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

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Outline

- Concepts: domain, grid, boundary conditions, finite-volume method
- Turbulence Modelling
  - Reynolds-Averaged Navier Stokes (RANS): steady and unsteady
  - Large Eddy Simulation (LES)
- Atmospheric boundary layers
- CFD Software
- Case studies
  - Source terms: flashing jets, overfilling tanks
  - Local-scale atmospheric dispersion: Jack Rabbit II
Turbulence Modelling (just to recap)

What is Steady/Unsteady RANS and LES?

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

What is Steady/Unsteady RANS and LES?

Next slides focus on modelling atmospheric boundary layers with RANS

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

A few km
Modelling Atmospheric Boundary Layers

**Problem**: Atmospheric boundary layer profiles change along the domain

![Diagram showing wind speed and height profiles changing over a few km](image)
Modelling Atmospheric Boundary Layers

Cause:

- Standard $k$-$\varepsilon$ turbulence model tuned to produce 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 $k$-$\varepsilon$ specifically for ABLs

- Incompatibility problem: tuned $k$-$\varepsilon$ 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:


Advice on Modelling ABLs

Relevant academic papers:


CFD Modelling of ABLs at HSL

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 \( k-\varepsilon \) model with L&T profiles
  - \( k-\varepsilon \) model with modifications of A&M for both sets of inlet profiles
Results 1: Modified Turbulence models

- $u$ and $T$ under-predicted below about 10 m and over-predicted above 10 m
- $k$ and $\varepsilon$ are over-predicted for all $z$
Results 2: Modified Turbulence models

- 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?

- 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 $\varepsilon$ 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

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

McQuaid and Roebuck (1985)

Barad (1958)
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 near the inlet is similar to case with fixed profiles

Release 1 km downwind is affected by changed ABL profiles

@ Height $z = 1.5$ m
Prairie Grass PG36: stable ABL

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 $z = 0.1 \text{ m}$ than at $z = 0.4 \text{ m}$

Results shown for standard $k$-$\varepsilon$ model. Alinot and Masson (2005) model was found to be numerically unstable and failed to produce results.

Modelling of wall roughness ($z_0$ or Smth) affects concentrations.
Thorney Island: dense gas, stable ABL

Mixing underestimated:
Very low concentrations at $z = 0.4\, \text{m}$

$Z = 0.4\, \text{m}$
Ground level
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 $k-\varepsilon$ 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

HSL Conference Papers


- 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


Turbulence Modelling

What is Steady/Unsteady RANS and LES?


SRANS

LES (coarse grid)

URANS

LES (fine grid)

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

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

Takes time (and distance downstream) for turbulence to become fully-developed
Large-Eddy Simulation Issues for ABLs

Inlet boundary conditions

2.) Precursor simulation

Periodic inlet/outlet boundary

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

- **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
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General-Purpose CFD Software

- ANSYS CFX/Fluent
- Siemens Star-CCM+
- Phoenics
- OpenFOAM
- Code Saturne
Application-Specific CFD Software

- **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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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

- **Toxic/flammable pressure-liquefied gas jets**
  - Kelsey (2001) Simulation of flashing propane jets, HSL Report CM/00/02

- **Water spray barriers**
Sprays and flashing two-phase jets

Buncefield Incident

- Coldrick S., Gant S.E. and Atkinson G.T. "Large scale evaporating liquid cascades -- an experimental and computational study" IChemE Hazards XXII Conference, Liverpool, UK, 11-14 April 2011
Sprays and flashing two-phase jets

- Buncefield Incident
Sprays and flashing two-phase jets

- Buncefield Incident
Sprays and flashing two-phase jets

- Buncefield Incident

Time = 0 [mins] 0 [sec]

Isosurface: Petrol Vapour Molar Fraction 1.6%
Sprays and flashing two-phase jets

- **Carbon Capture and Storage**
  - 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
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

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

**Figure 7.** CO₂ gas concentration along the centreline of the jet in INERIS Test 2.

**Figure 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.)
Flashing two-phase jets and sprays

- Coldrick S. and Gant S.E., "CFD modelling of oil mists for area classification", HSE Research Report RR1111, 2018

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Flammable mists

Figure 30 Contour plots of concentration (kg/m³, 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

- Jack Rabbit II chlorine releases

Play Videos

http://www.uvu.edu/esa/jackrabbit/
Flashing two-phase jets and sprays

Jack Rabbit II chlorine releases

- Gant S.E., McKenna B., Garcia M., Batt R., Witlox H.W.M., Stene J., Fernandez M. and Tickle G. "Integral dispersion model predictions for the proposed Jack Rabbit II experiments", 19th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, 9-10 June 2015, Fairfax, Virginia, USA


- Gant S.E. and Tucker H."CFD results for near-field dispersion in Jack Rabbit II ", 21st Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, Virginia, USA, 13-15 June 2017


Acknowledgements

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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