CHALLENGES OF DUST DEPOSITION MONITORING:

Pitfalls of dust monitoring results received when doing air quality modelling

3 December 2015
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• Airborne Particulate Characterisation
  ▪ Source Types
  ▪ Particulate Types
  ▪ Information Gaps

• ASTM 1739 Dustfall Rate Monitoring
  ▪ Comparison of different sampling methods

• Basic Dispersion Modelling Concepts
  ▪ AERMOD & CALPUFF
  ▪ Differences between Modelled and Sampled Deposition Rates
  ▪ Inadequacies and Information Gaps

• Questions and Answers

• Conclusions & Recommendations
Prominent Questions

• “Industry has collected records over many years in some cases using the four bucket system for dust monitoring, is this still of value or must it be discarded?”

• “Single bucket, shield/no shield, four-bucket directional - Are these comparable?”

• “What do we measure with dustfall monitoring equipment?”
More Questions

• “How suitable is dustfall monitoring data for use in air quality modelling studies?”

• “How do atmospheric dispersion models simulate airborne particulate matter?”

• “Are the National DustFall Standards applicable to modelled results?”
PARTICULATE CHARACTERISATION
Examples of Particulate Emissions

Wheel Entrainment

Dust Storm in Gobi Desert

July 2001 Mt. Etna’s eruption

Point source emissions

Materials handling
Forces Acting on Airborne Particle (Still Air)

**Gravitational Force:**

\[ F_G = \frac{\pi d^3}{6} \rho_p g \]

**Archimedes' Buoyancy Principle:**

Buoyant force \((F_B)\) exerted on a floating body is equal to the weight of the fluid displaced by the body:

\[ F_B = \frac{\pi d^3}{6} \rho_g g \]

**Newton's Resistance Equation:**

A sphere pushes aside a volume of gas equal to the projected area of the sphere times its velocity.

\[ F_D = C_D \frac{\pi d^2}{8} \rho_g V^2 \]

**Stokes Law (i.e., small Re):**

\[ C_D = \frac{24}{Re} \text{ where } Re = \frac{\text{inertial forces}}{\text{viscous forces}} = \frac{\rho_g V d}{\mu} \]

**Drag Coefficient**
Particle Settling Times – Unit Density Spheres

Still Air: Time to settle 1.5 m

Turbulent Air: Half-live of particles in 2.4 m depth of air

- 0.5 µm: 41 hours
- 1 µm: 12 hours
- 3 µm: 1.5 hours
- 10 µm: 8.2 minutes
- 100 µm: 5.8 seconds
Terminal Settling Velocity (Small Particles)

- Stokes’ Law:

\[ v_T = \frac{(\rho_p - \rho_g)gd^2}{18\mu} S_{CF} \]

Where the slip correction factor*, \( S_{CF} \), varies from 22.7 for 0.01 µm to \(~1.0\) for 10 µm (\( S_{CF}=1.168 \) for 1 µm)

- Stokes’ Law strictly not valid for \( Re > 0.1 \) (typically particles larger than 20 µm)

- This form is used in AERMOD and CALPUFF

* - also known as Cunningham correction
Terminal Settling Velocity (Large Particles)

- Stokes’ Law strictly not valid for $Re > 0.1$
  - At $Re = 0.3$ 5% error ($\sim 54 \mu m$)
  - At $Re = 1.0$ 12% error ($\sim 80 \mu m$)
  - For $\rho_p = 1000 \text{ kg/m}^3$

- The general equation for terminal settling velocity:
  \[
  v_T = \sqrt{\frac{4(\rho_p - \rho_g)gd^2}{3C_D\rho_g}}
  \]

  But not easily solved since $C_D$ depends on $v_T$

- This is not included in AERMOD nor CALPUFF, but ADMS employs an approximation of solved cases
Stokes’ Terminal Settling Velocity Error

Particle Density of 1000 kg/m³
Variety of Airborne Particulates

Coal Boiler Soot

Soot from Wild Fires
Terminal Settling Velocity – Non-Spherical

• Stokes’ Law (non-spherical particle):

\[ v_T = \frac{(\rho_p - \rho_g)gd^2}{18\mu\chi} S'_CF \]

Where the dynamic shape factor, \( \chi \), is mostly \( \geq 1.0 \) and \( S'_CF \) is the slip correction factor for irregular particle shapes (\( S'_CF \) 0 to 12% greater than \( S_{CF} \))

• Values for common dusts:
  - Bituminous coal : \( \chi = 1.05 \) to 1.11
  - Quartz : \( \chi = 1.36 \)
  - Sand : \( \chi = 1.57 \)
  - Talc : \( \chi = 1.88 \)
# Shape Factor

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<tr>
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<th>Ratio of Axis</th>
<th>Factor</th>
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<td>Three (triangle)</td>
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<td>Three (inline)</td>
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<td>1.34 – 1.40</td>
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<td>Four (inline)</td>
<td>4</td>
<td>1.56 – 1.58</td>
</tr>
</tbody>
</table>

*Source: Chamberlain (1975) and Johnson et al (1987)*
Non-Spherical Particles

Stokes’ Equivalent Diameter, \( d_s = 4.3 \, \mu m \)

\[ \rho_p = 4000 \, \text{kg/m}^3 \]
\[ \chi = 1.36 \]

Equivalent Volume Diameter, \( d_e = 5 \, \mu m \)

\[ v_T = 2.2 \, \text{mm/s} \]

Aerodynamic Diameter, \( d_a = 8.6 \, \mu m \)

\[ v_T = 2.2 \, \text{mm/s} \]

Aerodynamic Diameter: the diameter of the spherical particle with a density of 1000 kg/m³ and the same settling velocity as the irregular particle

\[ \rho_p = 1000 \, \text{kg/m}^3 \]

\[ v_T = 2.2 \, \text{mm/s} \]
Particle Motion

- **Particle Character**
  - Particle Size ($d$)
  - Particle Density ($\rho_p$)
  - Particle Shape and Agglomeration
    - All equations assume spherical shape
    - Non-spherical - Use dynamic shape factor ($\chi$) or the aerodynamic diameter ($d_a$), or Stokes’ equivalent diameter ($d_s$)

- **Airborne Motion**
  - Larger, dense and spherical particles deposit closer to source of origin
  - Smaller, light and highly irregular shaped particles travel longer distances
ASTM 1739 DUSTFALL RATE MONITORING
Tailings Dam Multi-Vertical Sampling (MVS)

- Fugitive Dust (<20μm)
- Suspension (20-70μm)
- Saltation (70-500μm)
- Sandblasting
- Lifting of small particles
- Surface Creep (>500μm)

Wind direction is indicated on the right side of the diagram.
Bucket Without Shield (2 m/s)

Contours of Velocity Magnitude (m/s)
Bucket With Shield (2 m/s)

Pathlines Colored by Velocity Magnitude (m/s)  
ANSYS Fluent Release 16.2 (3d, dp, pbns, sstkw)

By permission from Prof Ken Craig (UP)
Bucket Without Shield (1 m/s)

Contours of Velocity Magnitude (m/s)

Nov 24, 2015
ANSYS Fluent Release 16.2 (3d, dp, pbns, stikw)

By permission from Prof Ken Craig (UP)
Bucket With Shield (1 m/s)

Contours of Velocity Magnitude (m/s)

By permission from Prof Ken Craig (UP)
BASIC DISPERSION MODELLING CONCEPTS
Gaussian Plume Model

Stockie (2011)
Regulatory Model: AERMOD

\[ C(x, y, z) = \frac{Q}{2\pi u\sigma_y(x)\sigma_z(x)} g(x, z) \exp \left( -\frac{y^2}{2\sigma_y^2(x)} \right) \]

\[ g(x, z) = \exp \left( -\frac{(z - H)^2}{2\sigma_z^2(x)} \right) + \exp \left( -\frac{(z + H)^2}{2\sigma_z^2(x)} \right) \]

Horizontal Spread

Vertical Spread

Reflection Term
Tilted Gaussian Plume Model

Concept: Ermak (1977)
TILTED Gaussian Plume Model

\[ g(x, z) = \exp\left(-\frac{(z - H + v_t x / u)^2}{2\sigma_z^2(x)}\right) \]

\[ + \alpha(x_G)\exp\left(-\frac{(z + H - v_t x / u)^2}{2\sigma_z^2(x)}\right) \]

\[ v_t = \text{terminal settling velocity} \]

\[ \alpha(x_G) = \text{reflection coefficient} (= 0 \text{ to } 1) \]

\[ \text{function of particle size \& density; and wind speed and atmospheric stability} \]

GAUSSIAN PUFF MODEL
Regulatory Model: CALPUFF

\[ C(x, y, z, t) = \frac{Q}{2\pi \sigma_x(t) \sigma_y(t)} g(z, t) \exp \left( -\frac{(x - x_0)^2}{2\sigma_x^2(t)} \right) \exp \left( -\frac{(y - y_0)^2}{2\sigma_y^2(t)} \right) \]

Horizontal Spread

Vertical Spread

\[ g(x, z) = \frac{2}{\sqrt{2\pi} \sigma_y(t)} \left[ \exp \left( -\frac{(z - H)^2}{2\sigma_y^2(t)} \right) + \exp \left( -\frac{(z + H)^2}{2\sigma_y^2(t)} \right) \right] \]
TILTED Gaussian Puff Model

\[ g(z, t) = \frac{2}{\sqrt{2\pi} \sigma_y(t)} \left[ \exp \left( -\frac{(z - H + \nu_t t)^2}{2\sigma_z^2(t)} \right) \right. \\
+ \left. \alpha(x_G) \exp \left( -\frac{(z + H - \nu_t t)^2}{2\sigma_z^2(t)} \right) \right] \]

\( \nu_t = \text{terminal settling velocity} \)
\( \alpha(x_G) = \text{reflection coefficient} \ (= 0 \text{ to } 1) \)
Deposition Rate

\[ D(x, y, t) = v_d C(x, y, z = 0, t) \]

\( D \) = deposition rate (mass per unit area per time)
\( C \) = concentration at ground level (mass per volume)
\( v_d \) = deposition velocity (length per time)

\[ v_d = f \text{ (aerodynamic and substrate resistances)} + v_t \]
Fig. 10.3 Laboratory and field measurements of deposition speeds of particles to grass. [From T. A. McMahon and P. J. Denison, Empirical Atmospheric Deposition Parameters—A Survey, Atmos. Environ., 13: 1000 (1979); by permission of Pergamon Press, Ltd.]
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<thead>
<tr>
<th>Wind Speed (m/s)</th>
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Very Stable Conditions

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<tr>
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<table>
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<tr>
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<table>
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</tr>
<tr>
<td>8</td>
<td>-2%</td>
<td>1%</td>
<td>8%</td>
</tr>
</tbody>
</table>

Values in white not likely combination

“-ve” Model over-predicts measurement

Model similar to measurement
Model Inadequacies

- Ignores interaction between particles (model applied to each size as if independent)
- Ignores non-spherical particle orientation which may change during travel
- AERMOD & CALPUFF apply Stokes’ Law for all sizes, which could result in 10% to 40% over-estimate of fallout rate for 50 to 150 µm
- Assume all particle sizes to have same particle density
- Discretisation of particle size distribution may be inadequate (AERMOD limited to 20)
Inadequacies in Application of Model

• Deposition calculation at ground level vs. measurement at 2 m above ground level

Should the fallout be calculated at the height of measurement?

• Particles are not always perfectly spherical
  ▪ Cylindrical ±30% variation in terminal velocity
  ▪ Particle conglomerates
    ➢ ±40% (three spheres)
    ➢ ±58% (four spheres)

Particle sizes should be corrected for shape, but not always known.
Information Gaps

- Particle size distribution ill-defined or often not known – rely on “typical” distributions (e.g. US EPA AP42 emission factors)
- Particle shape is seldom known – mostly non-spherical, but normally assume to be spherical
- Particle density is seldom known and may often very between sizes in same emission (e.g. smelter emissions – smaller particles could contain more volatile metals than larger particles)
Question & Answers
<table>
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<th>Release Height</th>
<th>Measurement</th>
<th>Modelling</th>
<th>Comparable?</th>
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</thead>
<tbody>
<tr>
<td>Wind erosion, wheel entrainment</td>
<td>May under estimate</td>
<td>Model accommodates release height</td>
<td>Model &gt; Measurement More significant under night-time, stable atmospheric conditions</td>
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<tr>
<td>Material handling</td>
<td>Not certain</td>
<td>Fallout normally calculated at z=0</td>
<td>✓</td>
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<tr>
<td>Tall stacks</td>
<td>May be acceptable</td>
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<table>
<thead>
<tr>
<th>Particle Character</th>
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<tr>
<td>Density</td>
<td>Not restricted</td>
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<tr>
<td>Distribution</td>
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<td>Shape</td>
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### Is Dustfall Sampling = Deposition Modelling?

<table>
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<tr>
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<td>Simulated at z=0</td>
<td>✗ Approximation possible by using modelled concentration at z=2m instead of z=0m</td>
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<tr>
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<td>Prevents</td>
<td>Not simulated</td>
<td>✗</td>
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<td>Windshield</td>
<td>Slows flow</td>
<td>Not simulated</td>
<td>? Further investigation</td>
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<tr>
<td>Depth/Diameter</td>
<td>Slows flow</td>
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<td>Shield≡None</td>
<td>No restriction</td>
<td>✓? Wind flow over directional buckets uncertain</td>
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<tr>
<td>Direction</td>
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“Industry has collected records over many years ….. is this still of value or must it be discarded?”

- **Useful & Cost Effective** method of providing **trend analysis** of dust deposition over a **period of time**

- Provides **indication** of the main **areas of dust generation** – e.g. directional buckets

- **Comparison** to SA Dustfall Standard for **nuisance purposes** – appropriate method **must** be used
“How suitable is dustfall monitoring data for use in air quality modelling studies?”

• When considering the vertical concentration profiles, even **similar sources** of particulate emissions could potentially result in **different measurements** if the **release heights** are different.

• **Multi-vertical samplers** are most likely more appropriate for **comparison to dispersion models**.
“How do atmospheric dispersion models simulate airborne particulate matter?”

• When considering the complexities of particle behaviour in the atmosphere, most mathematical models probably suffer from comparably simplistic treatments. However, the lack of detailed particle knowledge may not allow more complicated models.

• The use of some Dispersion models (e.g. AERMOD) is limited in that the treatment of particles larger than around 30 (more dense) to 50 micron (less dense) would result in over-predicted fallout rates closer to source of emission (ADMS bound to result in better predictions).
“Are the two comparable?”

- There are **fundamental differences** between dustfall rate **measurement** (as required by Standard) and the output from **dispersion models** (see table of comparison).

- Perhaps **favourable comparisons** between simulated and measured results are more likely to be **(educated) luck** than science?
“Are the DustFall Standards applicable to modelled results?”

- **Measurement** at $z \neq 0$ and **dispersion models** calculate deposition at $z = 0$

- **Atmospheric** conditions and **particle behaviour** different at two heights
Conclusions

• Some dispersion models do not simulate airborne particle dispersion adequately for larger particles

• Dispersion models calculate deposition at ground level (z=0m), whereas dustfall measurements are done at z=2m

• Modelled results higher than dustfall with larger particles and increased stability, but fairly similar during unstable atmospheric conditions

• Measurement with wind shield may result in similar values as model, but needs further investigation
Recommendations

• Dispersion Models:
  ▪ Use models that adequately simulate terminal settling velocity such as ADMS
  ▪ Incorporate shape factor in specification of particle diameter – should perhaps consider lower (i.e. spherical) and upper values. This will offer the opportunity place upper and lower bounds on the computed deposition results, which is really all the accuracy that can be expected with the present state of the art
  ▪ In addition to model’s default deposition results, calculate “deposition rate” at 2 m above ground level
Recommendations

• Reconciliation between measurement and model - require regulatory models to apply a “ground surface” at a height $z = 2m$

• Since the two methods are likely to give different results it is perhaps more appropriate to have two different standards for dispersion model predictions and measurements, respectively
Recommendations

• Would be great if an extensive dustfall sampling campaign could be conducted using MVS near different source types (mining, smelters, tailings dams, light industries, roadways, etc.)

• Wind speed and direction must be included

• Determine ratio of dust collected at different MVS heights and base height

• From this determine a surrogate standard at reference height