, HF
- Problem: lack of experimental data
  - Field experiments
    - Jack Rabbit I: 1-2 tons chlorine releases in shallow depression (data unavailable)
    - Burro Trial 8: LNG spill in water pool in low wind speed (source conditions uncertain)
    - Porton Down: Instantaneous Freon releases (lacking concentration measurements)
  - Wind-tunnel experiments
    - BA-Hamburg: zero wind, neutral stability
    - Surrey University MODITIC: two-dimensional hill

    } Simple geometries; Scale effects

Further field-scale experiments are needed for dense-gas dispersion with terrain

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Discussion

- Scale of UK land-use planning requirements
  - Three-zone maps for around 2000 major hazard sites and 28,000 km of pipelines
  - For each site, e.g. medium-sized chemicals facility, currently modelling 700 scenarios
  - Using a CFD model to resolve obstacles/terrain: need to simulate each wind direction
    - e.g. 700 scenarios × 12 wind directions = 8,400 scenarios for one site
- Consistent modelling approach needed across all sites
  - So that risks can be compared
- Using CFD for all sites is impracticable
  - Thousands of CFD simulations required for every site
  - Massive effort needed to collect data, build models and post-process results
  - Disproportionate cost

Discussion

- Use CFD for just those sites with terrain, and use DRIFT for "flat" sites?
  - Problem: need for consistent modelling approach across all sites
    - Need to compare risks from different sites on equal basis
    - Challenge from developers, planners and public interest groups to use one or other model that gives them the "favourable" outcome
  - Solution? conduct benchmarking exercise between CFD and DRIFT for "flat" scenarios
    - Experience shows that the two models would probably give different results
    - Adjust model results to make them equivalent?
      - Scientifically dubious
      - Difficult to implement in practice
  - Challenge remains to validate CFD models
    - Particularly for dense-gas dispersion in complex terrain
    - Field-scale experiments needed

Discussion

Modelling philosophy

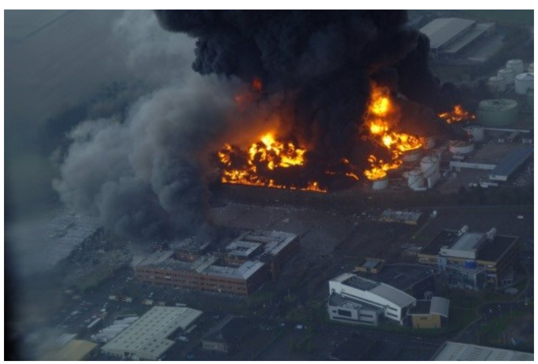
- Intricate and costly models like CFD are best suited to problems where:
  - Conditions are reasonably well defined, e.g. incident investigations
  - Model physics needs to be adapted, e.g. exploratory studies
  - Cases where extensive field-trial data exists, e.g. offshore oil and gas fire/explosion

- Land-use planning involves, in contrast:
  - Full spectrum of credible accident scenarios and all weather conditions
  - Scope of the modelling effort is very wide and not tightly focussed
  - Modelling methodology must be applied consistently across all sites in the long term

- Significant challenges to the use of CFD in land-use planning
  - Efforts could be better spent on reducing other uncertainties e.g. toxicology, failure frequencies, scenario selection?

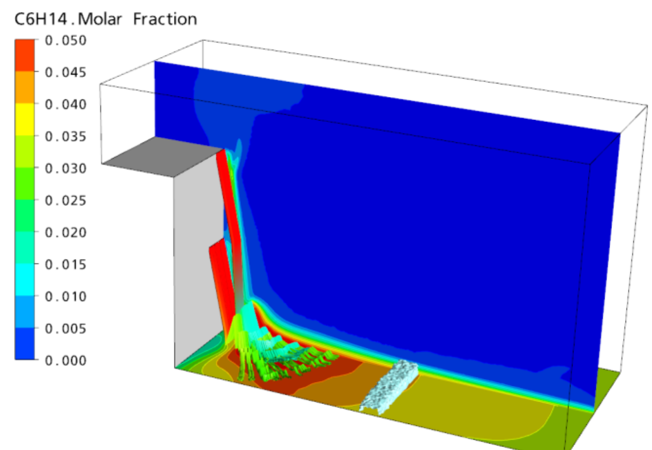
- CFD may be appropriate in a different context to land-use planning where particular hazards need to be studied in more detail

Example: Buncefield Incident Investigation



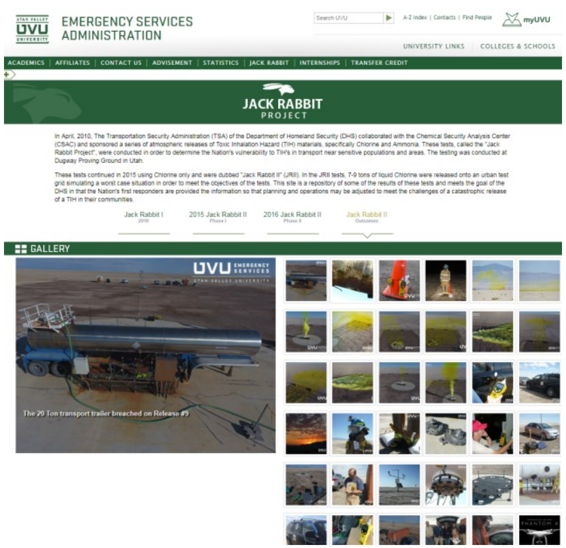
Guidance on assessing tank over-filling hazards published in FABIG TN12

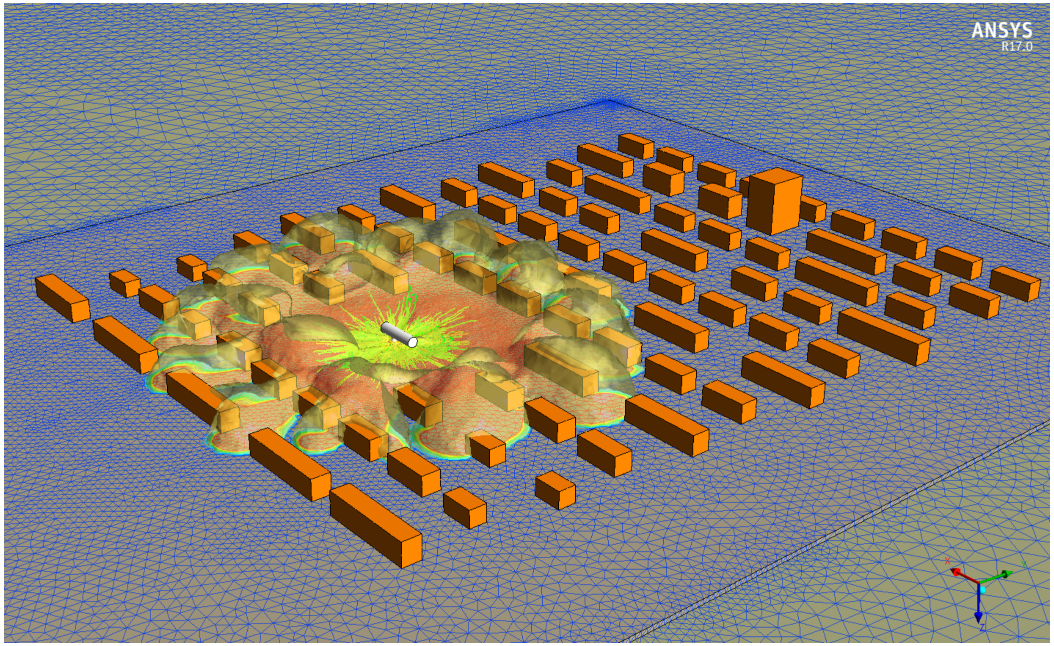
CFD used to determine the flow rate of flammable vapor from gasoline cascade

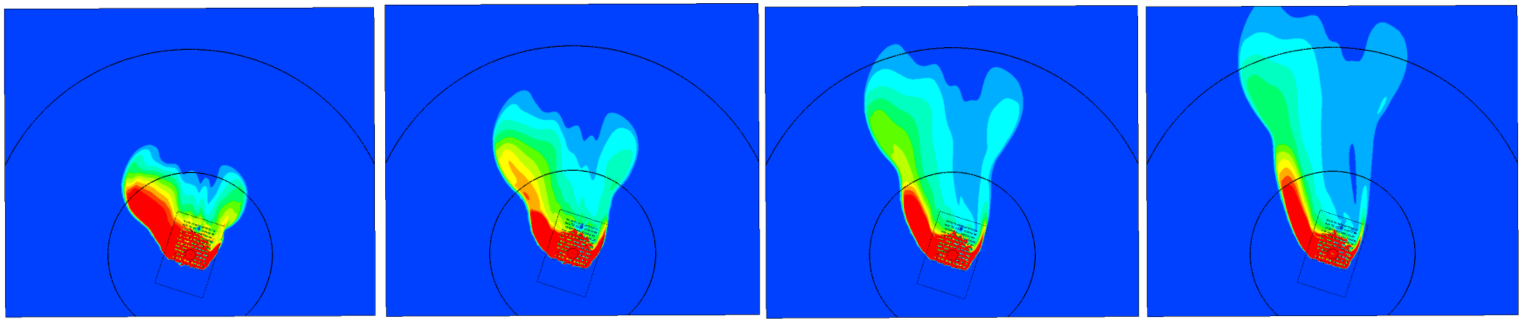


Examples: Jack Rabbit II

http://www.uvu.edu/esa/jackrabbit/







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Summary

- Overview of UK regulatory framework
  - Land-use planning, hazardous substance consent, COMAH safety cases, emergency plans
  - Differences in modelling approach depending upon application

- CFD issues
  1. Problems in sustaining realistic atmospheric boundary layers
  2. Treatment of wind meandering and averaging times
  3. Uncertainty in source models for complex releases
  4. Verification and grid resolution issues
  5. Variability from user effects
  6. High costs and long computing times
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  Identified where further work is needed

- Discussed challenges to the use of CFD in land-use planning
  - Scale of problem, need for consistency, unresolved CFD issues, lack of confidence in results

- CFD useful in other contexts, e.g. incident investigation, developing understanding, certain risk assessments (e.g. offshore oil and gas)

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