CFD modelling of dispersion in neutral and stable atmospheric boundary layers:

Results for Prairie Grass and Thorney Island

9th May 2016

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Overview

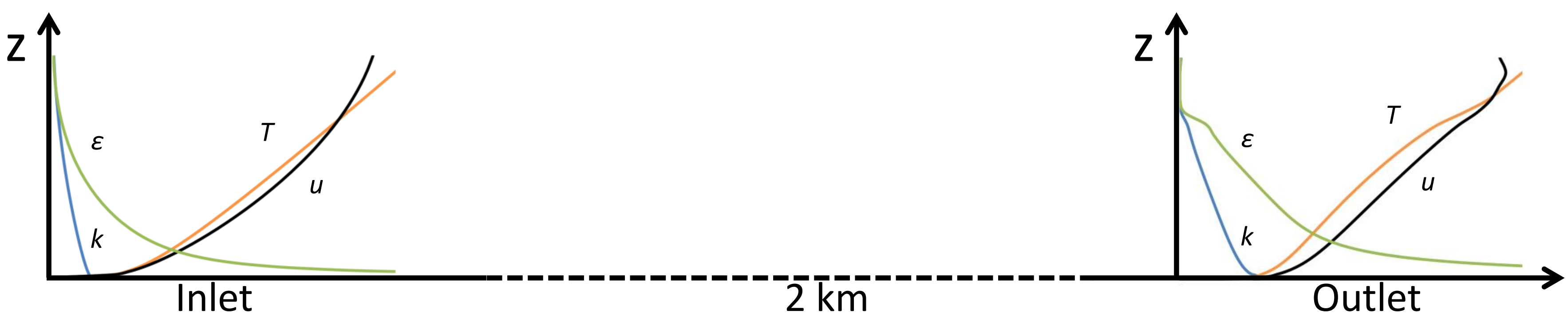
- Introduction
- Test cases
- CFD model
- Results
- Conclusions

Introduction – Are CFD models suitable for risk assessment?

- Growing interest in the use of CFD to assess risks from releases of toxic and flammable gases from industrial sites
- How do CFD models perform for stably-stratified atmospheric conditions, which often produce the largest hazardous zones in industrial risk assessments?

Literature – Known problems with standard *k-ε* for atmospheric dispersion

- Best practice guidance (BPG) available: Franke et al (2007), French Working Group (2015)
- Difficult to maintain the correct atmospheric boundary layer (ABL) profiles in CFD codes with *k-ε* turbulence model
  - Various solutions in the literature (discussed in Batt et al. 2016)
  - Many are complex and difficult to implement
  - Little is known about effects on gas dispersion



Test cases – 'simple', well-defined, large-scale field trials

What is the impact on dispersion predictions of errors introduced by CFD models of ABLs?

- Prairie Grass (Barad, 1958)
  - Flat, empty terrain
  - Continuous passive gas releases (SO2)
  - 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)
- Cases chosen are not sufficient to provide a statistical evaluation of the CFD model's capabilities

CFD Model – User judgement required

- Wind speed and direction assumed constant, no meandering
- 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 TI
- Input parameters and mesh statistics in the table below

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

Roughness specification – Incompatible with mesh requirements

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

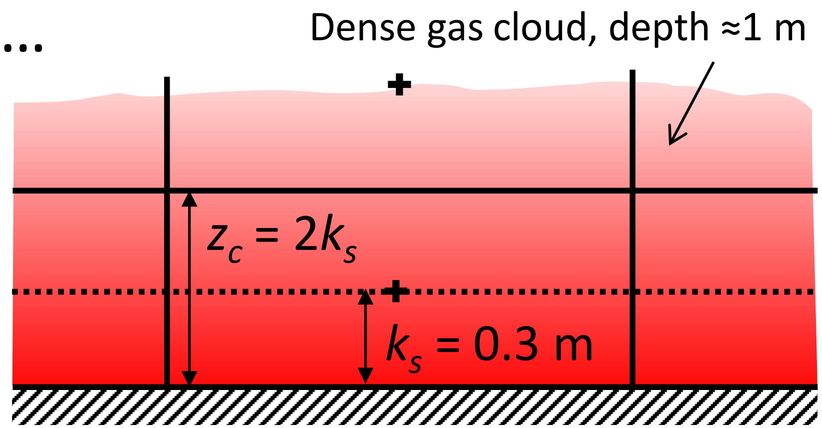
In CFX $k_s \approx 30z_0$ and wall functions for k-ε turbulence model have limit on near-wall cell height of $z_c > 2k_s$.
So, for TI47 with $z_0 = 0.01$ m:

$k_s = 0.3$ m

and

$z_c > 0.6$ m

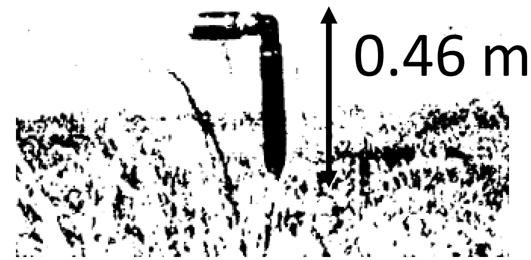
THE DENSE GAS CLOUD IS ONLY ABOUT 1M DEEP!



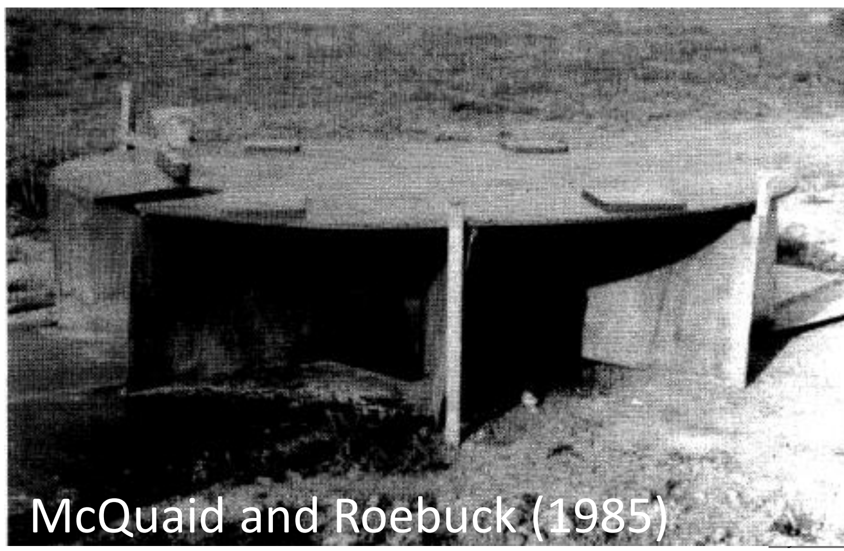
- z_0 on the wall was limited by the mesh to 0.0008 m or smooth
- z_0 in the ABL profiles on the inlet was correct at 0.01 m
- We expect the profiles to change but how much will this affect the gas dispersion?

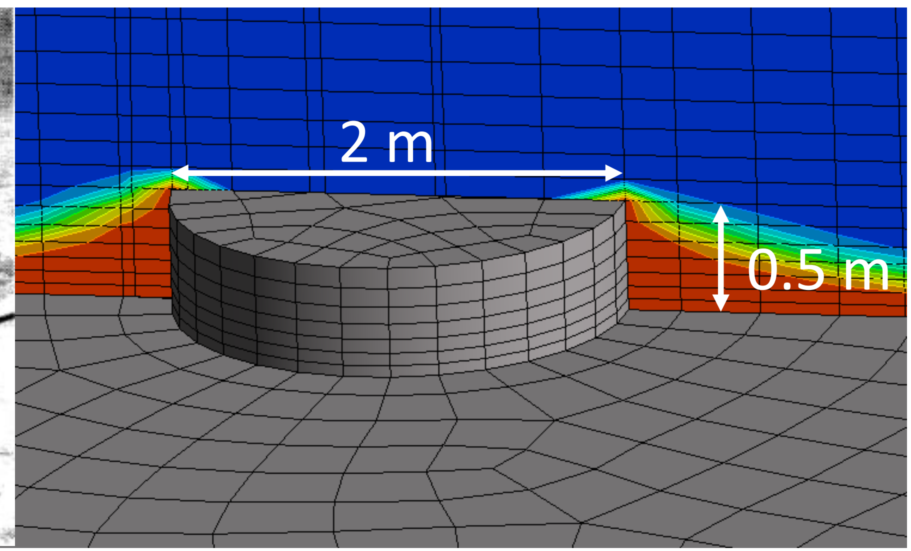
Source resolution – Difficult to reconcile with far field resolution

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



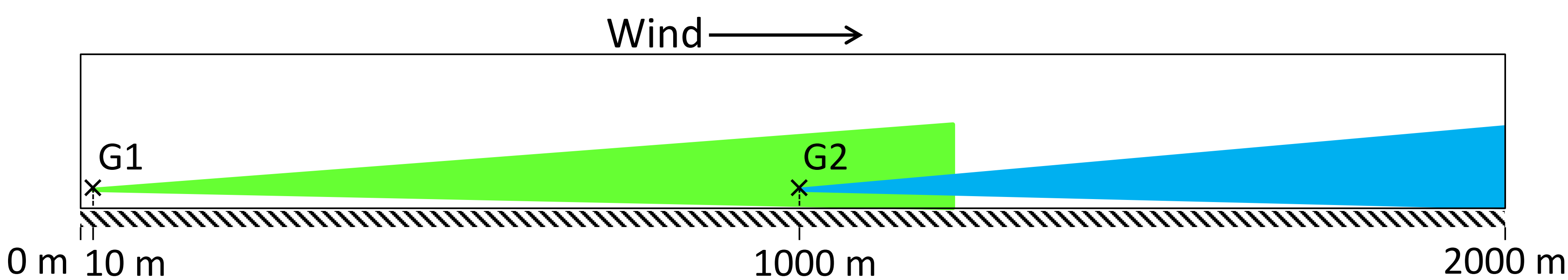
Barad (1958)


McQuaid and Roebuck (1985)

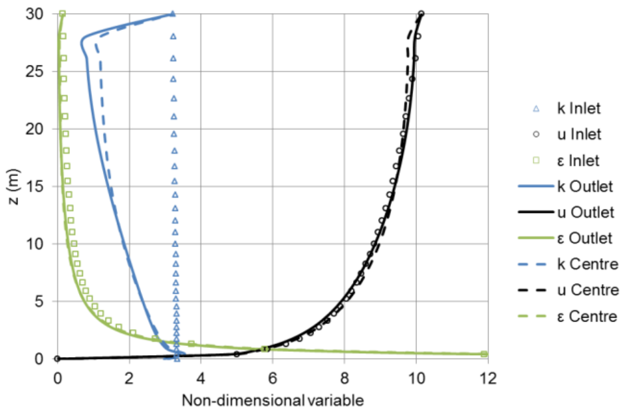


Assessing effects of profile change with multiple release points and fixed profiles

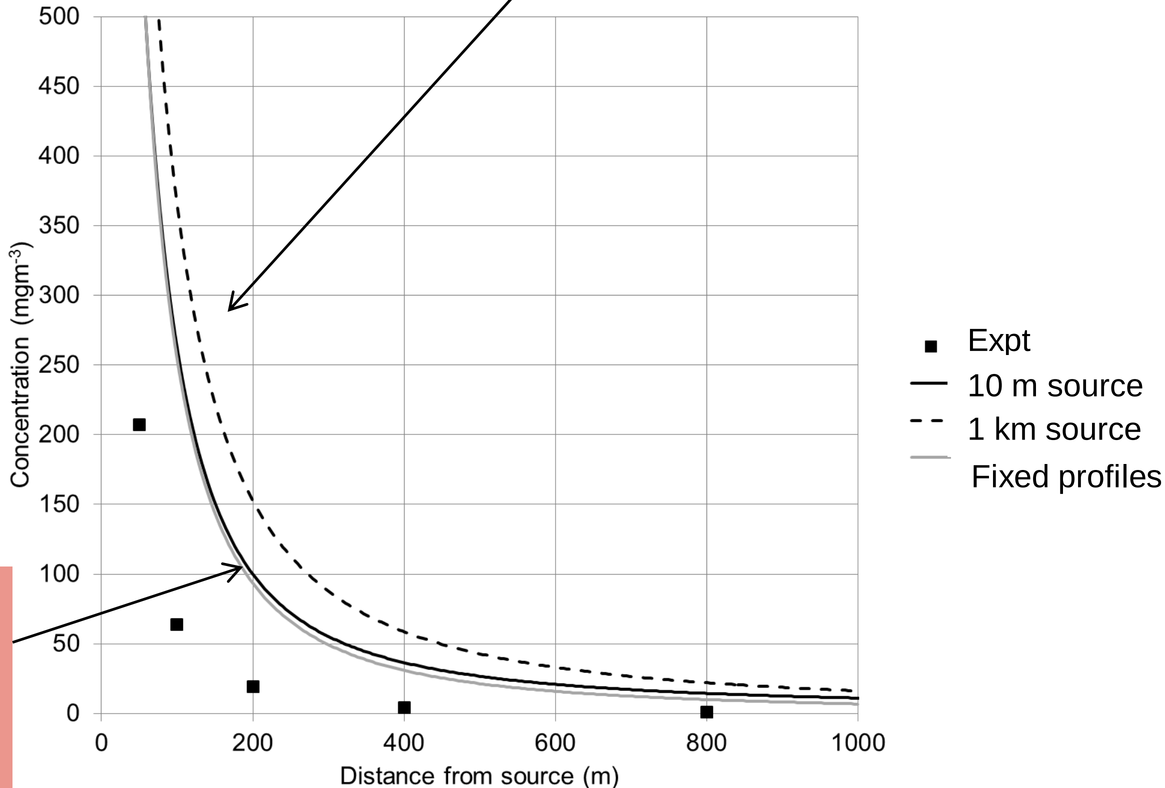
- Prairie Grass only
- Solving the full transport equations for all variables
  - Passive scalar was injected at two locations
  - If the profiles change gas will disperse differently
- ABL profiles ‘fixed’ throughout the domain as a reference case



Prairie Grass, neutral atmosphere – Profile changes increase concentration



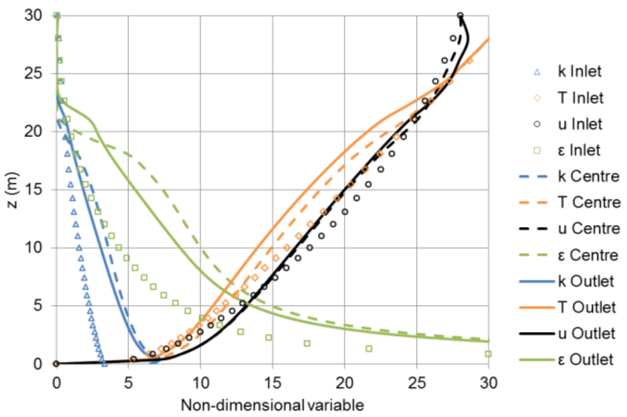
Release 1 km downwind



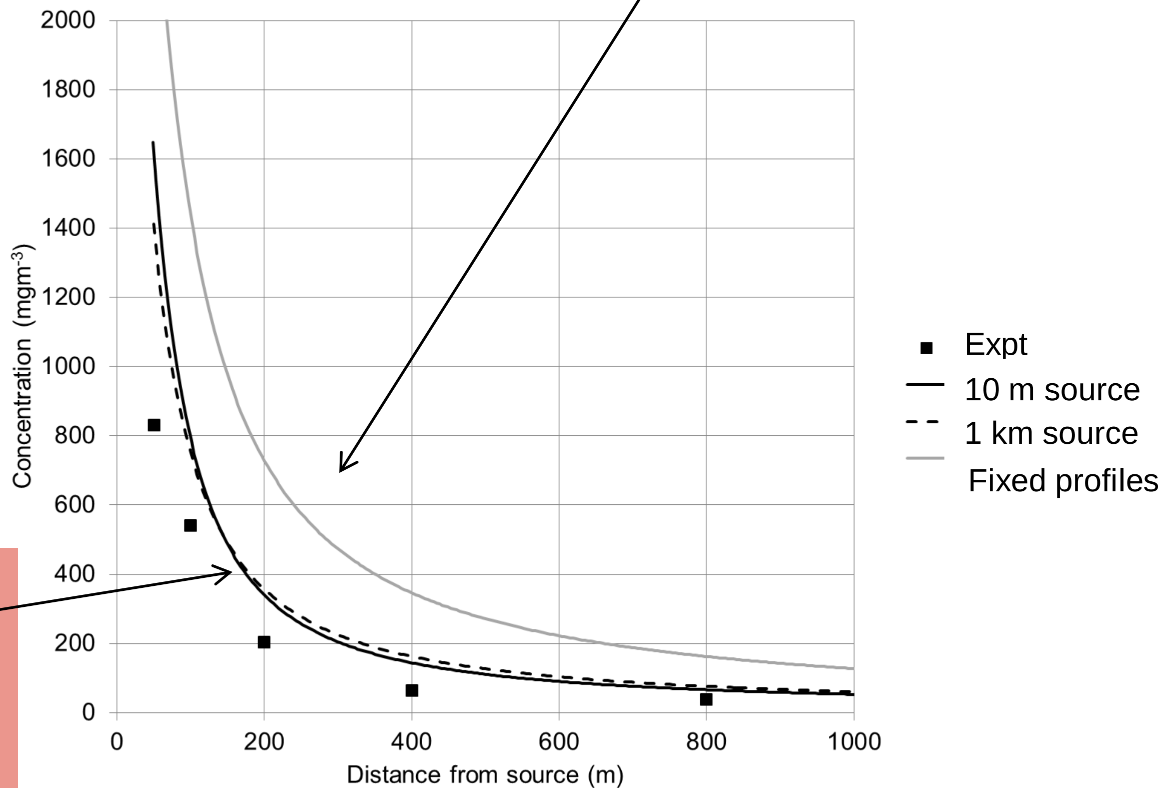
Release near the inlet is similar to case with fixed profiles

@ z = 1.5 m

Prairie Grass, stable atmosphere – Profile changes reduce concentration



Release with fixed flow profiles



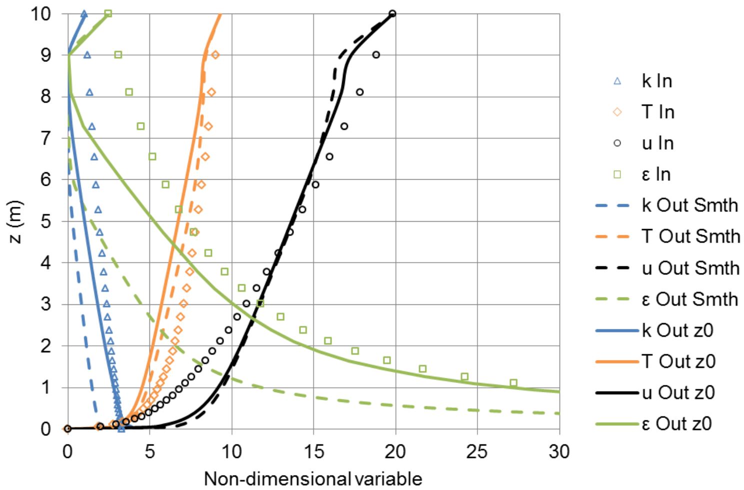
Release near the inlet is similar to release at 1 km downwind

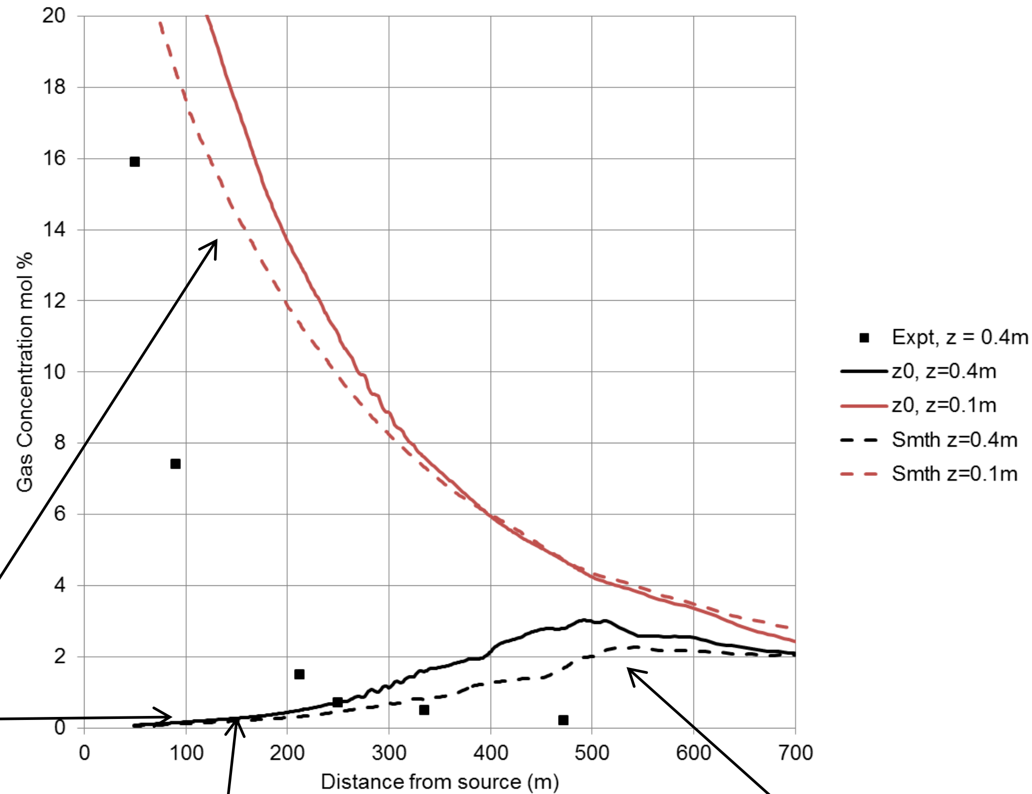
@ z =1.5 m

Passive dispersion – Minor changes in the ABL profiles impact on dispersion

- Minimise the effects of profile changes in the neutral case by putting the source near the inlet
- Predicted concentrations are up to 30 times larger than the experiments
  - Mixing is globally underestimated in the model
  - No wind meander
  - Crude source model but difficult with domain scale
  - Only two tests

Thorney Island, stable atmosphere – Insufficient vertical mixing





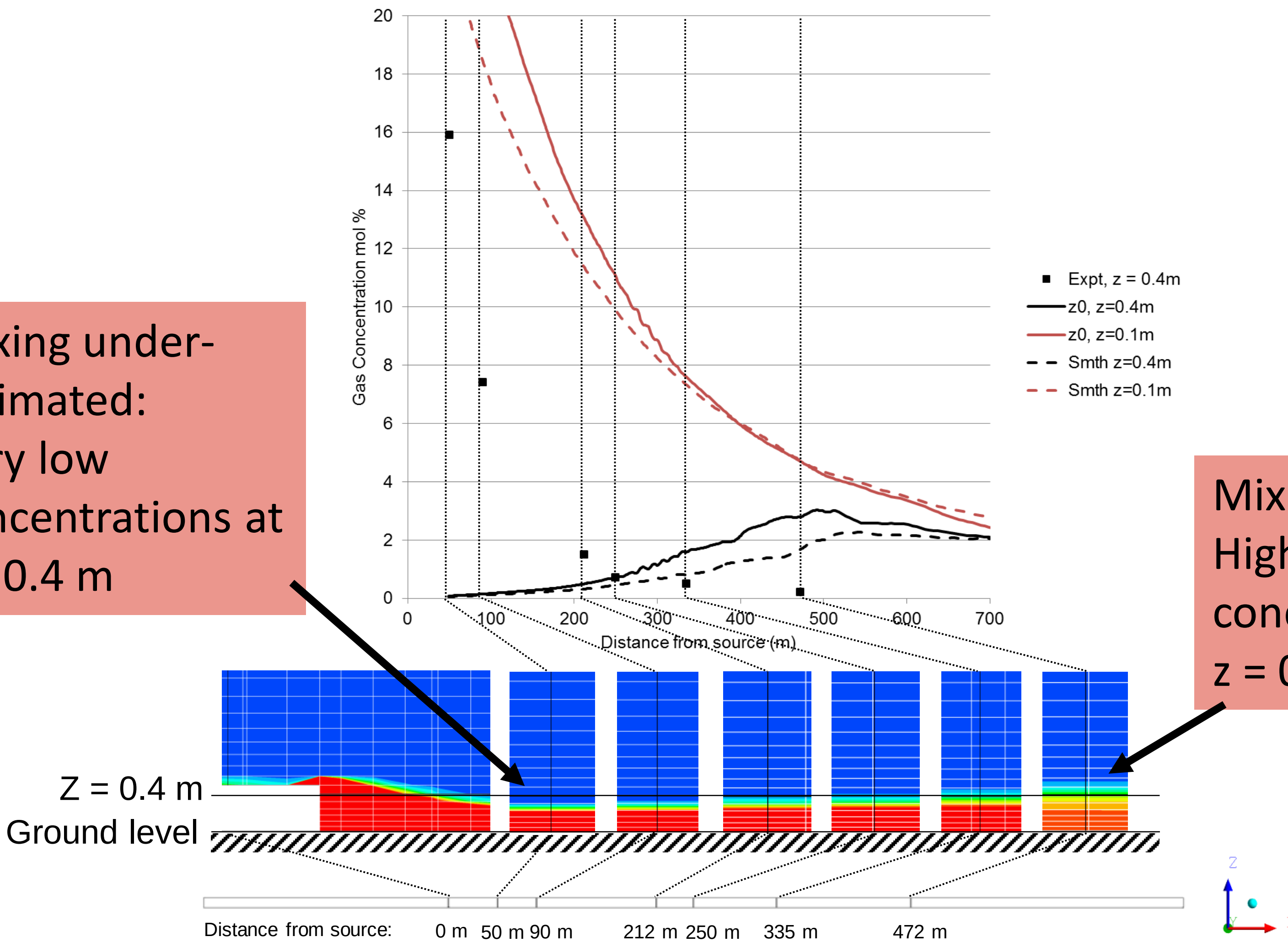
Strong vertical gradient in concentration

Under-predicts

Over-predicts

Thorney Island, stable atmosphere – Insufficient vertical mixing

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



Mixing increased:
Higher concentrations at z = 0.4 m

CFD models face several challenges for atmospheric dense-gas dispersion

- CFD results with the standard *k*-*ε* model show poor agreement with measurements
- The roughness length was smaller than in the experiments but…
- The correct roughness length could not be used in the CFD model
  - Requires near-wall grid cell to be at least 0.6 m high
- Our Alinot and Masson (2005) model was found to be numerically unstable with the dense gas present and failed to produce results

Conclusions – Are CFD models suitable for use in risk assessment?

- Minor changes in ABL profiles impact on dispersion
- Difficult to reconcile the mesh required at the source with the ultimate scale of the release
- Limited ability to handle roughness - mesh requirements for roughness and dense gas dispersion are incompatible
- For cases like Prairie Grass and Thorney Island alternative models might be better

It is important that risk assessments using CFD results take into account the uncertainties introduced by the limitations of the *k*-*ε* turbulence model and issues relating to surface roughness and grid resolution

Disclaimer

This publication and the work it describes were funded by the Health and Safety Executive (HSE). Its contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy

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