Introduction to CFD modelling of source terms and local-scale atmospheric dispersion (Part 2 of 2)

Atmospheric Dispersion Modelling Liaison Committee (ADMLC) meeting

15 May 2018

Simon Gant, Fluid Dynamics Team

Outline

- Concepts: domain, grid, boundary conditions, finite-volume method
- Turbulence Modelling
  - Reynolds-Averaged Navier Stokes (RANS): steady and unsteady
  - Large Eddy Simulation (LES)

Part 1

- Atmospheric boundary layers
- CFD Software
- Case studies
  - Source terms: flashing jets, overfilling tanks
  - Local-scale atmospheric dispersion: Jack Rabbit II

Part 2

Turbulence Modelling (just to recap)

What is Steady/Unsteady RANS and LES?

P.R. Spalart / Int. J. Heat and Fluid Flow 21 (2000) 252–263

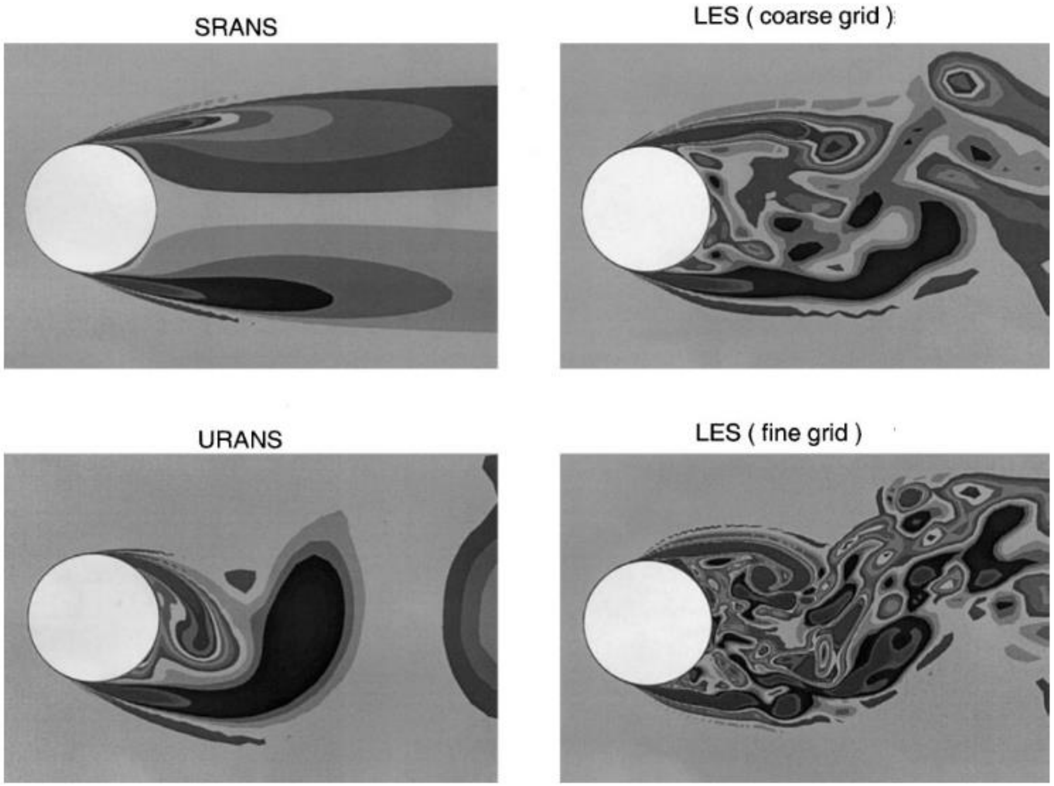

Fig. 4. Simulation of flow past circular cylinder by various approaches (Shur et al., 1996; Travin et al., 2000).

Turbulence Modelling (just to recap)

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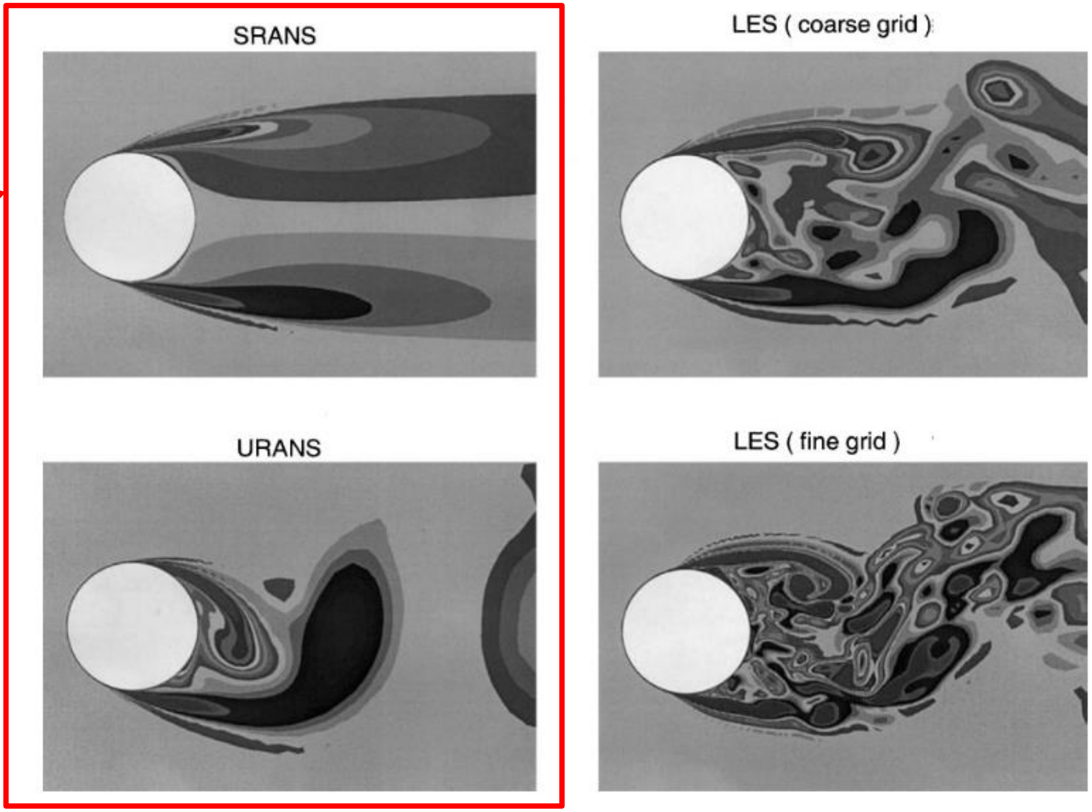
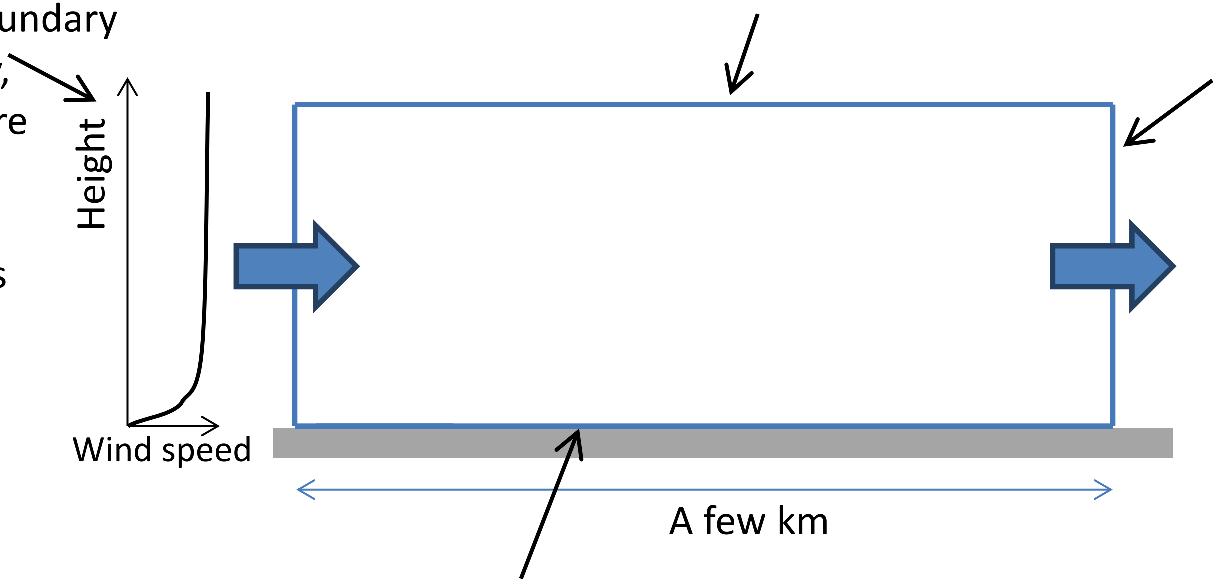


Fig. 4. Simulation of flow past circular cylinder by various approaches (Shur et al., 1996; Travin et al., 2000).

Next slides focus on modelling atmospheric boundary layers with RANS

Modelling Atmospheric Boundary Layers

Task: to model air flow over flat, open terrain



Boundary layer profiles specified on inlet boundary for velocity, temperature and turbulence parameters

“Slip” conditions, prescribed shear-stress or prescribed wind speed on the top boundary

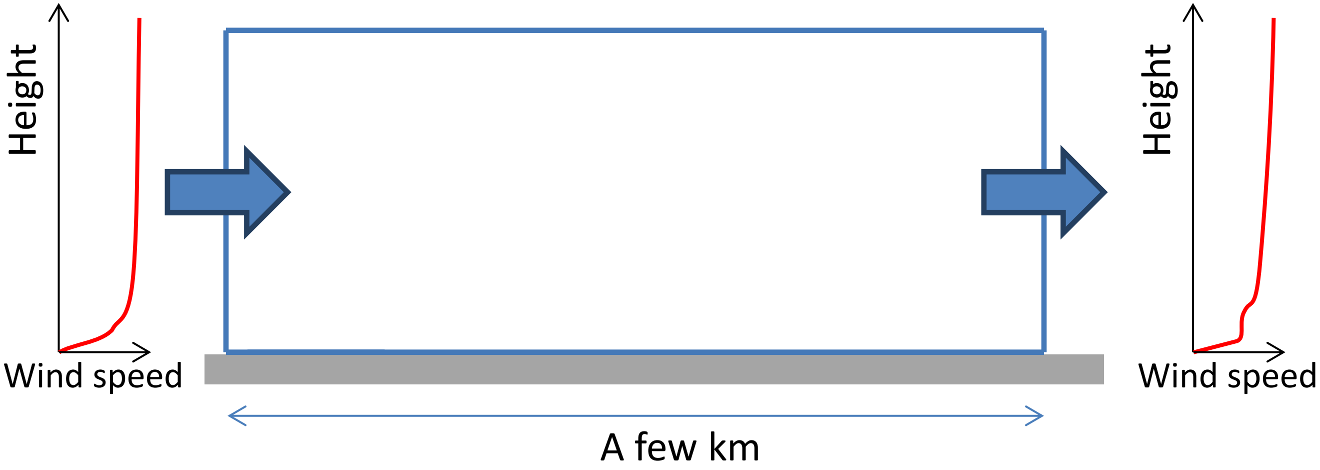
Constant pressure conditions applied on outflow boundary

(needs to account for density variation with height if air is treated as an ideal gas or temperature variations are modelled)

Air velocity set to zero on the ground boundary:
wall functions

Modelling Atmospheric Boundary Layers

Problem: Atmospheric boundary layer profiles change along the domain



Modelling Atmospheric Boundary Layers

Cause:

- Standard *k-ε* turbulence model tuned to produced reasonable predictions in range of engineering flows (e.g. plain jet, pipe flow, wall jet, coaxial jet, cavity flow, film cooling, turbine blade boundary layer)
- Model constants were chosen as a compromise
  - Not tuned specifically for ABLs
- Solutions have been proposed to tune *k-ε* specifically for ABLs
- Incompatibility problem: tuned *k-ε* models for ABLs probably perform poorly for other important flows relevant to gas dispersion, e.g. jets, wakes, gravity-driven flows
- Pope (2000) “*[when] modified models are applied to a range of flows, the general experience is that their overall performance is inferior to that of the standard model*”

Advice on Modelling ABLs

Good-practice guidance on RANS modelling of ABLs:

- Franke J., Hellsten A., Schlünzen H., Carissimo B. (Eds.), 2007, *Best practice guideline for the CFD simulation of flows in the urban environment*, COST Action 732 “Quality assurance and improvement of microscale meteorological models”. COST Office, Brussels, Belgium.
- French Working Group, 2015, *Guide de Bonnes Pratiques pour la réalisation de modélisations 3D pour des scénarios de dispersion atmosphérique en situation accidentelle*. Available for download from http://www.ineris.fr/aida/liste_documents/1/86007/0

Advice on Modelling ABLs

Relevant academic papers:

- Duynkerke, P.G. 1988. *Application of the E-ε turbulence closure model to the neutral and stable atmospheric boundary layer*. J. Atmos. Sci. 45(5).865-880.
- Richards, P.J. and Hoxey, R.P., 1993. Appropriate boundary conditions for computational wind engineering models using the k-ε turbulence model, J. Wind Eng. Ind. Aero.,46-47, p145-153.
- Alinot, C. and Masson, C. 2005. *K-ε model for the atmospheric boundary layer under various thermal stratifications*. Transactions of the ASME. 127, p438 – 443.
- Hargreaves, D.M. and Wright N.G., 2007. *On the use of the k-ε model in commercial CFD software to model the neutral atmospheric boundary layer*, J. Wind Eng. Ind. Aero., 95, p355-369
- Blocken, B., Stathopoulos, T and Carmeliet, J. 2007. *CFD simulation of the atmospheric boundary layer: Wall function problems*. Atmos. Env. 41. Pp 238 – 252.
- Pontiggia M., Derudi M., Busini V., Rota R., 2009. *Hazardous gas dispersion: A CFD model for atmospheric stability classes*, J. Hazard. Mater., 171, 739-747

CFD Modelling of ABLs at HSL

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Aims

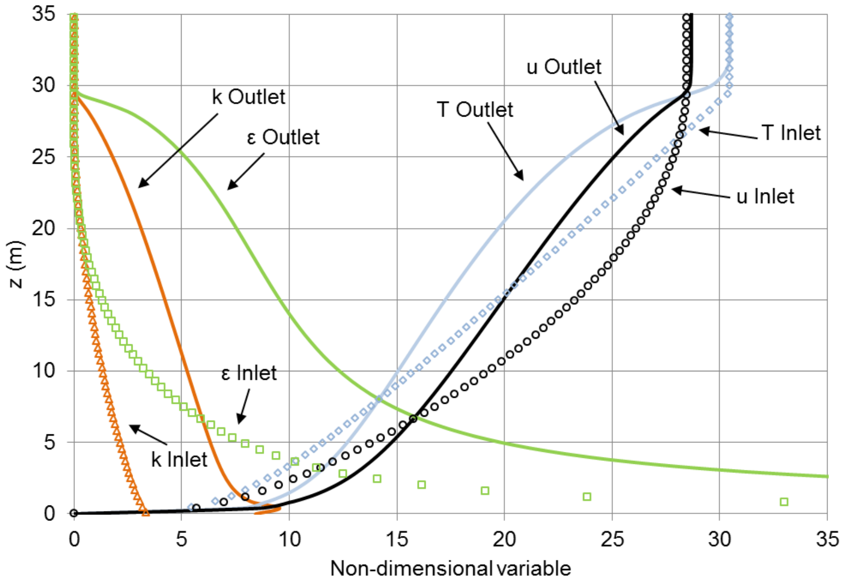
- What options are available to model stable ABLs in commercial CFD codes using RANS models?
- How well do they perform?
  - Can they sustain realistic ABL profiles?
- How do errors in the ABL profiles affect gas dispersion predictions?

CFD Modelling Approach

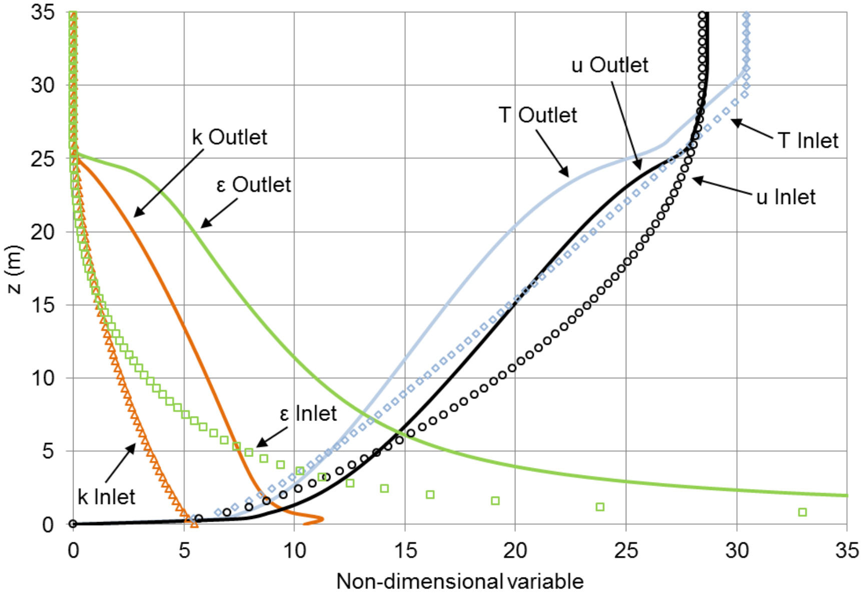
- Pasquill class F2.4
- Check profiles are maintained along an empty 2 km section (BPG)
- Large domain (> 200 m high) – suitable for complex geometry
- Fine near wall mesh – suitable for dense gas dispersion
- Test inlet profiles:
  - Lacome and Truchot (L&T, 2013)
  - Alinot and Masson (A&M, 2005)
- Test turbulence model:
  - Standard *k*-*ε* model with L&T profiles
  - *k*-*ε* model with modifications of A&M for both sets of inlet profiles

Results 1: Modified Turbulence models

Standard k-ε with L&T inlet profile



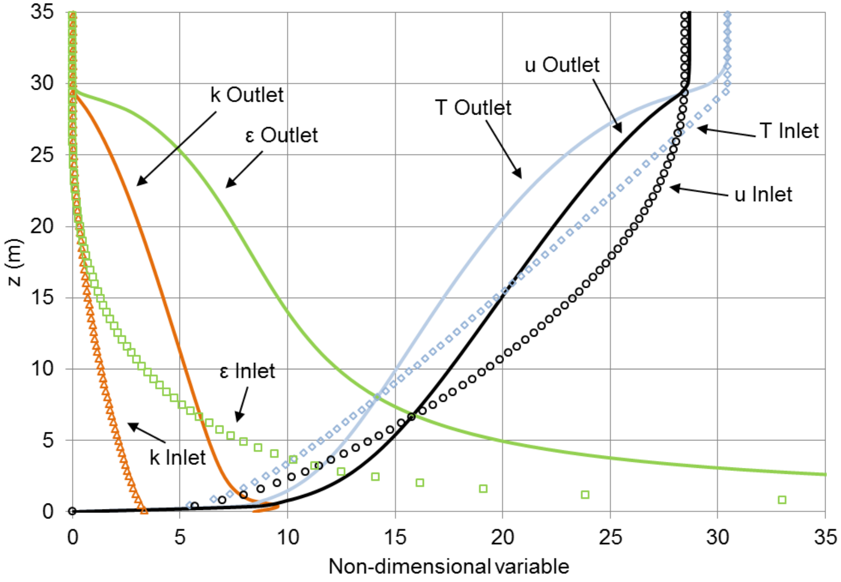
A&M k-ε model with L&T inlet profile



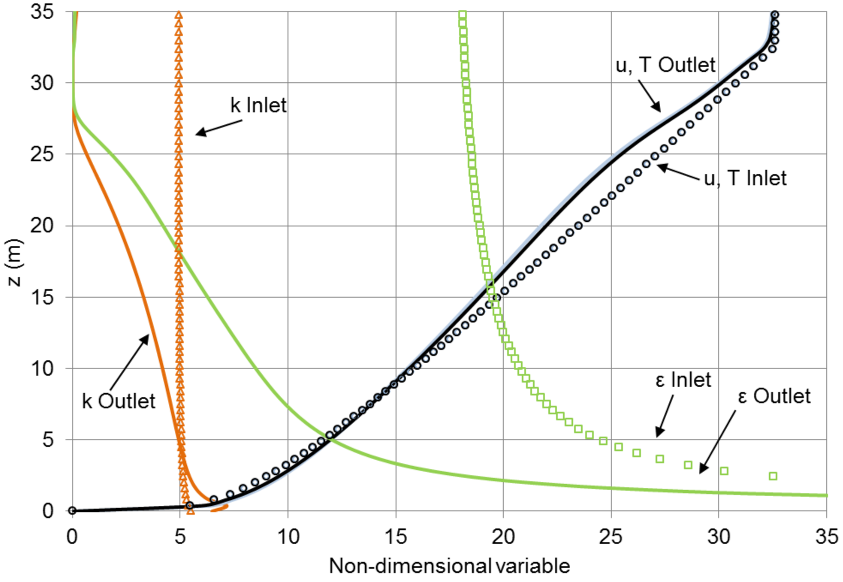
- *u* and *T* under-predicted below about 10 m and over-predicted above 10 m
- *k* and *ε* are over-predicted for all z

Results 2: Modified Turbulence models

Standard k-ε with L&T inlet profile

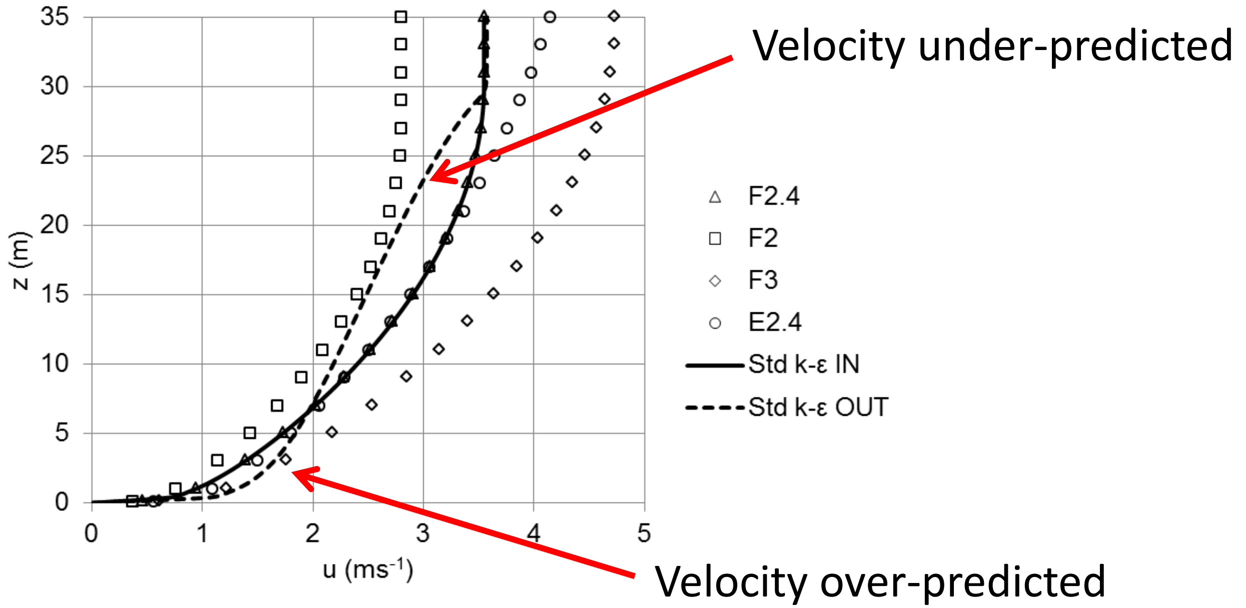


Complete A&M model



- Complete A&M (right) shows improvements but the profiles still change
- Difficult to make other adjustments to improve consistency further due to constrains of commercial ANSYS-CFX CFD software

What might this mean?



Velocity under-predicted

Velocity over-predicted

- Outlet profile not necessarily representative of the same stability class as the inlet profile
- If used in a dispersion calculation, the higher velocity near the ground could artificially increase dilution rates producing an unrealistic reduction in the hazard range … but by how much?

Case Studies

- Prairie Grass (Barad, 1958)
  - Flat, empty terrain
  - Continuous passive gas releases (SO_2)
  - Neutral (PG33) and stably-stratified (PG36) conditions
- Thorney Island (McQuaid and Roebuck, 1985)
  - Flat, empty terrain
  - Continuous dense gas releases (Freon/Nitrogen mix)
  - Stably-stratified (TI47)

CFD Model Setup

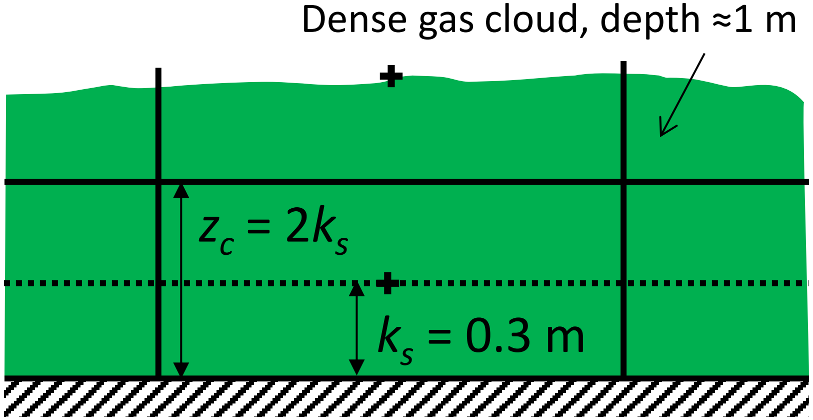
- Inlet ABL profiles of *U*, *k* and *ε* from Lacome and Truchot (2013) with temperature profile *T* from Alinot and Masson (A&M, 2005)
- Hexahedral cells used for PG, hex-dominant (prisms) for Thorney Island
- Wind speed and direction assumed constant, no meandering

Trial	**PG33**	**PG36**	**TI47**
Atmos. stability (Pasquill class)	Neutral (D)	Stable (F)	Stable (F)
Wind speed (ms^{-1})	8.5	1.9	1.5
Wind reference height (m)	2	2	10
Roughness length, z_0 (m) – ABL	0.006	0.006	0.01
Roughness length, z_0 (m) – Wall	0.006	0.006	0.0008 and smooth
Domain size (m × m × m)	2000 × 100 × 30	2000 × 100 × 30	1000 × 800 × 10
Total grid nodes (millions)	1.6	1.6	2.9
Near-wall cell height (m)	0.4	0.4	0.05
Turbulence model	Standard *k*-*ε*	Standard *k*-*ε*	Standard *k*-*ε* and A&M

Wall roughness model – incompatible with mesh requirements

- For Thorney Island it was not possible to use z_0 from the experimental measurements…

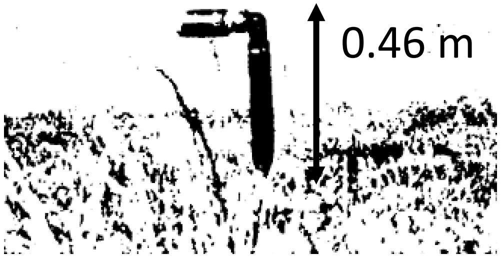
In CFX $k_s \approx 30z_0$ and wall functions for k-ε turbulence model have limit on near-wall cell height of $z_c > 2k_s$.
So, for TI47 with $z_0 = 0.01$ m:
$k_s = 0.3$ m
and
$z_c > 0.6$ m
THE DENSE GAS CLOUD IS ONLY ABOUT 1M DEEP!



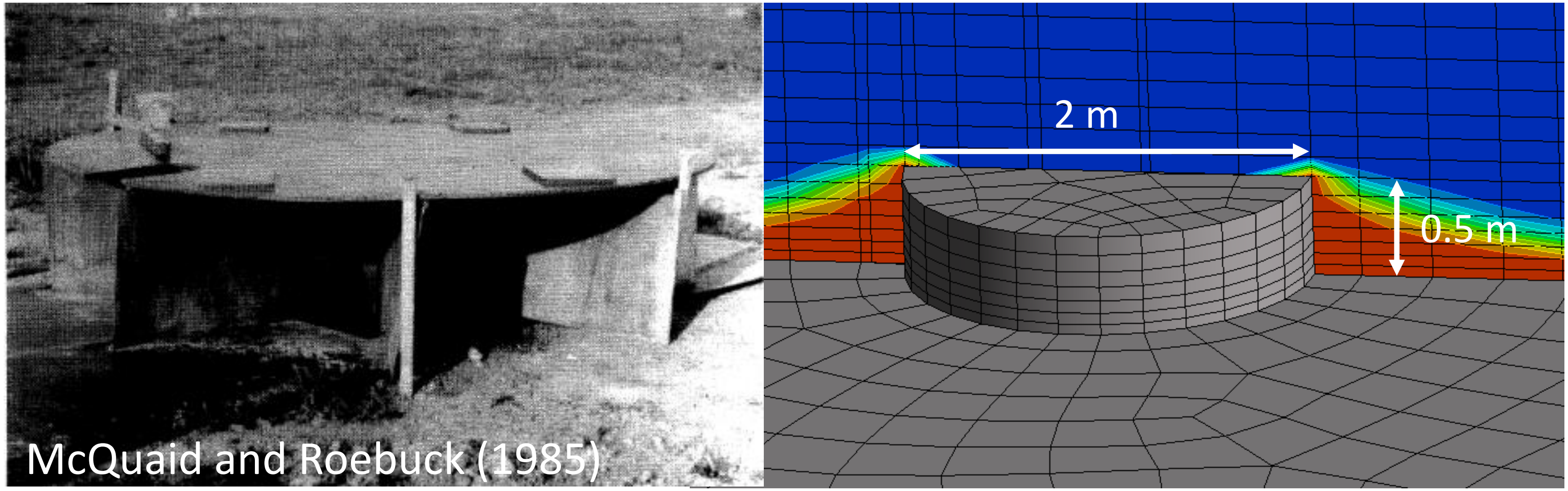
- In the experiment: $z_0 = 0.01$ m
- In the model: z_0 limited by the mesh to be $z_0 = 0.0008$ m or smooth
- How much will this affect the gas dispersion?

Source resolution – difficult to reconcile with far field resolution

- Prairie grass: point source
- Thorney Island: mass flow inlet



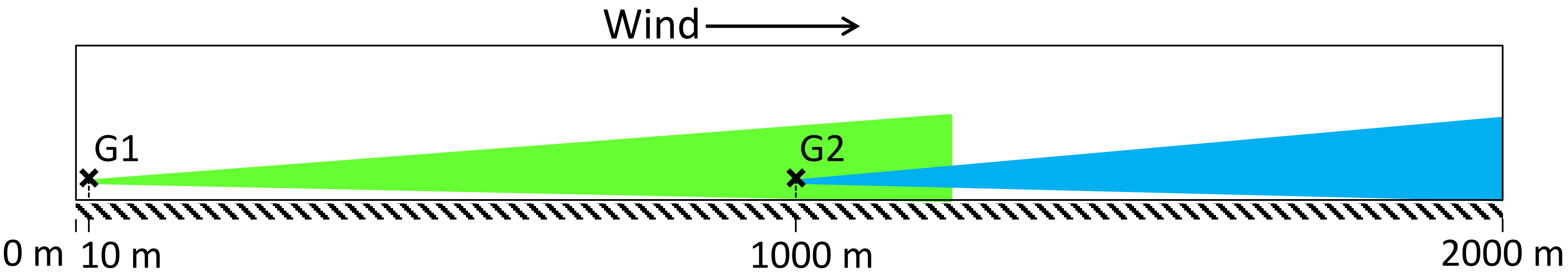
Barad (1958)



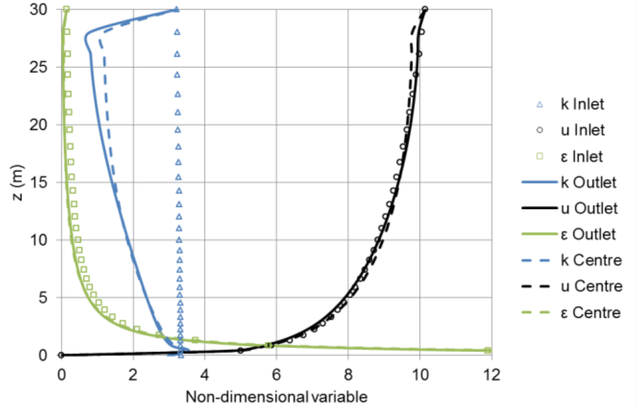
McQuaid and Roebuck (1985)

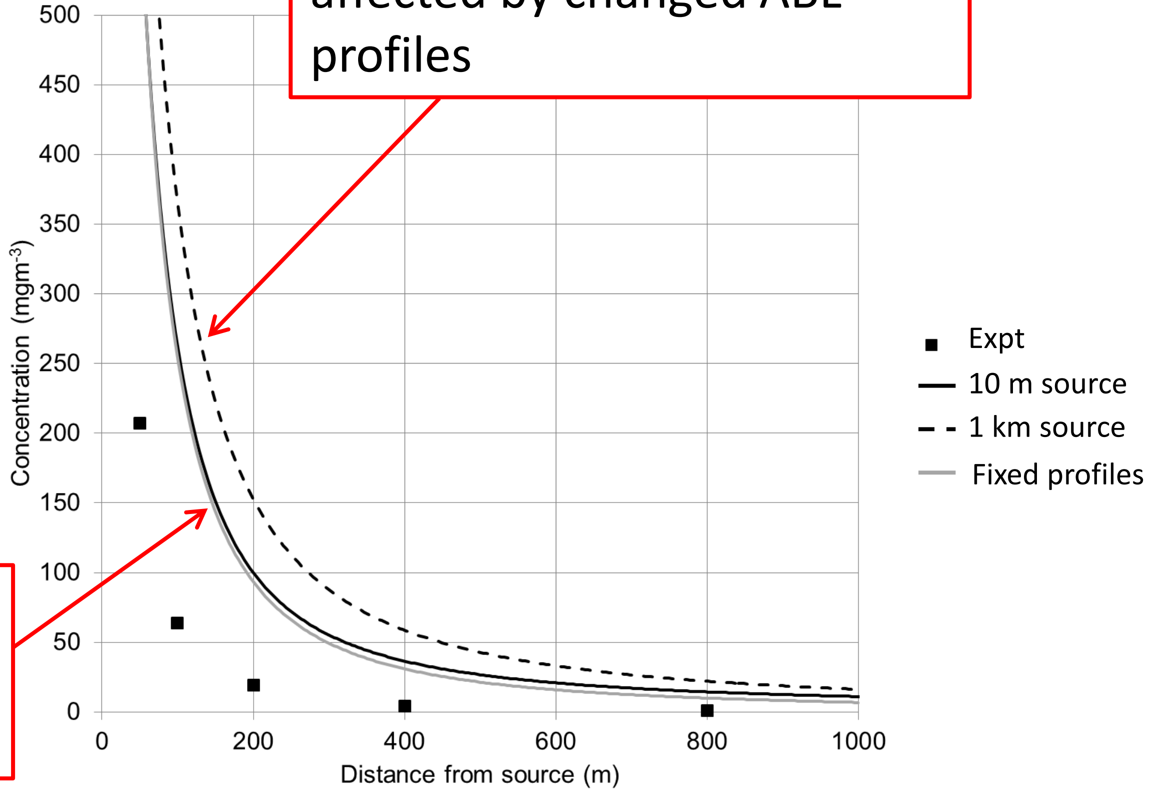
Assessing effects of profile change with multiple release points and fixed profiles

- Prairie Grass only
- Solving the full transport equations for all variables
  - Passive scalar was injected at two locations
  - If the profiles change, the gas will disperse differently
- Correct ABL profiles ‘fixed’ throughout the domain as a reference case (only possible with passive gas)



Prairie Grass PG33: neutral ABL





Release 1 km downwind is affected by changed ABL profiles

Release near the inlet is similar to case with fixed profiles

@ Height z = 1.5 m

Prairie Grass PG36: stable ABL

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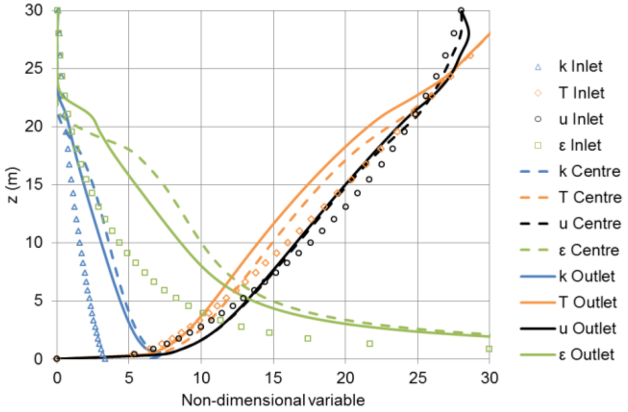
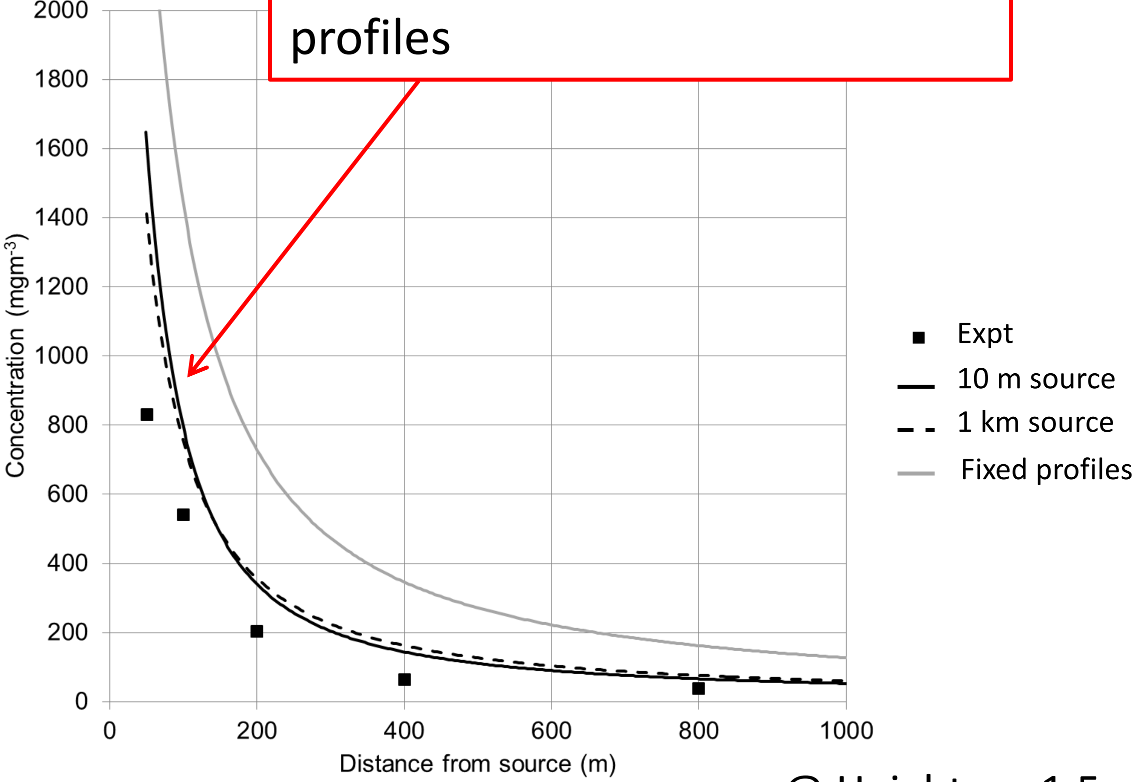
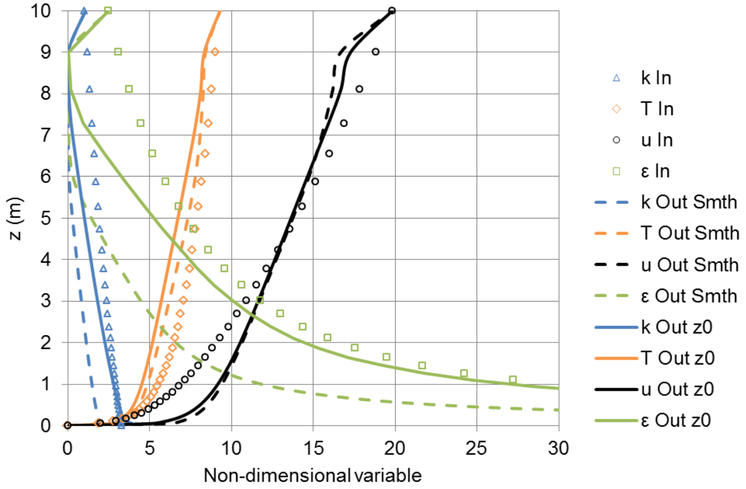


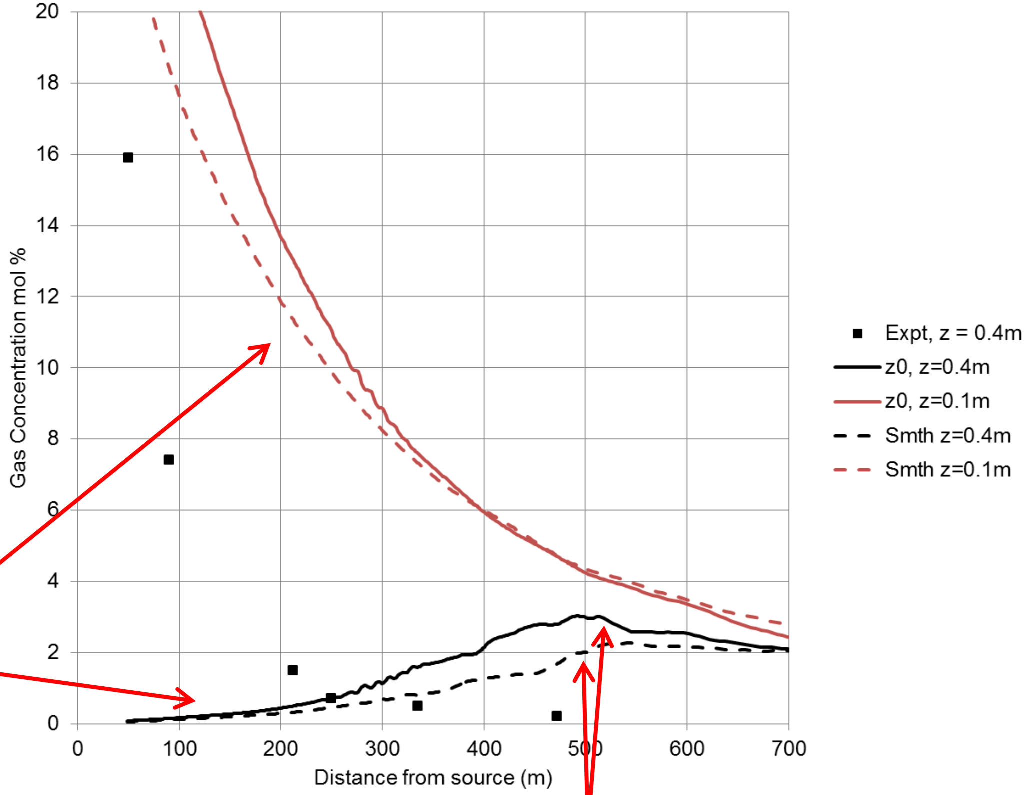
Releases at both 10 m and 1 km are affected by changed ABL profiles



@ Height z = 1.5 m

Thorney Island: dense gas, stable ABL





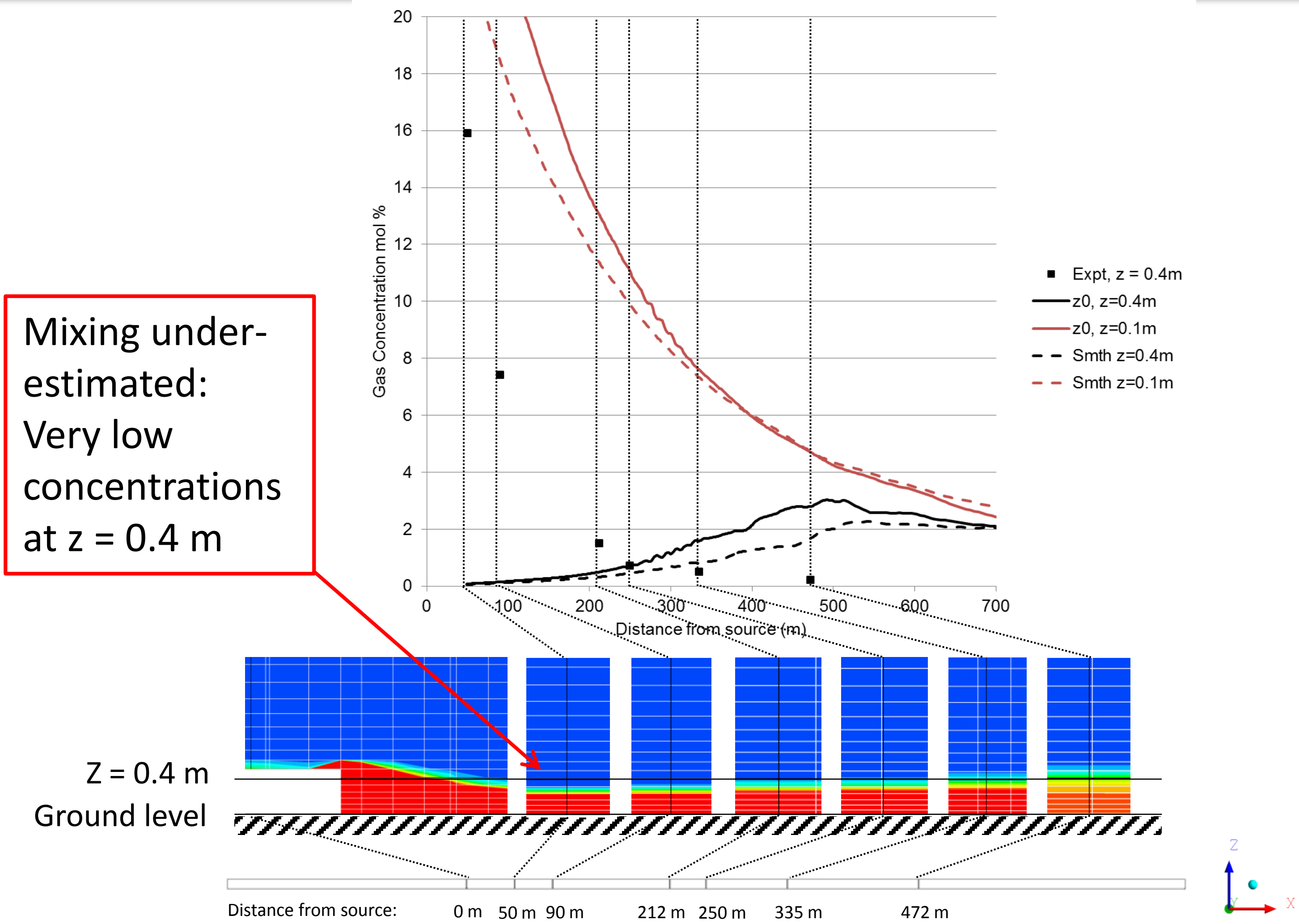
Strong vertical gradient: concentrations much higher at z = 0.1 m than at z = 0.4 m

Modelling of wall roughness (z0 or Smth) affects concentrations

Results shown for standard *k-ε* model
Alinot and Masson (2005) model was found to be numerically unstable and failed to produce results

Thorney Island: dense gas, stable ABL

Mixing under-estimated: Very low concentrations at z = 0.4 m



Case Study Conclusions

- Minor changes in ABL profiles affect dispersion predictions
- To minimise the effects of ABL profile changes put the source near the inlet (but it worked only for neutral ABL with Prairie Grass)
- Surface roughness
  - Mesh requirements for roughness and dense gas dispersion are incompatible
  - May be responsible for poor results in Thorney Island
- Unstructured grid useful to resolve fine details of source and span dispersion distances of kilometres
- Risk assessments using CFD with k-ε turbulence model should take into account the limitations of the model and issues relating to surface roughness and grid resolution

CFD Modelling of ABLs at HSL

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HSL Conference Papers

- Batt R., Gant S.E., Lacome J.-M. and Truchot B., 2016. *Modelling of stably-stratified atmospheric boundary layers with commercial CFD software for use in risk assessment*, 15th International Symposium on Loss Prevention and Safety Promotion in the Process Industries (Loss Prevention 2016), Freiburg, Germany, 5-8 June 2016
- Batt R., Gant S.E., Lacome J.-M., Truchot B. and Tucker H., 2016. *CFD modelling of dispersion in neutral and stable atmospheric boundary layers: Results for Prairie Grass and Thorney Island*, 17th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (Harmo-17), Budapest, Hungary, 9-12 May 2016
- Gant S.E. and Tucker H., 2017. *Computational Fluid Dynamics (CFD) modelling of atmospheric dispersion for land-use planning around major hazards sites in the UK* , 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (Harmo-18), Bologna, Italy, 9-12 October 2017

HSL Journal Papers

- Batt, R., Gant, S.E., Lacome, J.-M., Truchot, B. and Tucker, H. (2018) *CFD modelling of dispersion in neutral and stably stratified atmospheric boundary layers: results for Prairie Grass and Thorney Island*, International Journal of Environment and Pollution (In press)
- 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 (In press), https://doi.org/10.1016/j.jlp.2018.03.015

Turbulence Modelling

What is Steady/Unsteady RANS and LES?

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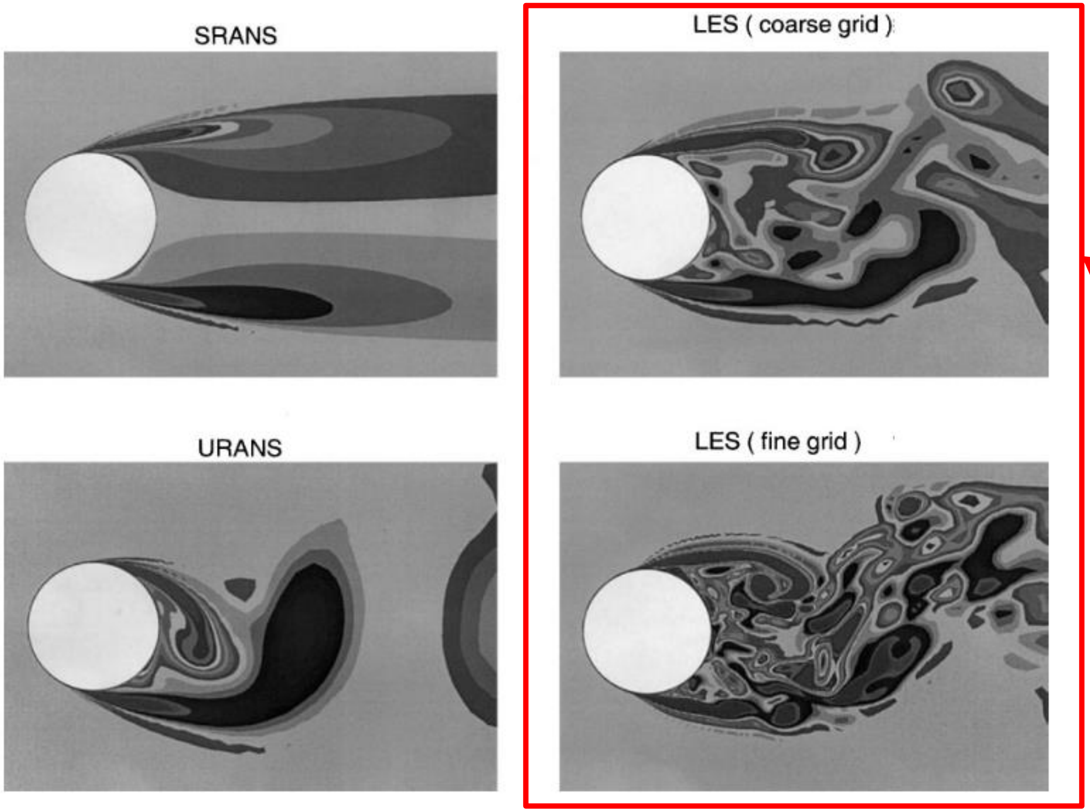
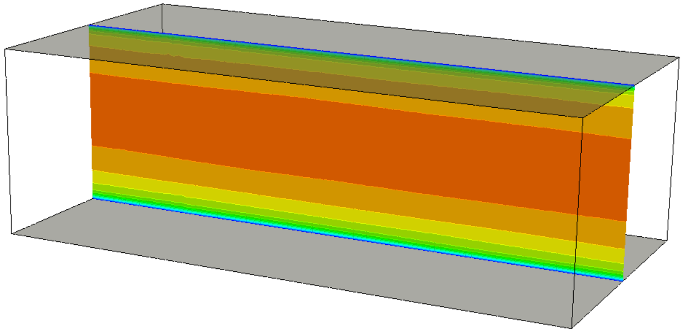


Fig. 4. Simulation of flow past circular cylinder by various approaches (Shur et al., 1996; Travin et al., 2000).

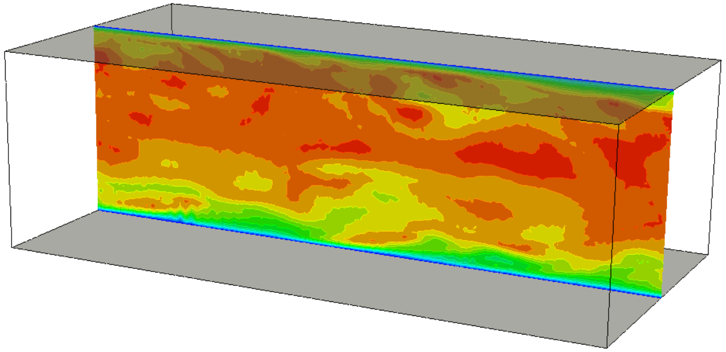
What about LES for atmospheric boundary layers?

Turbulence Modelling

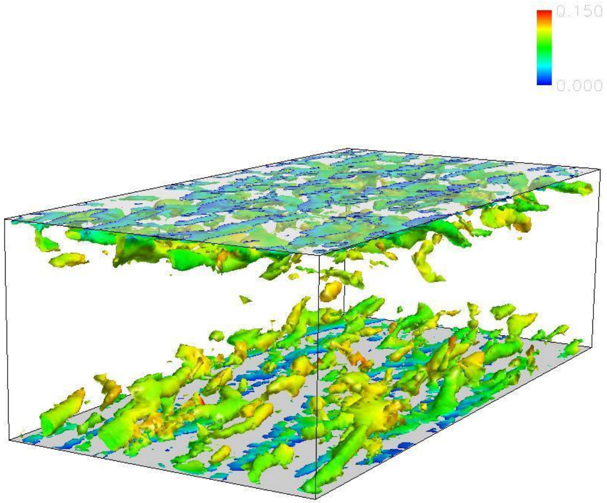
RANS



Large-Eddy Simulation (LES)



Streamwise velocity contours



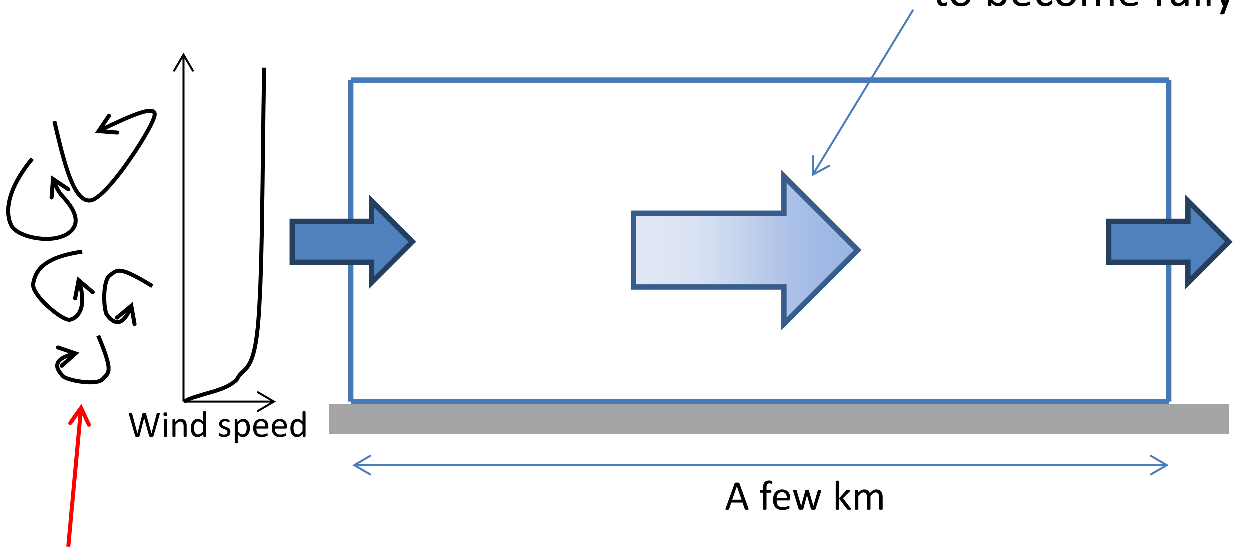
Coherent eddy structures

Large-Eddy Simulation Issues for ABLs

Inlet boundary conditions: two options

1.) Synthetic turbulence

Takes time (and distance downstream) for turbulence to become fully-developed

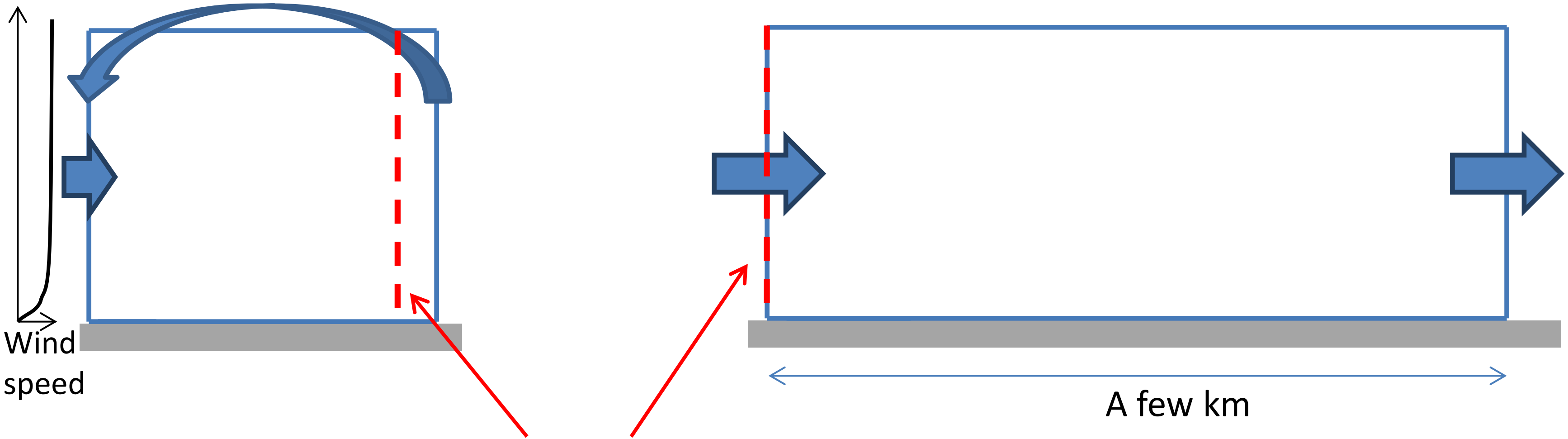


Generate time-varying coherent vortex structures with representative temporal and spatial scales of turbulence spectra, e.g. Synthetic Eddy Method (Jarrin *et al*., 2006)

Large-Eddy Simulation Issues for ABLs

Inlet boundary conditions

2.) Precursor simulation



Periodic inlet/outlet boundary

Wind speed

A few km

Once flow is fully-developed in precursor simulation, conditions are mapped onto inlet to domain (sometimes, with re-scaling)

Large-Eddy Simulation Issues for ABLs

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- Inflow profiles
  - 1.) Synthetic methods
    - Flexible and fast to apply
    - Flow within the domain can take time to generate realistic turbulence
  - 2.) Precursor simulations
    - Computing time needed for precursor simulation, but can store profiles for later use
    - Flow usually is fully developed from inlet (unless there are issues with re-scaling)
- Grid resolution
  - Must be fine enough to resolve turbulent structures or else turbulence will decay and flow become more laminar
- Options for resolving roughness
  - 1.) Resolve obstacles 2.) momentum forcing 3.) prescribed wall shear stress
  - E.g. Vasaturo, *et al*., 2018. *Large-eddy simulation of the neutral atmospheric boundary layer: performance evaluation of three inflow methods for terrains with different roughness*, J. Wind Eng. Ind. Aero, 173, p241-261.

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- Concepts: domain, grid, boundary conditions, finite-volume method
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  - Reynolds-Averaged Navier Stokes (RANS): steady and unsteady
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Part 1

- Atmospheric boundary layers
- CFD Software
- Case studies
  - Source terms: flashing jets, overfilling tanks
  - Local-scale atmospheric dispersion: Jack Rabbit II

Part 2

General-Purpose CFD Software

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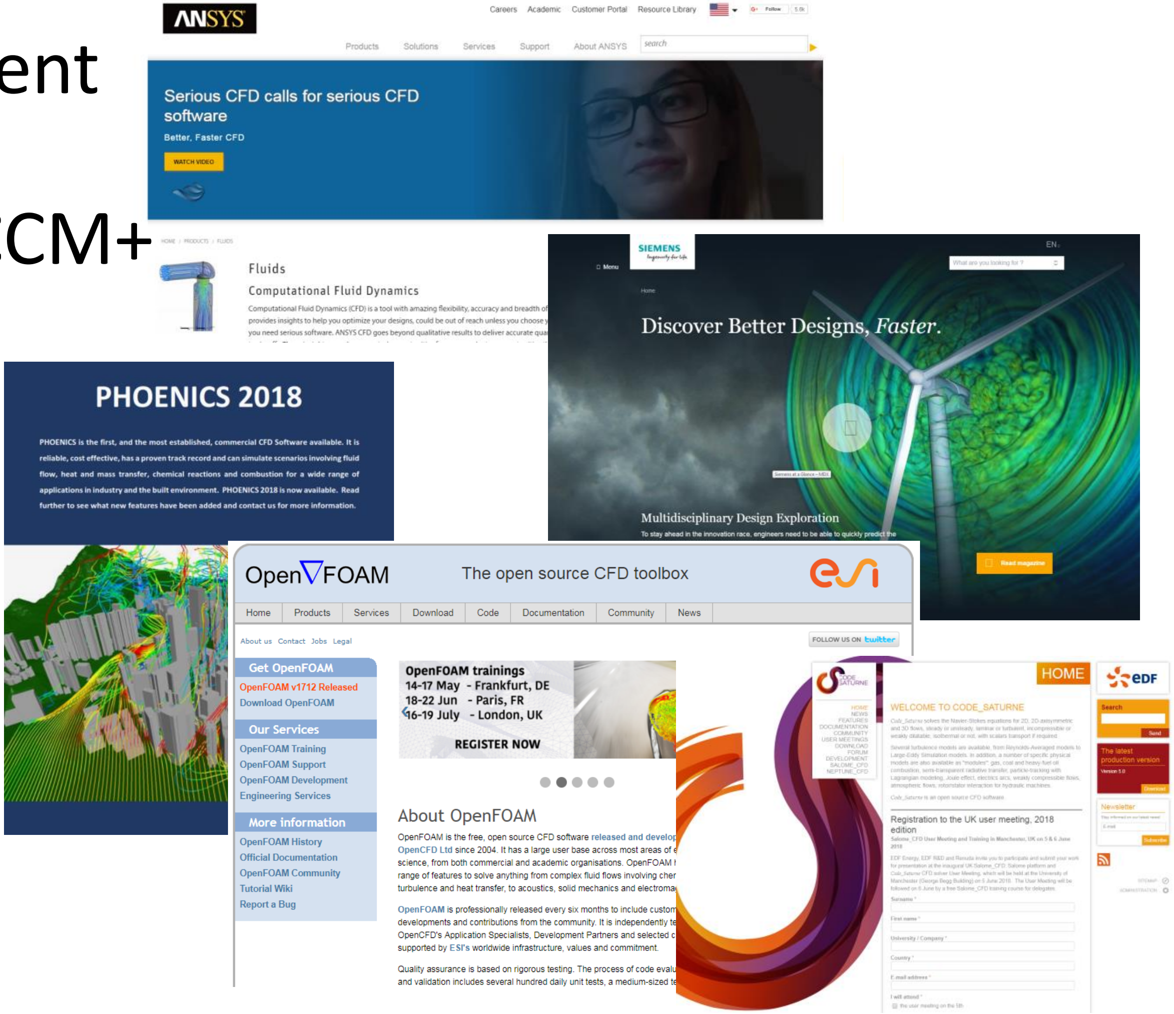
- ANSYS CFX/Fluent
- Siemens Star-CCM+
- Phoenics
- OpenFOAM
- Code Saturne



Serious CFD calls for serious CFD software

Better, Faster CFD

Fluids

Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) is a tool with amazing flexibility, accuracy and breadth of
provides insights to help you optimize your designs, could be out of reach unless you choose y
you need serious software. ANSYS CFD goes beyond qualitative results to deliver accurate qua

Discover Better Designs, *Faster*.

Multidisciplinary Design Exploration

To stay ahead in the innovation race, engineers need to be able to quickly predict the

PHOENICS 2018

PHOENICS is the first, and the most established, commercial CFD Software available. It is reliable, cost effective, has a proven track record and can simulate scenarios involving fluid flow, heat and mass transfer, chemical reactions and combustion for a wide range of applications in industry and the built environment. PHOENICS 2018 is now available. Read further to see what new features have been added and contact us for more information.

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OpenFOAM trainings
14-17 May - Frankfurt, DE
18-22 Jun - Paris, FR
16-19 July - London, UK

About OpenFOAM

OpenFOAM is the free, open source CFD software released and develop
OpenCFD Ltd since 2004. It has a large user base across most areas of e
science, from both commercial and academic organisations. OpenFOAM h
range of features to solve anything from complex fluid flows involving cher
turbulence and heat transfer, to acoustics, solid mechanics and electroma

OpenFOAM is professionally released every six months to include custom
developments and contributions from the community. It is independently te
OpenCFD's Application Specialists, Development Partners and selected c
supported by ESI's worldwide infrastructure, values and commitment.

Quality assurance is based on rigorous testing. The process of code evalu
and validation includes several hundred daily unit tests, a medium-sized te

WELCOME TO CODE_SATURNE

Code_Saturne solves the Navier-Stokes equations for 2D, 2D-axisymmetric and 3D flows, steady or unsteady, laminar or turbulent, incompressible or weakly dilatable, isothermal or not, with scalars transport if required.

Several turbulence models are available, from Reynolds-Averaged models to Large-Eddy Simulation models. In addition, a number of specific physical models are also available as "modules": gas, coal and heavy-fuel oil combustion, semi-transparent radiative transfer, particle-tracking with Lagrangian modeling, Joule effect, electrics arcs, weakly compressible flows, atmospheric flows, rotor/stator interaction for hydraulic machines.

Code_Saturne is an open source CFD software

Registration to the UK user meeting, 2018 edition

Salome_CFD User Meeting and Training in Manchester, UK on 5 & 6 June 2018

EDF Energy, EDF R&D and Renuda invite you to participate and submit your work for presentation at the inaugural UK Salome_CFD: Salome platform and Code_Saturne CFD solver User Meeting, which will be held at the University of Manchester (George Begg Building) on 5 June 2018. The User Meeting will be followed on 6 June by a free Salome_CFD training course for delegates.

Surname *

First name *

University / Company *

Country *

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I will attend *

☐ the user meeting on the 5th

The latest production version

Application-Specific CFD Software

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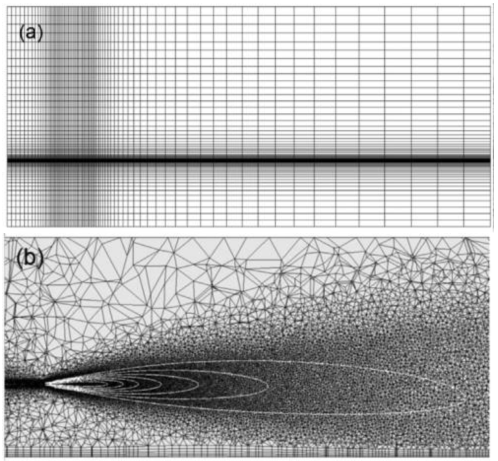
- Gexcon FLACS-Dispersion
  - Originally an explosion model for oil/gas industry
  - Porosity Distributed Resistance for sub-grid scale obstructions
  - Lagrangian particle-tracking model for sprays
  - Shallow-layer model for evaporating spills
- DNV GL Kameleon FireEx – KFX
  - Originally jet-fire model for oil/gas industry
  - Some similar capabilities to FLACS
- Fluidyn-Panache
  - Atmospheric pollution and industrial risk analysis
- Fire Dynamics Simulator (FDS)
  - Developed by NIST, LNG dispersion model validation

Main weakness: Cartesian grid



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  - Source terms: flashing jets, overfilling tanks
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Part 2

CFD Case Studies: Common Factors

Why use CFD in these examples?

- Complex flow behaviour
  - Geometry, e.g. multiple spray nozzles, liquid cascade around rim of tank
  - Coupled flow, e.g. evaporation of droplets with re-entrainment of vapour into the jet
  - Interaction of jet with obstacles and terrain, e.g. impinging jets
  - Nil-wind dispersion modelling
- Unable to use integral models
- Experimental data available to validate/tune CFD model
- Need to calculate quantities that cannot easily be measured, e.g. integrated vapour flow rate (not discrete point values)
- Ability to conduct parametric studies that would be costly to perform experimentally

Sprays and flashing two-phase jets

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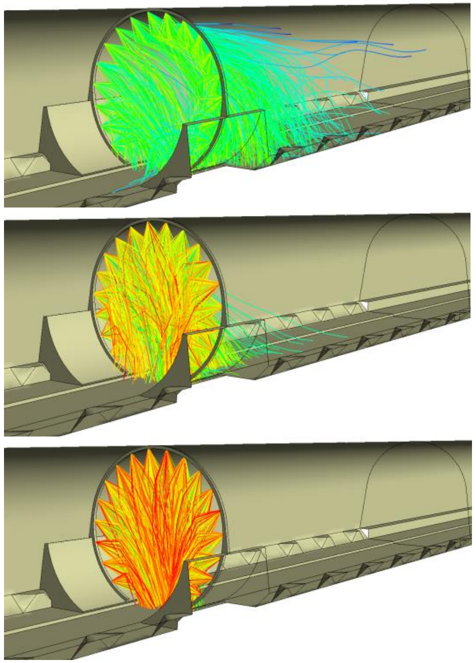

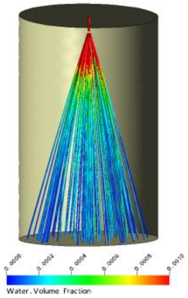

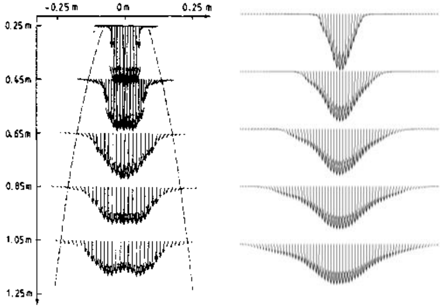

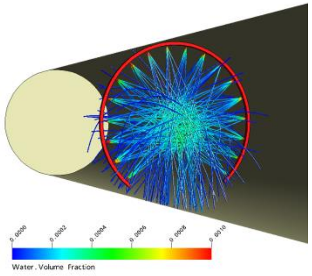

Sprays and flashing two-phase jets

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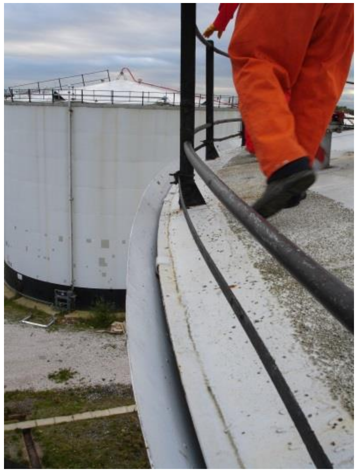
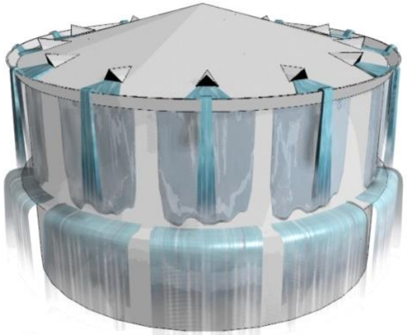
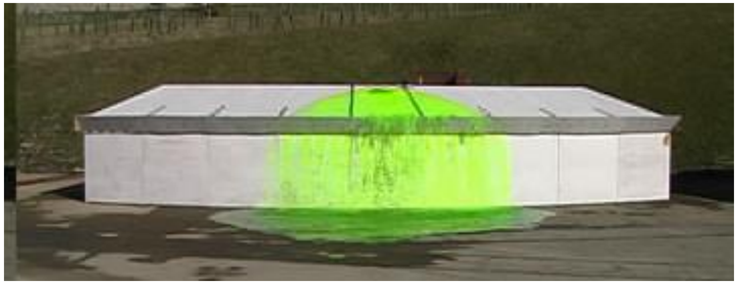
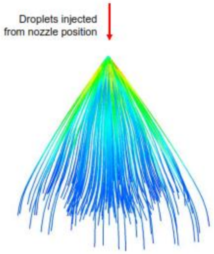


Sprays and flashing two-phase jets

- Buncefield Incident







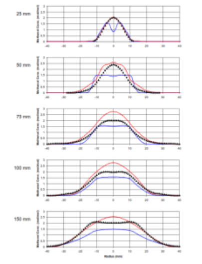
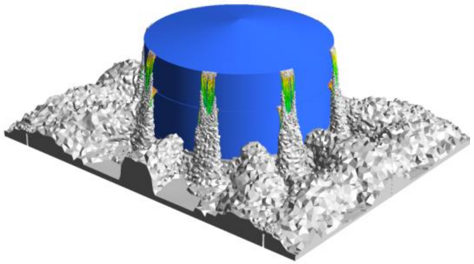
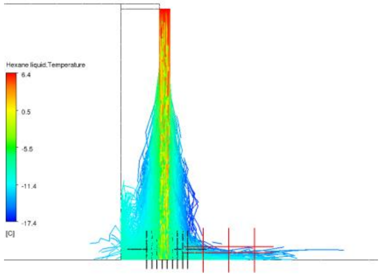
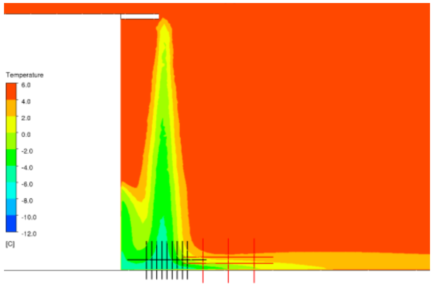


Figure 24 Predicted vapour concentrations for the RSA02 spray with different inlet conditions: — using experimental data; — using a 'best-guess' with no tuning; ▲ McDonell & Samuelsen experiments.





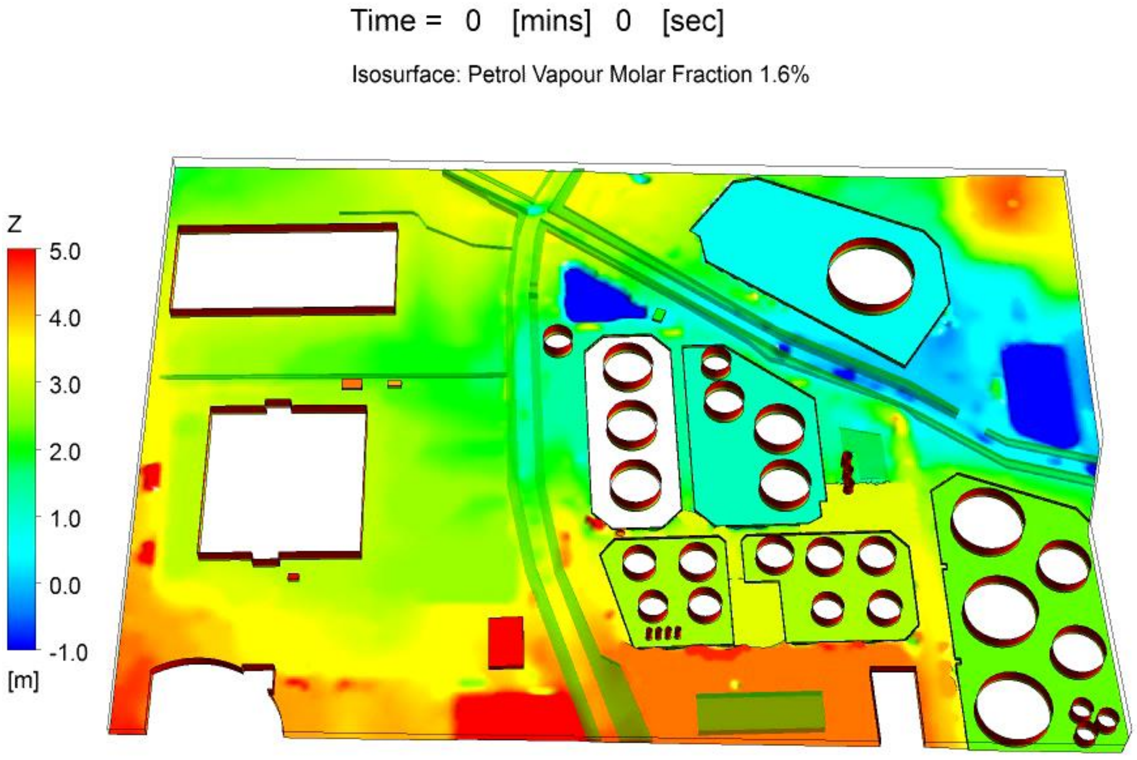


Sprays and flashing two-phase jets

- Buncefield Incident

Sprays and flashing two-phase jets

- Buncefield Incident



Sprays and flashing two-phase jets

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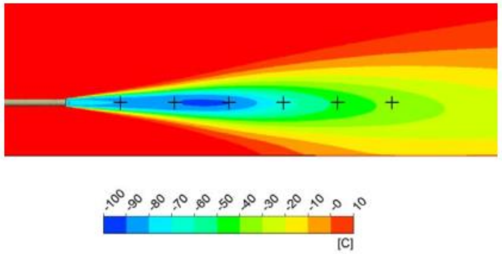
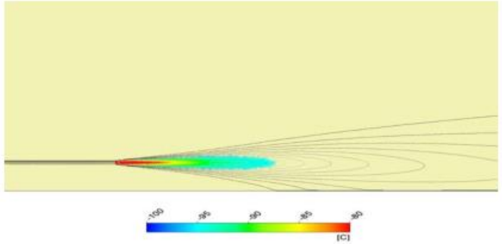
Sprays and flashing two-phase jets

- Carbon Capture and Storage





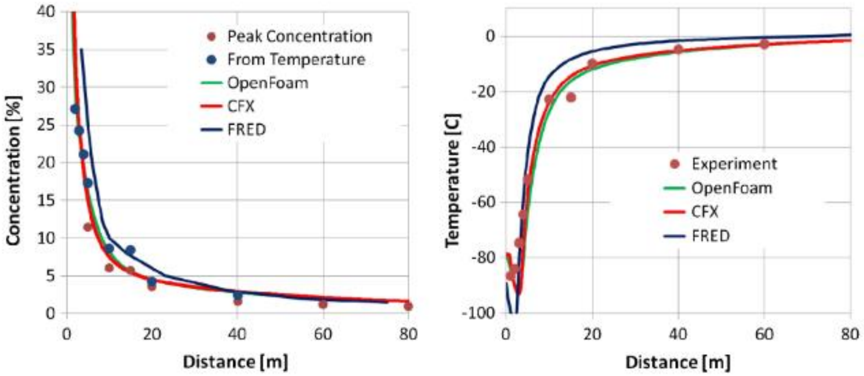


Figure 3. Measured and predicted centreline mole fraction (left) and temperatures (right) for Test 11

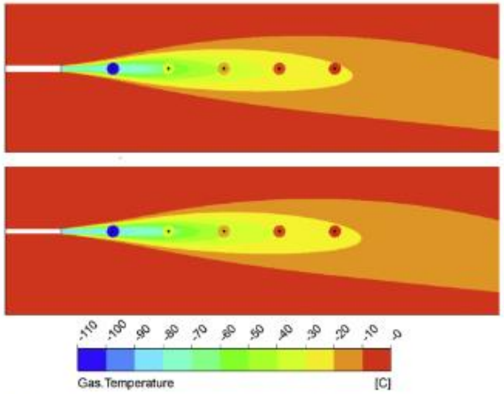


Fig. 8. Contours of predicted temperature for INERIS Test 2 using ANSYS-CFX with the full University of Leeds inlet profiles (top) and averaged inlet profiles (bottom). Coloured circles show the experimental values. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

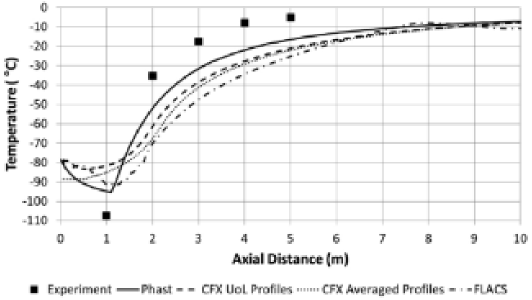


Fig. 6. Temperature along the centreline of the jet in INERIS Test 2.

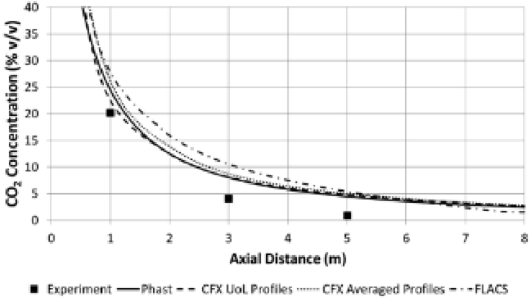


Fig. 7. CO_2 gas concentration along the centreline of the jet in INERIS Test 2.

Flashing two-phase jets and sprays

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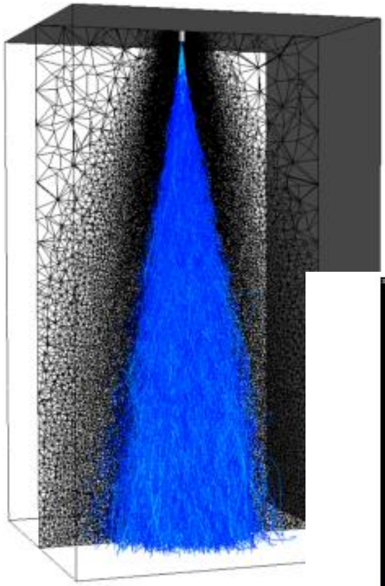
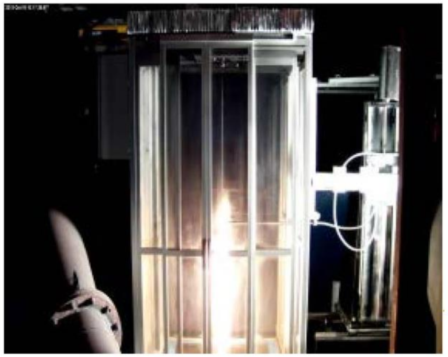




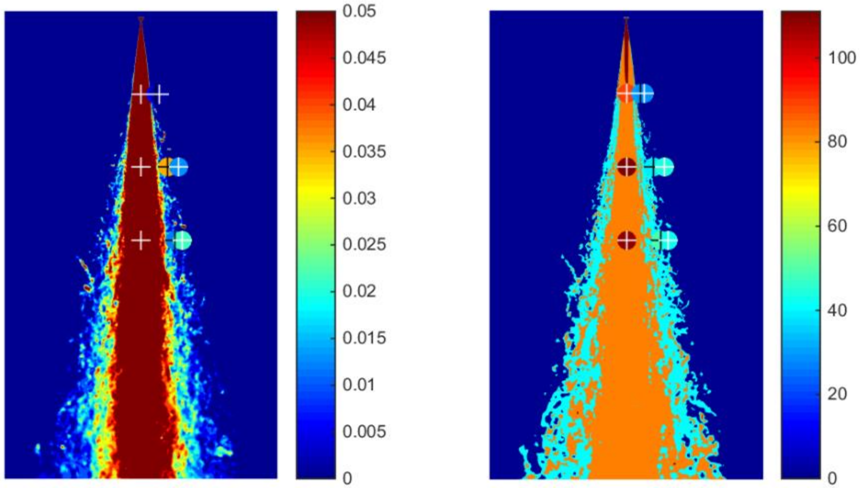
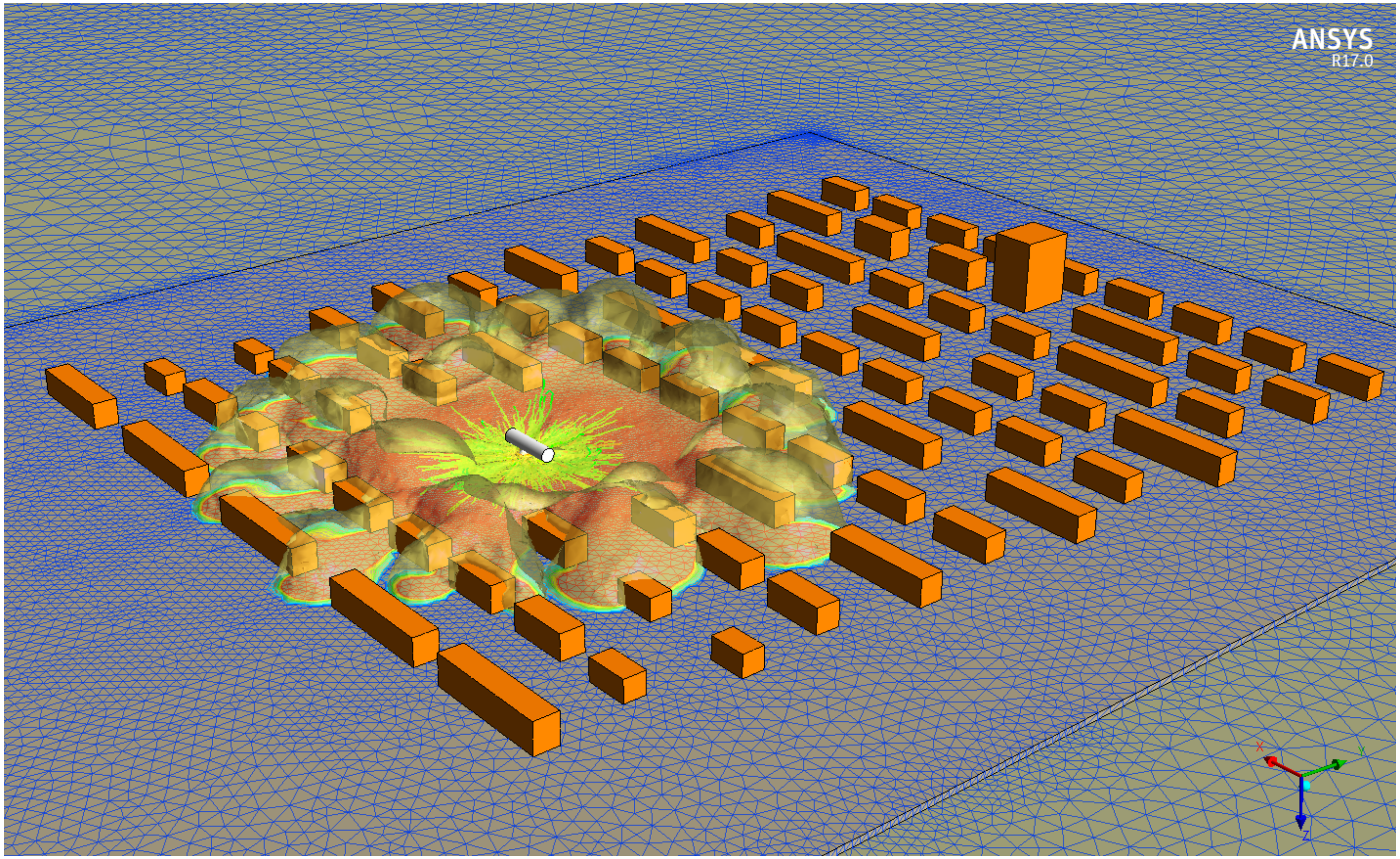


Figure 30 Contour plots of concentration (kg/m^3, left) and Sauter Mean Diameter (µm, right) for the DNV Phase III JIP RR primary breakup model

Flashing two-phase jets and sprays

- Jack Rabbit II chlorine releases



Flashing two-phase jets and sprays

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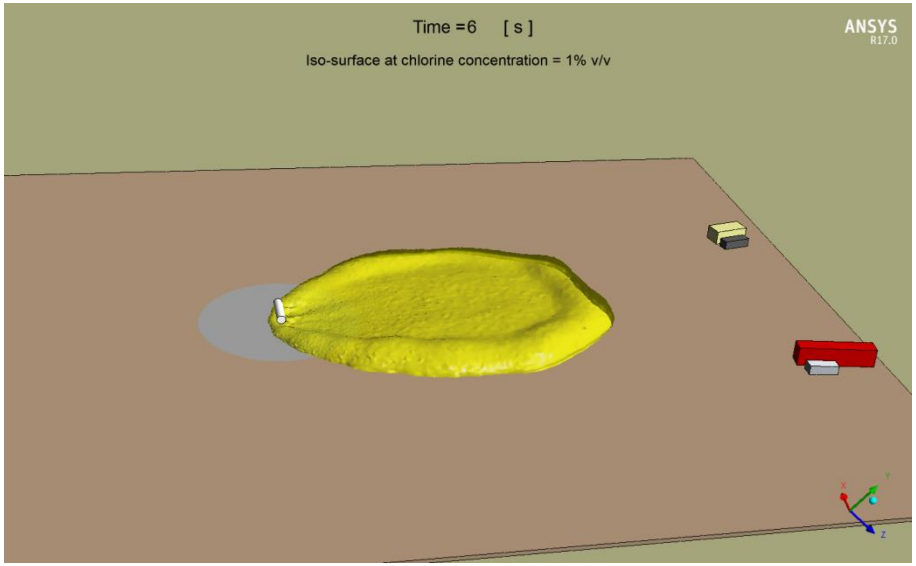
- Jack Rabbit II chlorine releases



Play Videos

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

Flashing two-phase jets and sprays

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- Jack Rabbit II chlorine releases
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Acknowledgements

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Sincere thanks to the organisations responsible for funding and managing the Jack Rabbit II trials (primarily the U.S. Department of Homeland Security and Defence Threat Reduction Agency) and the MWG coordinators and participants , in particular:

- Shannon Fox (DHS), Ronald Meris (DTRA), Richard Babarsky (US Army), Thomas Mazzola and John Magerko (Engility), Steven Hanna (Hanna Consultants), Joseph Chang (RAND), Thomas Spicer (Arkansas University),, Nathan Platt, Jeffry Urban and Kevin Luong (IDA), Jeffrey Weil (NCAR), John Boyd (ARA), Steven Herring (DSTL), Chlorine Institute, Andy Byrnes (UVU)

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