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
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- ASTM 1739 Dustfall Rate Monitoring
  - Comparison of different sampling methods
- Basic Dispersion Modelling Concepts
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  - Differences between Modelled and Sampled Deposition Rates
  - Inadequacies and Information Gaps
- Questions and Answers
- Conclusions & Recommendations

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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?"*

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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?"*

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PARTICULATE CHARACTERISATION

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Examples of Particulate Emissions

Dust Storm in Gobi Desert

Materials handling

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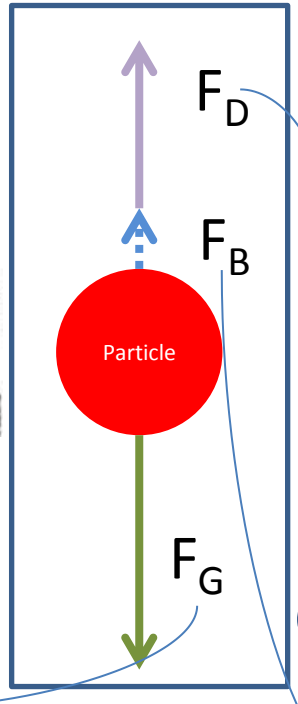
Forces Acting on Airborne Particle (Still Air)



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):

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

Drag Coefficient

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:

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

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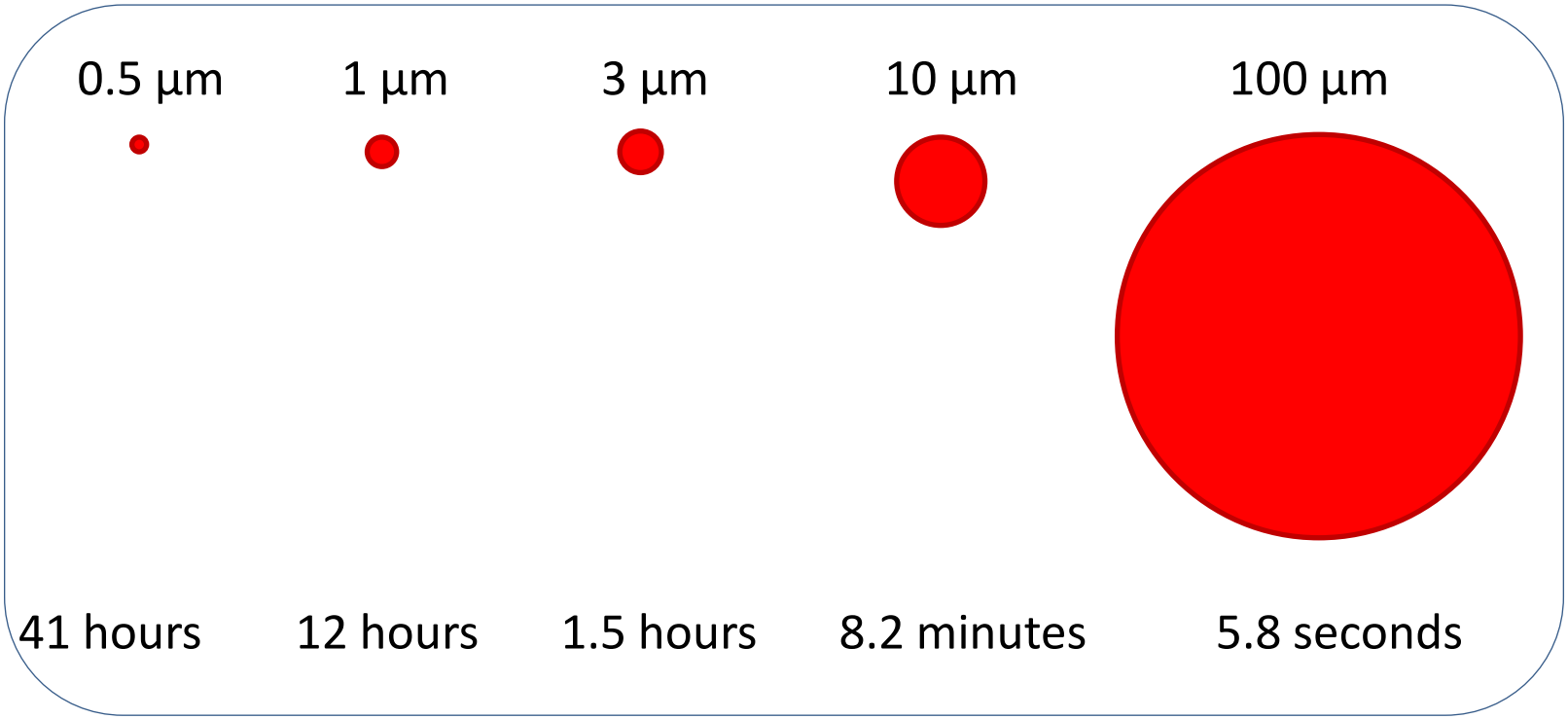
Particle Settling Times – Unit Density Spheres

Still Air: Time to settle 1.5 m

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



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Terminal Settling Velocity (Small Particles)

- Stokes' Law:

$$v_T = \frac{(\rho_p - \rho_g) g d^2}{18\mu} S_{CF}$$

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

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Terminal Settling Velocity (Large Particles)

- Stokes' Law strictly not valid for *Re > 0.1*
  - At *Re = 0.3* 5% error (~54 µm)
  - At *Re = 1.0* 12% error (~80 µm)
  - For $\rho_p = 1000$ kg/m³

Even Smaller for higher densities

- 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**

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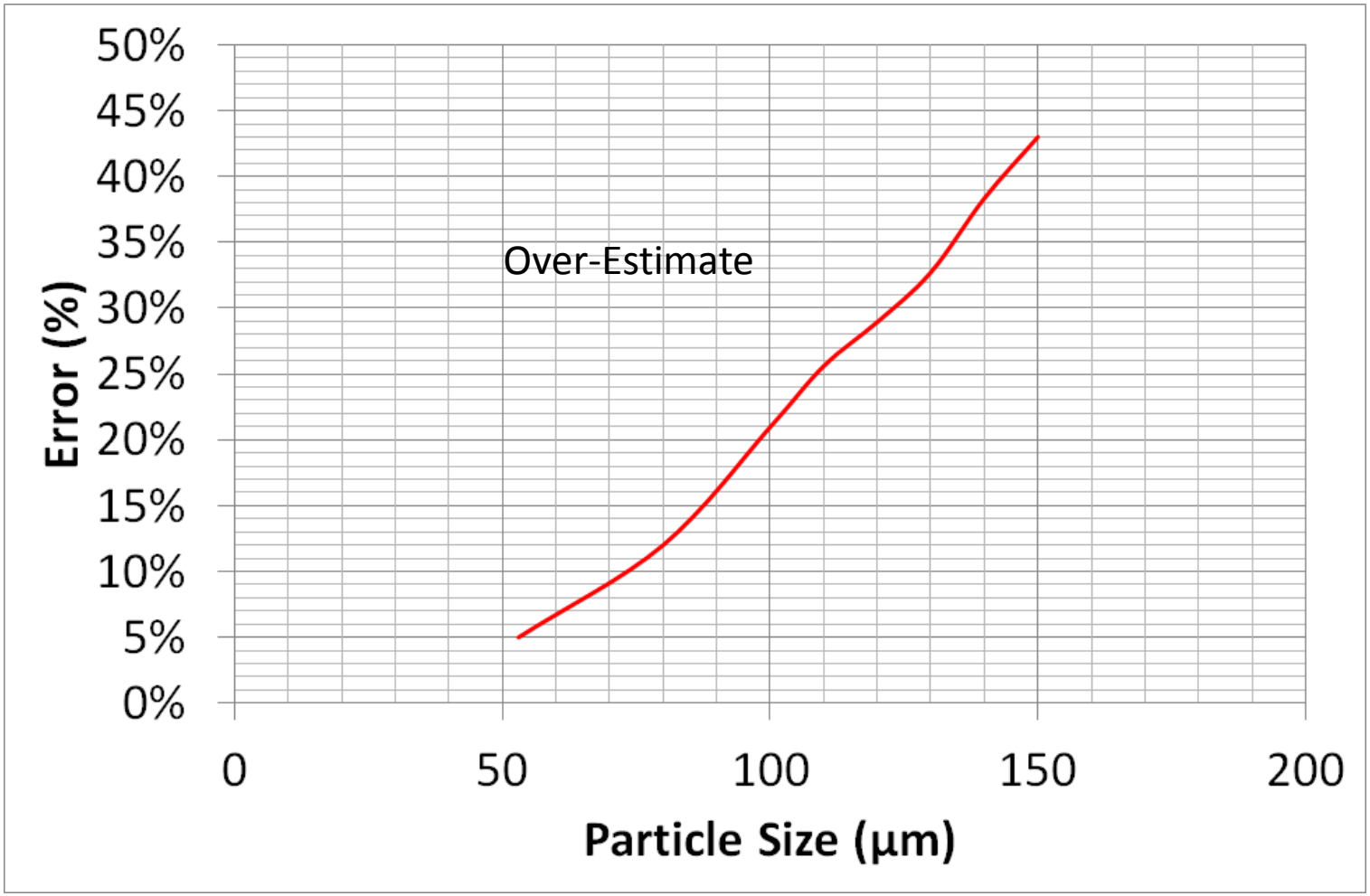
Stokes' Terminal Settling Velocity Error



Particle Density of 1000 kg/m³

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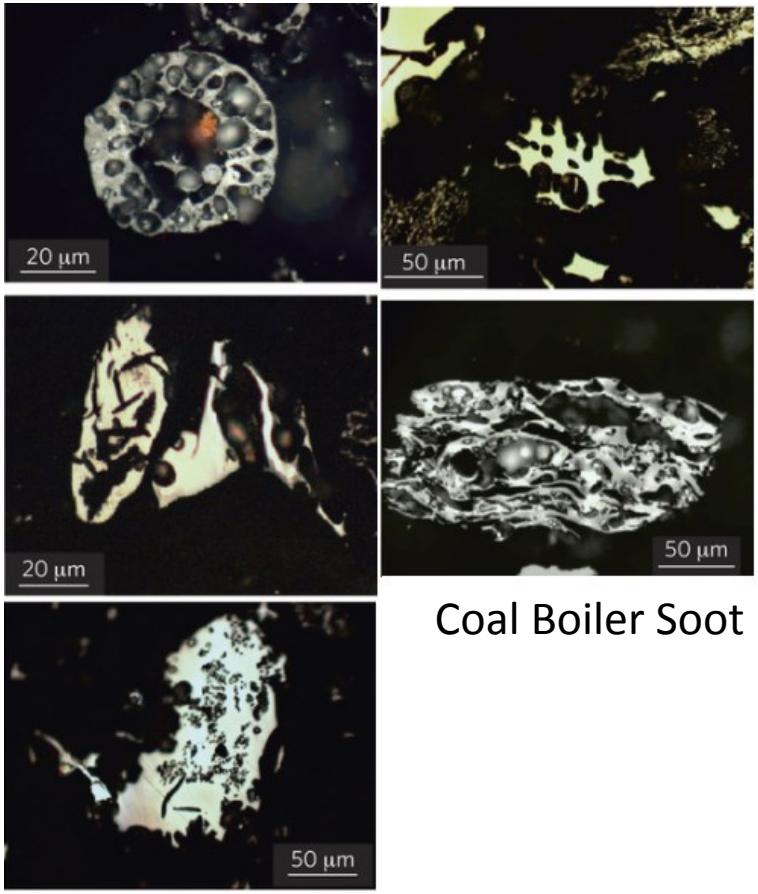
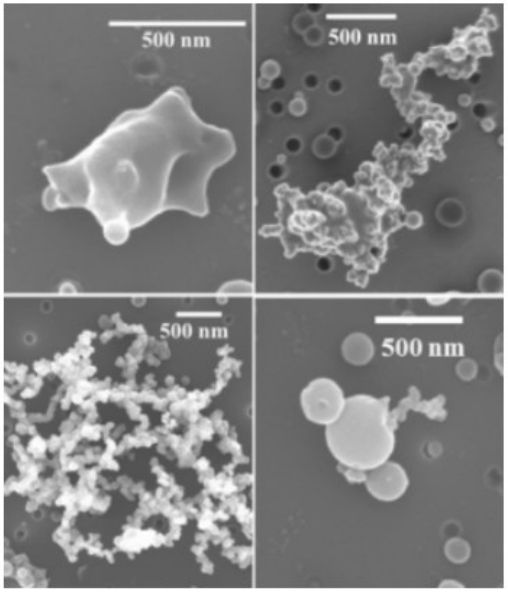
Variety of Airborne Particulates



Coal Boiler Soot



Soot from Wild Fires

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Terminal Settling Velocity – Non-Spherical

- Stokes' Law (non-spherical particle):

$$v_T = \frac{(\rho_p - \rho_g) g d^2}{18 \mu \chi} S'_{CF}$$

Where the dynamic shape factor, χ, is mostly ≥1.0 and S'_{CF} is the slip correction factor for irregular particle shapes (S'_{CF} 0 to12% greater than S_{CF})

- Values for common dusts:
  - Bituminous coal : χ = 1.05 to 1.11
  - Quartz : χ = 1.36
  - Sand : χ = 1.57
  - Talc : χ = 1.88

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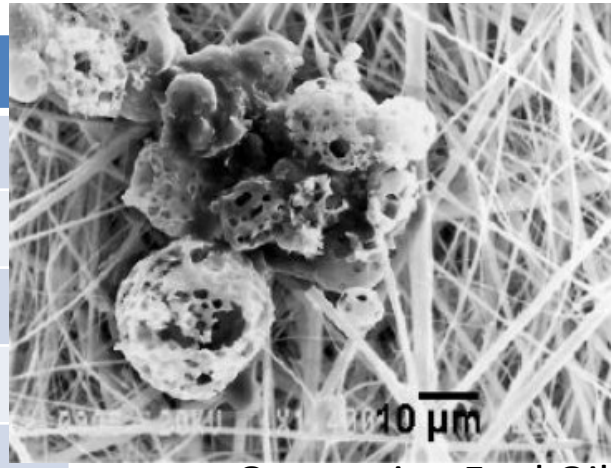
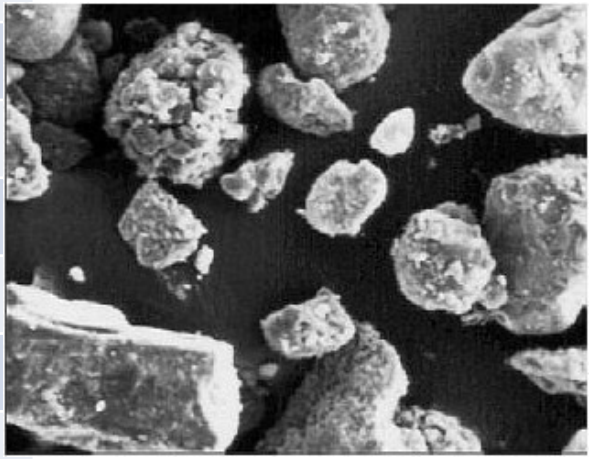
Shape Factor

Shape	Ratio of Axis	Factor
Sphere		1.00
Cube		1.08
Ellipsoid	4	1.28
Cylinder	1	1.06
	2	1.14
	3	1.24
	4	1.32
Touching Spheres		
Two	2	1.10 – 1.17
Three (triangle)		1.20
Three (inline)	3	1.34 – 1.40
Four (inline)	4	1.56 – 1.58



Oven using Fuel Oil


Natural Mineral Particles

Source: Chamberlain (1975) and Johnson et al (1987)

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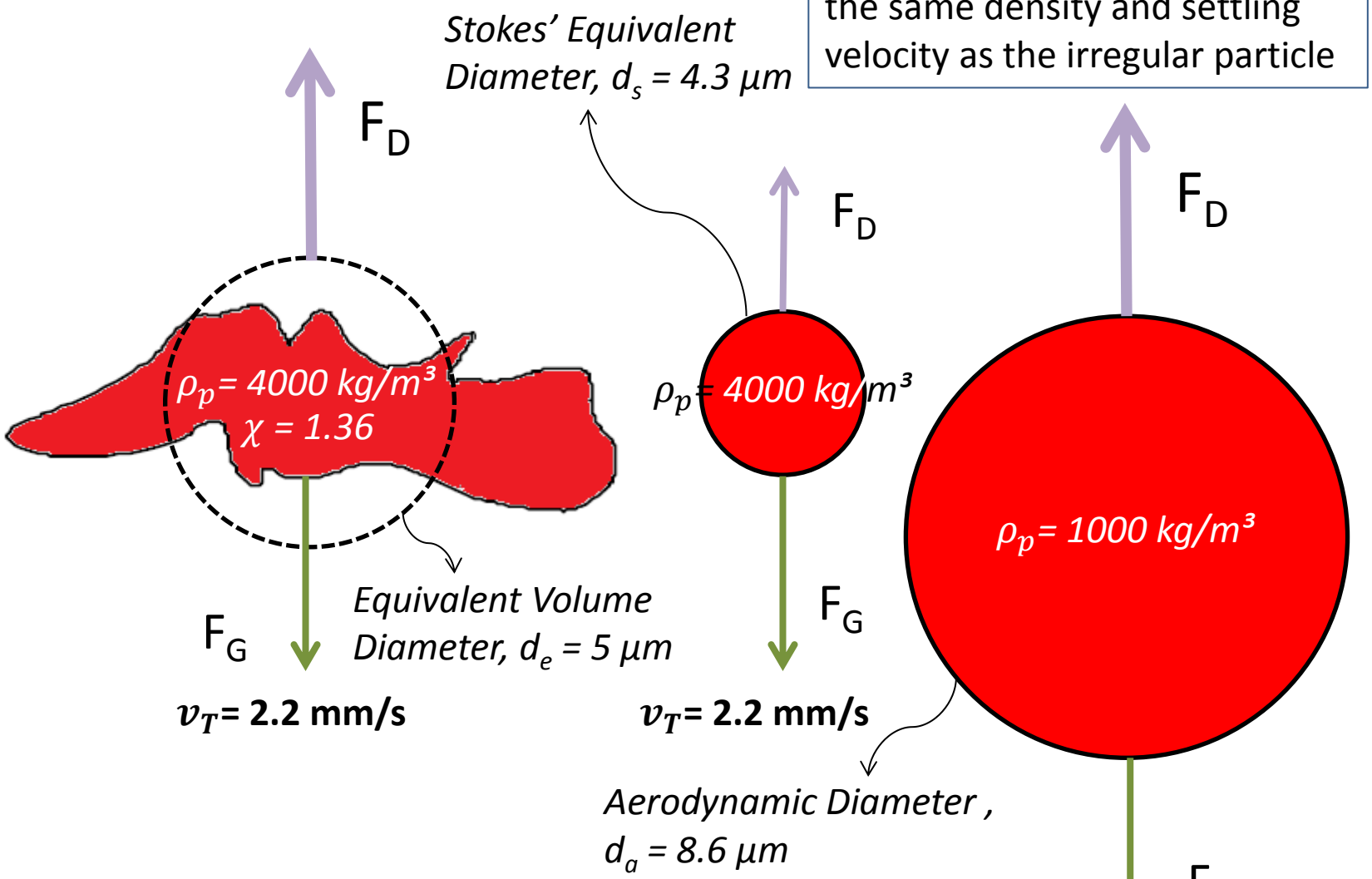
Non-Spherical Particles

Stokes' Diameter : the diameter of the spherical particle with the same density and settling velocity as the irregular particle



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

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Particle Motion

- Particle Character
  - Particle Size (d)
  - Particle Density (ρ_p)
  - Particle Shape and Agglomeration
    - All equations assume spherical shape
    - Non-spherical - Use dynamic shape factor (χ) 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

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ASTM 1739 DUSTFALL RATE MONITORING

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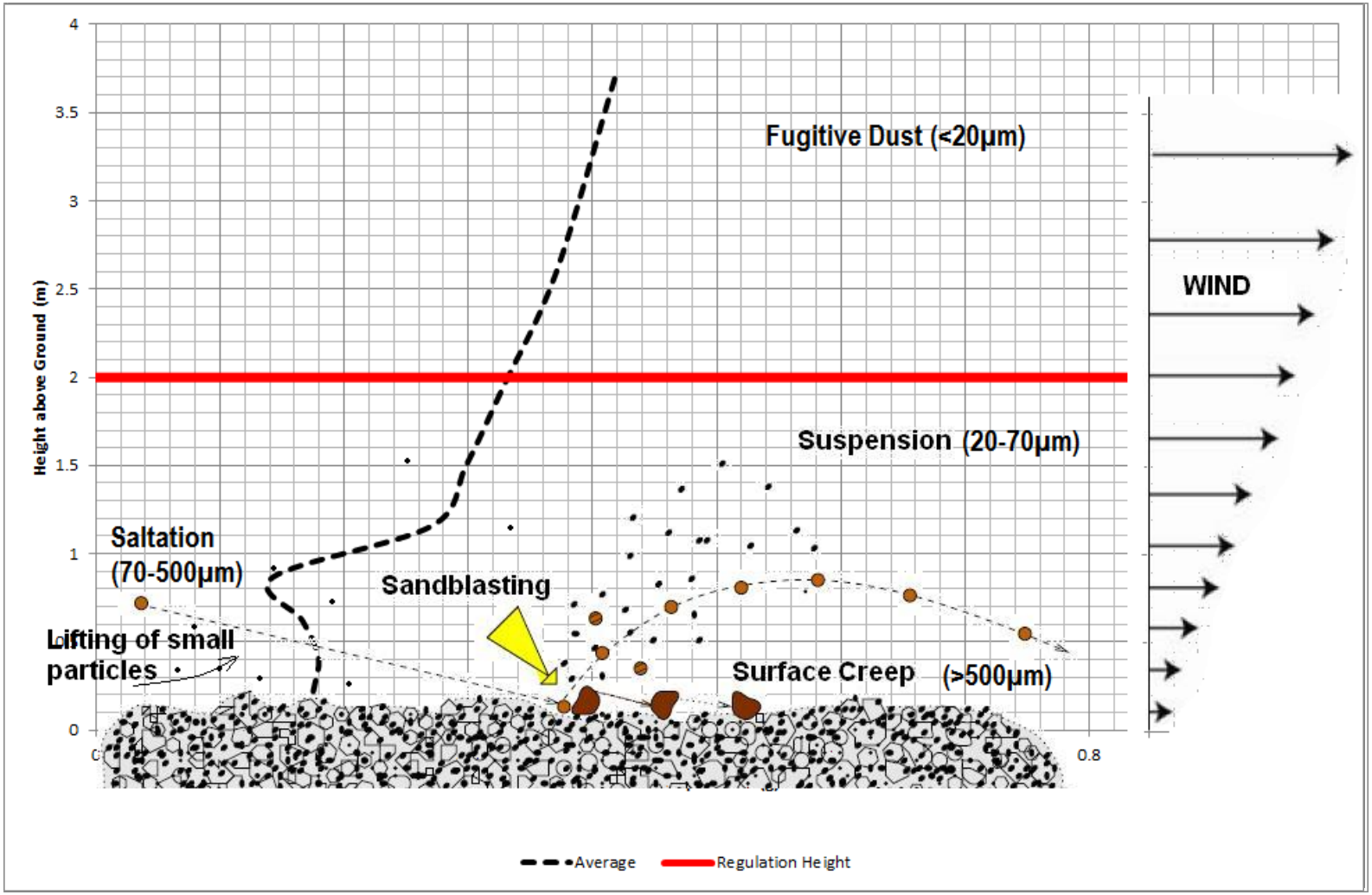
Tailings Dam Multi-Vertical Sampling (MVS)



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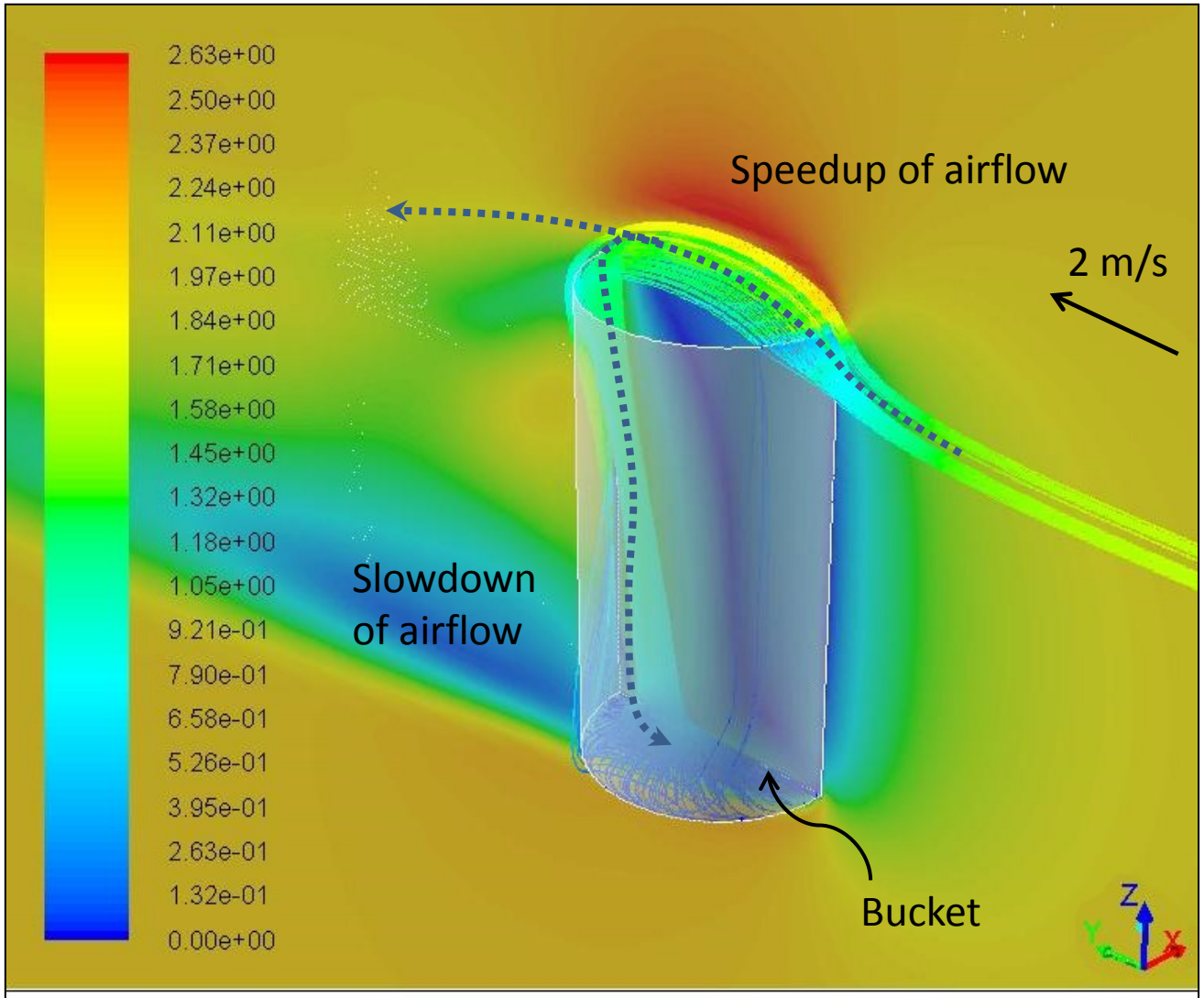
Bucket Without Shield (2 m/s)



Contours of Velocity Magnitude (m/s)

Nov 02, 2015
ANSYS Fluent Release 16.2 (3d, dp, pbns, sstkw)

By permission from Prof Ken Craig (UP)

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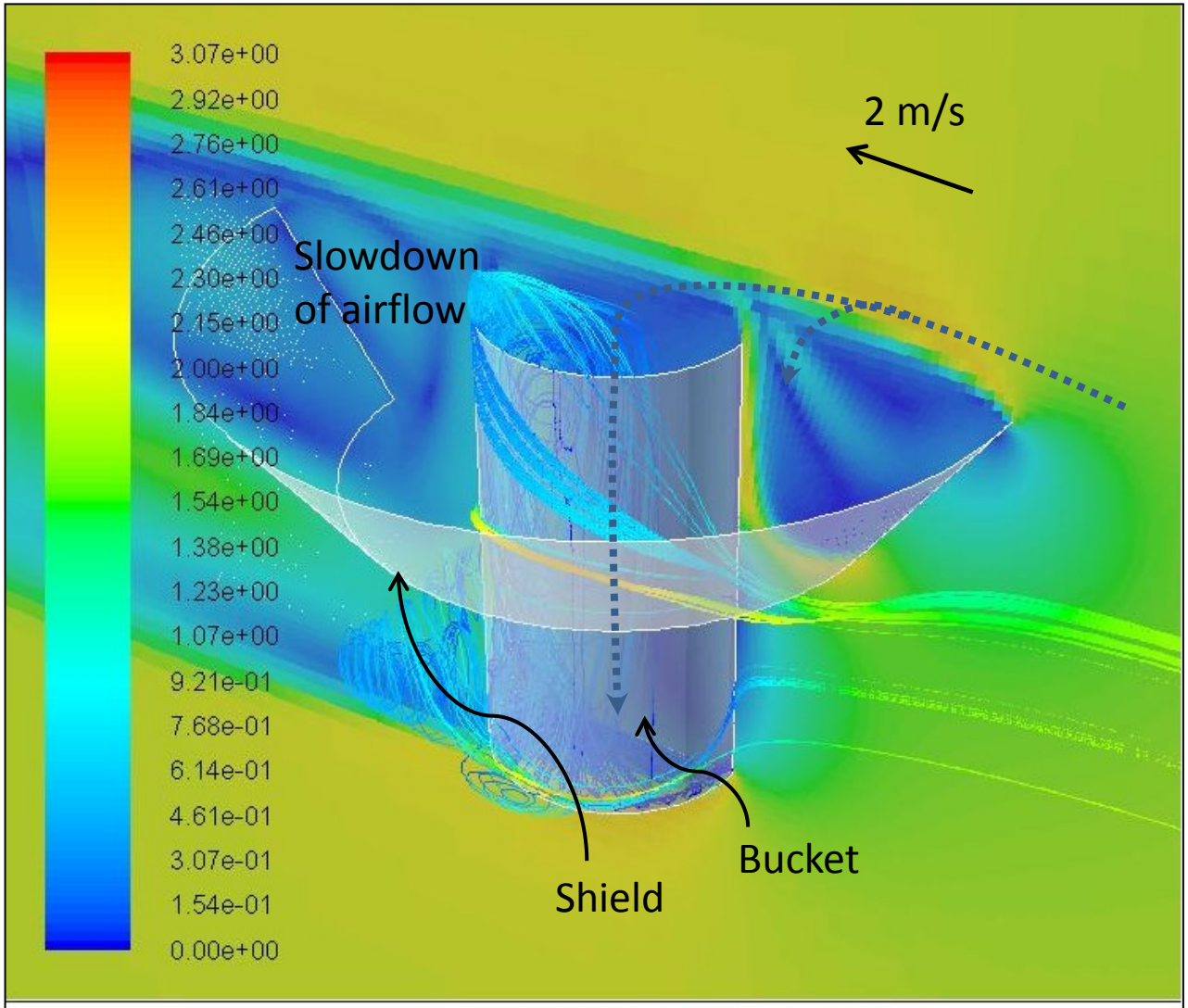
Bucket With Shield (2 m/s)



Pathlines Colored by Velocity Magnitude (m/s)

Nov 02, 2015

ANSYS Fluent Release 16.2 (3d, dp, pbns, sstkw)

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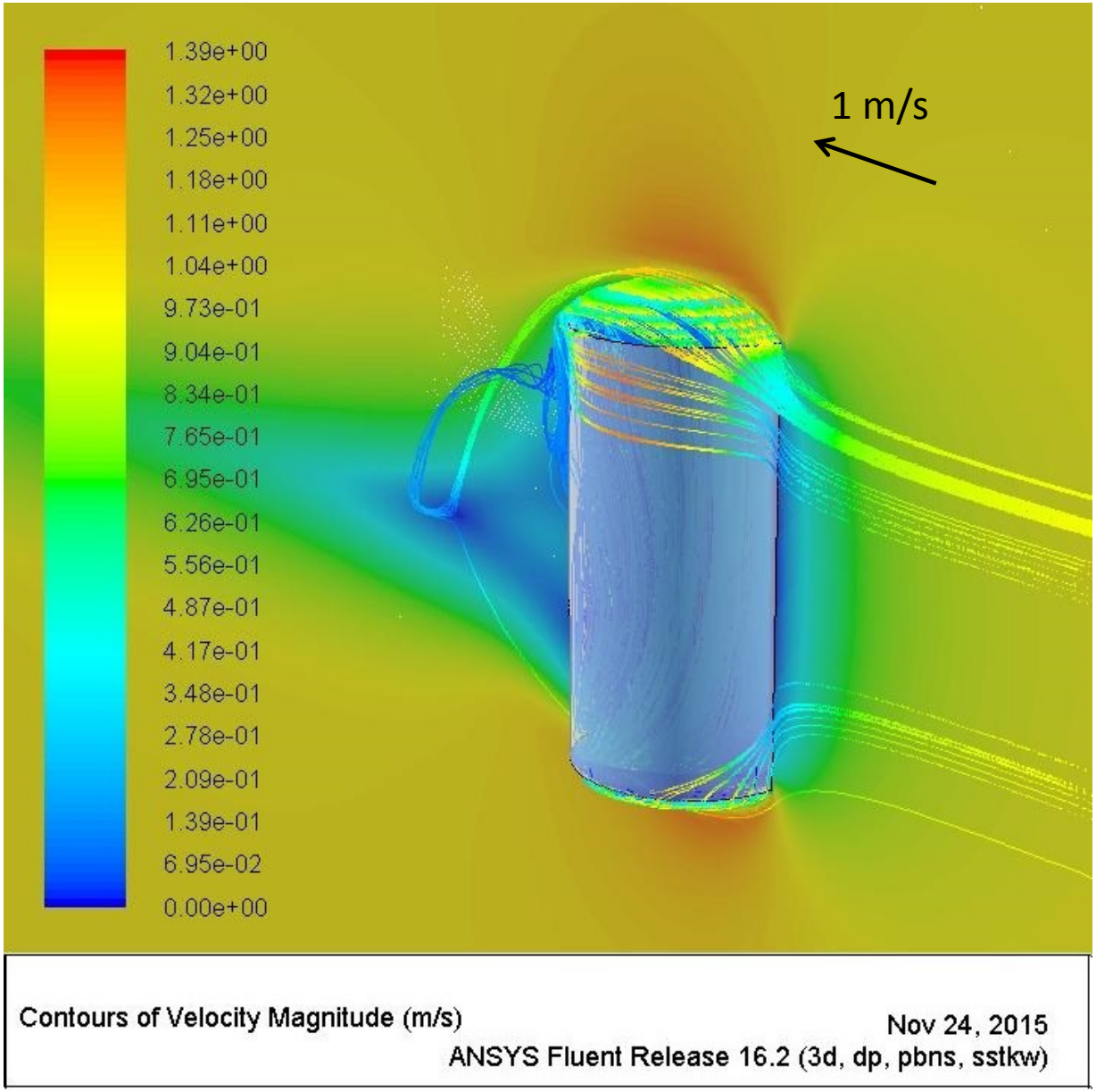
Bucket Without Shield (1 m/s)



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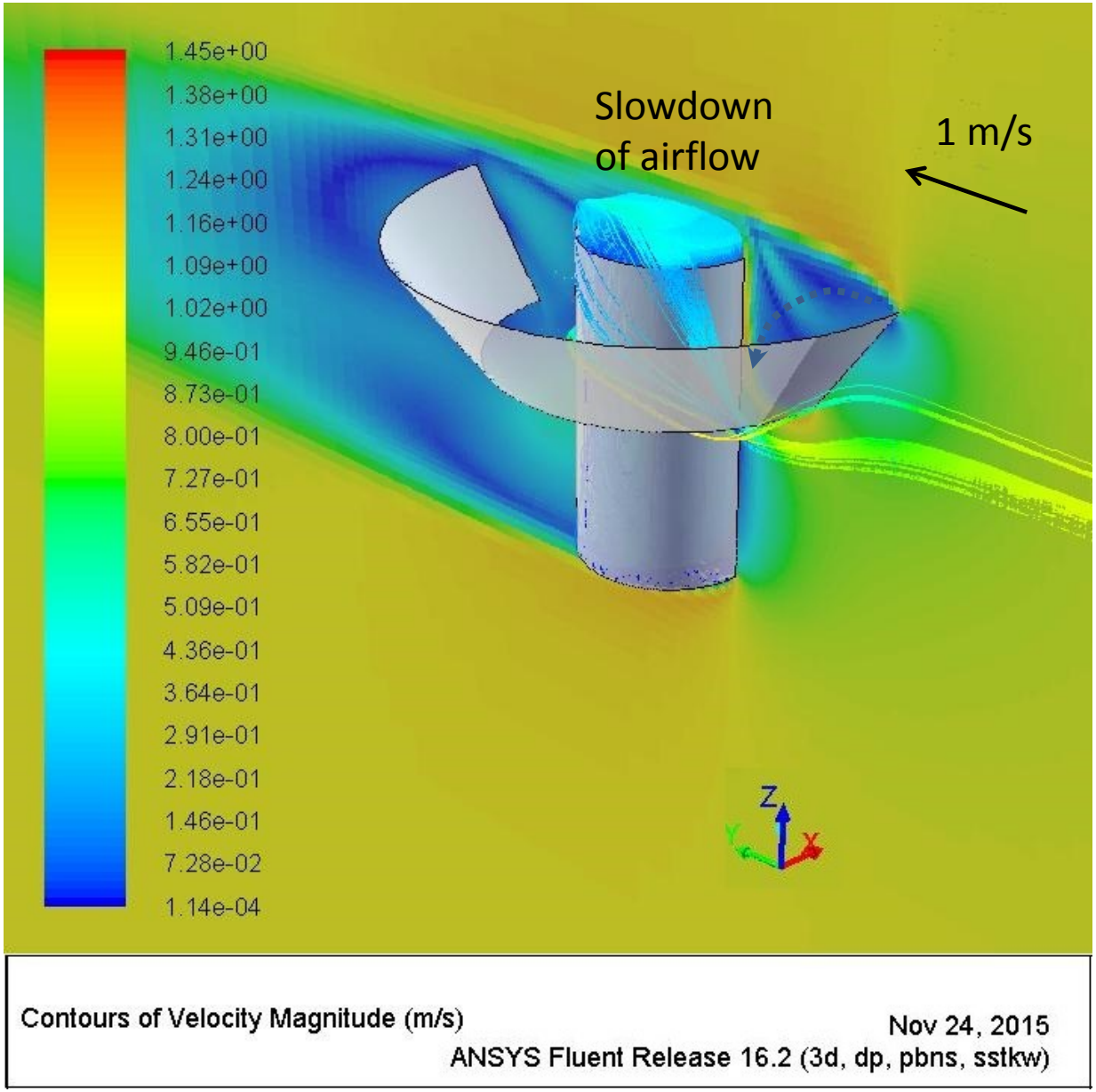
Bucket With Shield (1 m/s)



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BASIC DISPERSION MODELLING CONCEPTS

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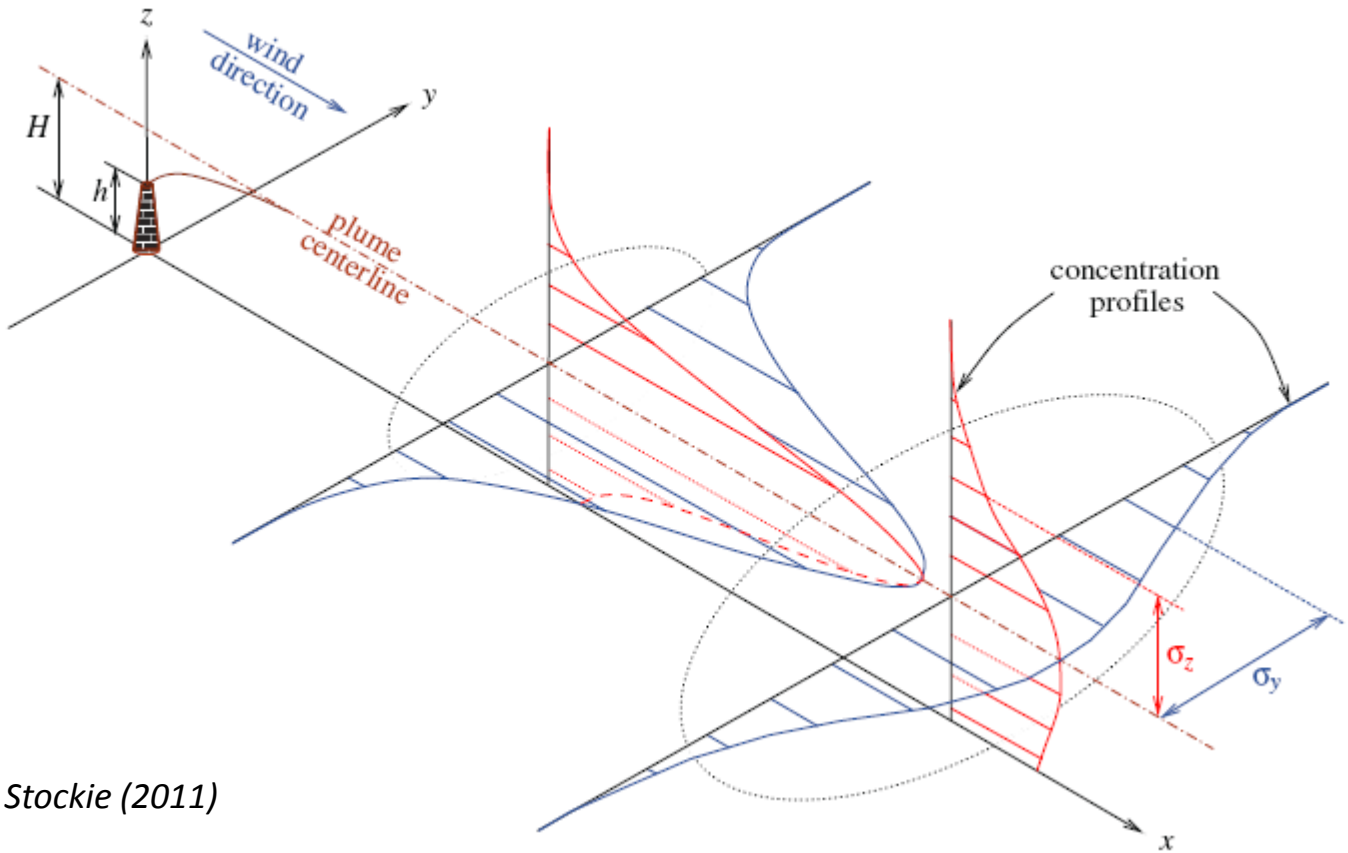

Stockie (2011)

Gaussian Plume Model

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Regulatory Model: AERMOD

Horizontal Spread

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

Vertical Spread

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

Reflection Term

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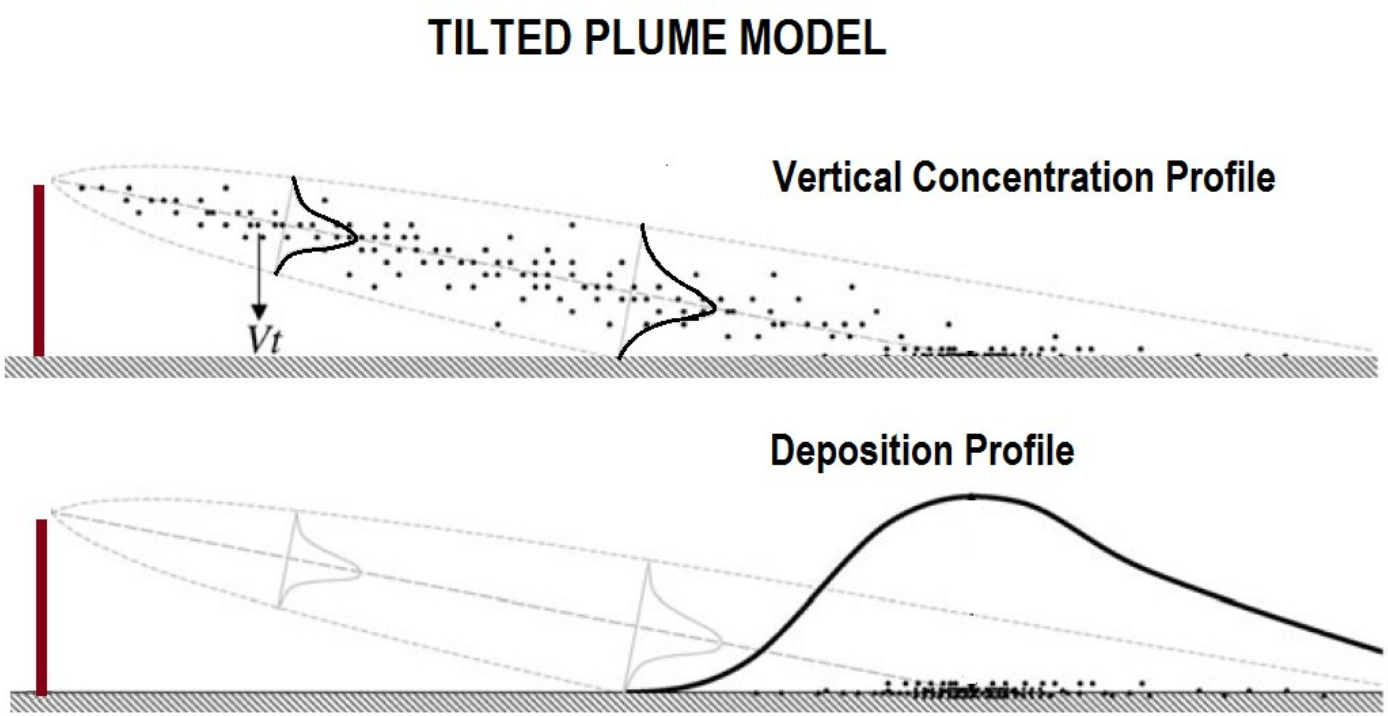

Tilted Gaussian Plume Model

Concept: Ermak (1977)

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TILTED Gaussian Plume Model

$$g(x,z) = exp\left(-\frac{(z-H+\boldsymbol{v_t}x/u)^2}{2\sigma_z^2(x)}\right) + \boldsymbol{\alpha(x_G)}exp\left(-\frac{(z+H-\boldsymbol{v_t}x/u)^2}{2\sigma_z^2(x)}\right)$$

Vertical Spread

Reflection Term

$\boldsymbol{v_t} = terminal\ settling\ velocity$

$\boldsymbol{\alpha(x_G)} = reflection\ coefficient\ (= 0\ to\ 1)$

$function\ of\ particle\ size\ \&\ density;$

$and\ wind\ speed\ and\ atmospheric\ stability$

Hanna et al (1982)

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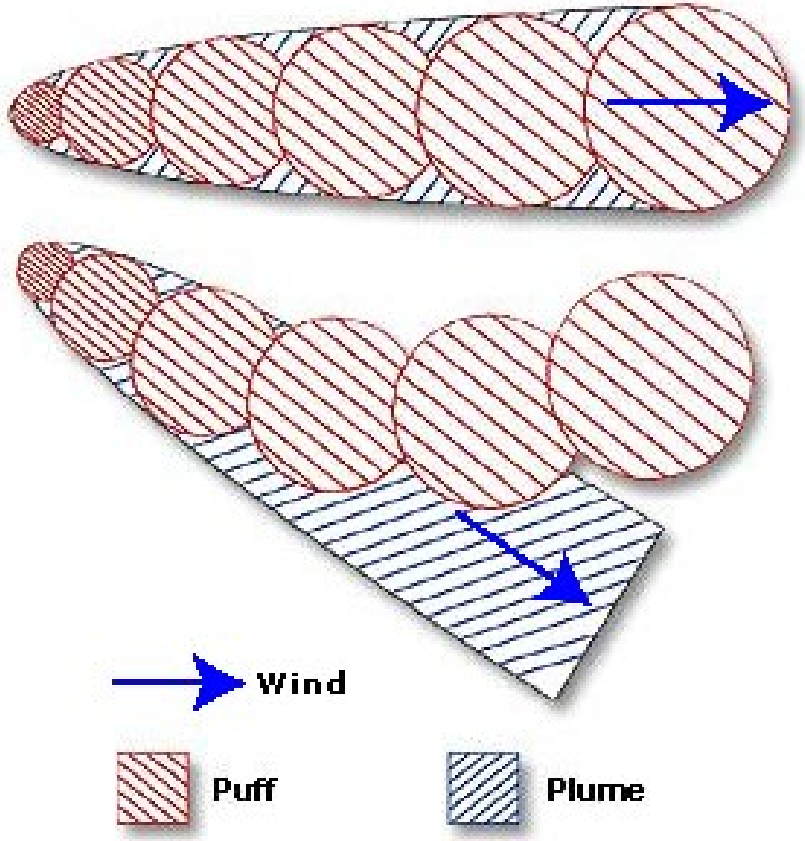

GAUSSIAN PUFF MODEL

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Regulatory Model: CALPUFF

Horizontal Spread

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

Vertical Spread

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

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TILTED Gaussian Puff Model

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

$v_t = terminal\ settling\ velocity$

$\boldsymbol{\alpha(x_G)} = reflection\ coefficient\ (= 0\ to\ 1)$

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Deposition Rate

$$D(x, y, t) = v_d C(x, y, z = 0, t)$$

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

$v_d = f(\text{aerodynamic and substrate resistances}) + v_t$

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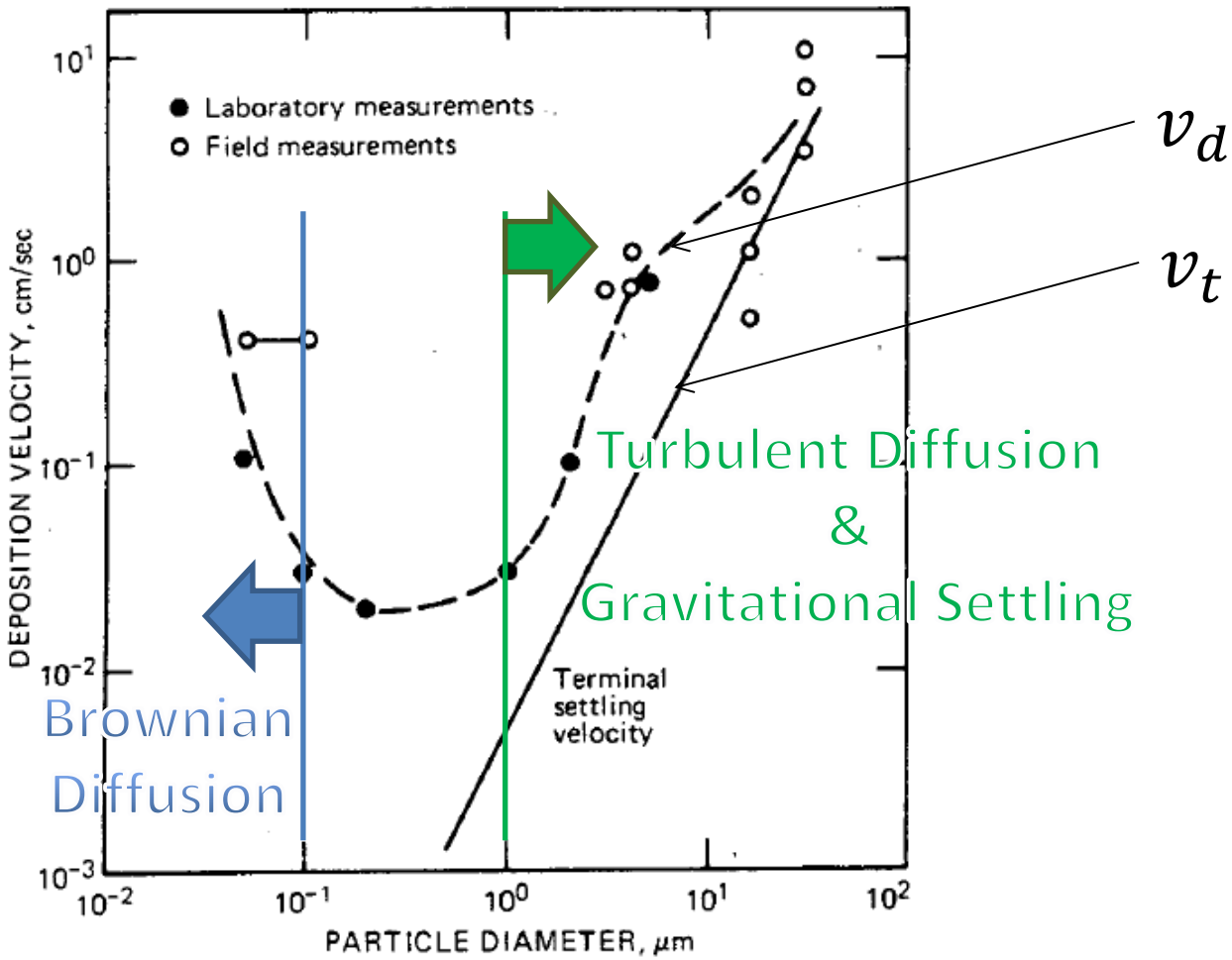

Fig. 10.3 Laboratory and field measurements of deposition speeds of particles to grass. [From T. A. McMahon and P. J. Denison, Empirical Atmospheric Deposition Parameters—A Survey, *Atmos. Environ.*, 13: 1000 (1979); by permission of Pergamon Press, Ltd.]

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Wind Speed (m/s)	Small Particles (20)			Medium Particles (50)			Large Particles (100)		
	H=1	H=2.5	H=5	H=1	H=2.5	H=5	H=1	H=2.5	H=5
	Very Stable Conditions								
1	-32%	-27%	-16%	-89%	-89%	-88%	-100%	-100%	-100%
2	-18%	-11%	5%	-68%	-67%	-64%	-98%	-98%	-98%
4	[illegible]	-2%	18%	-45%	-41%	-33%	-89%	-89%	[illegible]
[illegible]	[illegible]	4%	25%	-18%	4%	[illegible]	-68%	[illegible]	[illegible]
	Stable Conditions								
[illegible]	-16%	-13%	-7%	-63%	-62%	-61%	-97%	-97[illegible]	[illegible]
2	-8%	-5%	1%	-40%	-39%	-35%	-85%	-85%	[illegible]
4	-4%	-1%	6%	-23%	-21%	-16%	-63%	-62%	-61%
8	-2%	1%	8%	-8%	1%	-4%	-40%	-9%	-35%
	Neutral Conditions								
1	-8%	-7%	-4%	-41%	-40%	-39%	-85%	-85%	-85%
2	-4%	-3%	1%	-24%	-22%	-20%	-64%	-63%	-63%
4	-2%	0%	3%	-13%	-11%	-8%	-41%	-40%	-39%
8	-1%	1%	4%	-4%	1%	-2%	-24%	-5%	-20%
	Moderately Unstable Conditions								
1	-3%	-2%	-1%	-16%	-16%	-15%	-48%	-48%	-47%
2	-1%	-1%	0%	-9%	-8%	-7%	-29%	-29%	-28%
4	-1%	0%	1%	-4%	-4%	-3%	-16%	-16%	-15%
8	0%	0%	1%	-1%	0%	0%	-9%	-2%	-7%
	Unstable Conditions								
[illegible]	-1%	-1%	0%	-7%	-7%	-6%	-24%	-24%	-24%
[illegible]	-1%	0%	0%	-4%	-3%	-3%	-14%	-13%	-13%
[illegible]	0%	0%	1%	-2%	-2%	-1%	-7%	-7%	-6%
[illegible]	0%	0%	1%	-1%	0%	0%	-4%	-1%	-3%
	Convective Conditions								
1	0%	0%	0%	-3%	-3%	-2%	-9%	-9%	-9%
2	0%	0%	0%	-1%	-1%	-1%	-5%	-5%	-5%
4	0%	0%	0%	-1%	-1%	0%	-3%	-3%	-2%
8	0%	0%	0%	0%	0%	0%	-1%	0%	-1%

Values in white not likely combination

"-ve" Model over-predicts measurement

Model similar to measurement

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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)

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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.

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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)

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Question & Answers

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Is *Dustfall Sampling = Deposition Modelling?*

	Measurement	Modelling	Comparable?
Release Height			
Wind erosion, wheel entrainment	May under estimate	Model accommodates release height	Model>Measurement More significant under night-time, stable atmospheric conditions
Material handling	Not certain	Fallout normally calculated at z=0	
Tall stacks	May be acceptable		✓
Particle Character			
Density	Not restricted	Uniform	✓?
Distribution	Not restricted	AERMOD & CALPUFF – Stokes. ADMS unrestricted	AERMOD & CALPUFF may over-predict near the source. ADMS should perform better.
Shape	Not restricted	Spherical	User needs to correct

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Is *Dustfall Sampling = Deposition Modelling?*

	Measurement	Modelling	Comparable?
Resuspension			
Height	z=2m	Simulated at z=0	✗ Approximation possible by using modelled concentration at z=2m instead of z=0m
Presence of Liquid	Prevents	Not simulated	✗
Windshield	Slows flow	Not simulated	? Further investigation
Depth/Diameter	Slows flow	Not simulated	? Needs investigation
Wind Field			
Strong winds	Shield>None	No restriction	? Further investigation
Weak winds	Shield≡None		✓
Direction			✓? Wind flow over directional buckets uncertain

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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

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“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 <u>different measurements</u> if the <u>release heights</u> are <u>different</u>

- **Multi-vertical samplers** are most likely more appropriate for <u>comparison to dispersion models</u>

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"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)

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"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?

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"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

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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

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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 <u>really all the accuracy</u> 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

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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 <u>different results</u> it is perhaps more appropriate to have <u>two different standards</u> for dispersion model predictions and measurements, respectively

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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

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