Description and evaluation of particulate deposition modelling in ADMS



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ADMLC Dry deposition and Surface Chemical Reactivity seminar

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Cambridge Environmental Research Consultants Environmental Software and Services



Outline

- Introduction to deposition in ADMS
- Evaluation study
 - Measurement study
 - Modelling approaches
 - Deposition analysis
 - Modelling sensitivities
- Summary



Dry Deposition in ADMS (1)

- Dry and wet deposition model options
- Dry deposition rate, *F*, proportional to near-surface concentration, *C* :

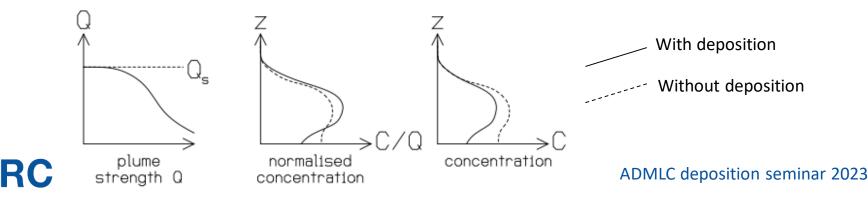
$$F = v_d C$$

• Deposition velocity, v_d , calculated as:

$$v_d = \frac{v_t}{1 - \exp(-v_t/v_d)}$$

 v_t - gravitational settling velocity v'_d - diffusive part of v_d $v_d \rightarrow v'_d$ as $v_t \rightarrow 0$ (gases)

- Removal of airborne material at surface leads to:
 - Reduced effective plume strength
 - Modified vertical distribution of concentration (shape factor)



Dry Deposition in ADMS (2)

- True deposition velocity depends on:
 - Nature of pollutant
 - Atmospheric state
 - Nature of surface
- Can change with time (e.g. due to diurnal and closing of leaf stomata) and/or space (e.g. due to land use changes over region of interest)
- In ADMS:
 - Gravitational settling velocity v_t (particulates only) assumed **fixed** and is **supplied by user** (either directly or calculated from particle diameter & density)
 - Diffusive part v'_d (particulates & gases) can be supplied by user **or** calculated by model. Supplied values can be:
 - Fixed
 - Temporally varying; Hourly or seasonal (day/night for Spring/Summer/Autumn/Winter) values
 - Spatially varying (via additional input file containing list of x, y, v'_d values)
 - Spatially and temporally varying (hourly factors applied to spatially varying values)

Dry Deposition in ADMS (3)

- Calculated v'_d based on resistance model
- $r = 1/v'_d$ taken as sum of three terms:
 - *r_a* Aerodynamic resistance
 - Ability of turbulent eddies to bring material close to surface
 - Based on momentum transfer between two

near-surface heights:
$$r_a = \frac{U(z_2) - U(z_1)}{u_*^2}$$

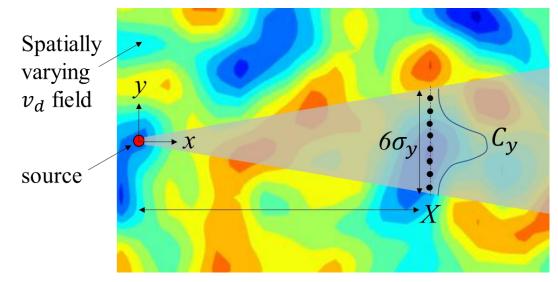
r_b - Sub-layer resistance

- Resistance to transfer across final zone adjacent to surface
- For smooth surfaces, r_b represents molecular and turbulent diffusion across laminar and transition sublayers: $r_b = \frac{1}{\kappa u_*} \ln(1 + \text{Sc})$. Schmidt number $\text{Sc} = \nu/D$, i.e. ratio of kinematic viscosity to molecular diffusivity. Sc = 1 assumed for gases. For e.g. $\text{PM}_{2.5}$, Sc $\approx 1 \times 10^6$ so $\ln(\text{Sc}) \approx 14$
- *r_s* Surface resistance
 - Gases: Affinity of surface (adsorption, absorption etc). Can be:
 - Estimated by model given nature of gas (reactive/non-reactive/inert) or
 - Supplied by user (same options as for v'_d , i.e. fixed, temporally and/or spatially varying)
 - Particulates: r_s taken as zero (particles assumed to adhere on contact)

| Atmosphere | Turbulent flow and advection | Aerodynamic resistance (R _a) | | |
|---------------------|---|---|--|--|
| Transition sublayer | | Sub-layer | | |
| Laminar sublayer | Molecular diffusion | resistance (R _b) | | |
| Surface | Adsorption/absorption/ chemical reaction, etc. | Surface resistance (R _s) | | |

Dry Deposition in ADMS (4)

- For spatially-varying v_d :
 - During dispersion calculations: Depletion and shape factor at downwind distance X calculated using v_d, a crosswind-concentration-weighted average of v_d at ~20 points across plume (between +/- 3σ_y)

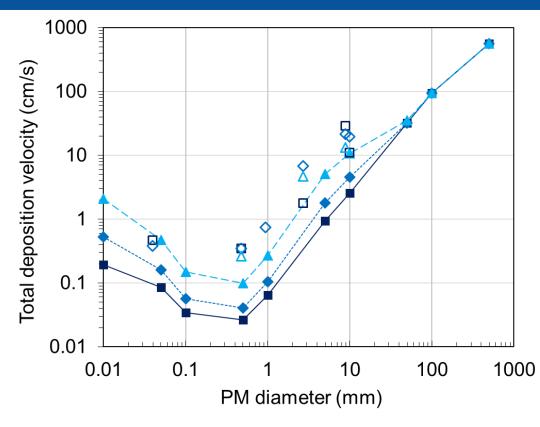


- Deposition at a given output point $F(x, y) = v_d C$:
 - v_d is value extracted at x, y
 - C is near-ground concentration at x, y, calculated using v_d-based depletion and shape factor



Dry deposition evaluation

- No routine measurements of dry deposition for evaluation
- Very few published studies with measurements of dry deposition fluxes available
- ADMS deposition velocity variation with wind speed and surface roughness validated against Sehmel (1980) measurements



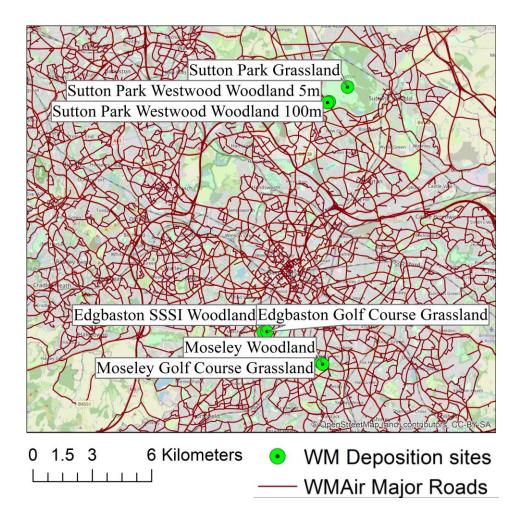
-■-ADMS (U* = 0.35 m/s)

- ----- ADMS (U* = 0.70 m/s)
- -▲-ADMS (U* = 1.40 m/s)
- observations (U* = 0.35 m/s, natural grass)
- observations (U* = 0.70 m/s, natural grass)
- △ observations (U* = 1.40 m/s, natural grass)

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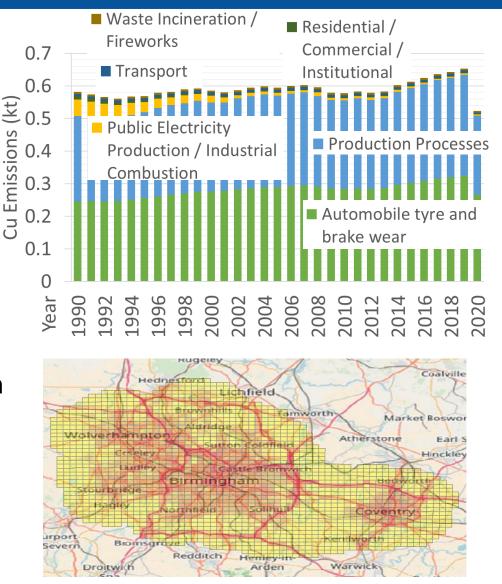
Evaluation study: Measured data

- Fowler et al. (2004) measured heavy metal concentrations in undisturbed soils in the West Midlands, UK
- 3 sets of nearby sites with grassland/forest land use, some information about tree species and grass length
- Soil concentrations represent longterm accumulated wet and dry deposition
 - Focus on Copper concentration data from surface layer (0-5 cm below ground level), most recent deposition



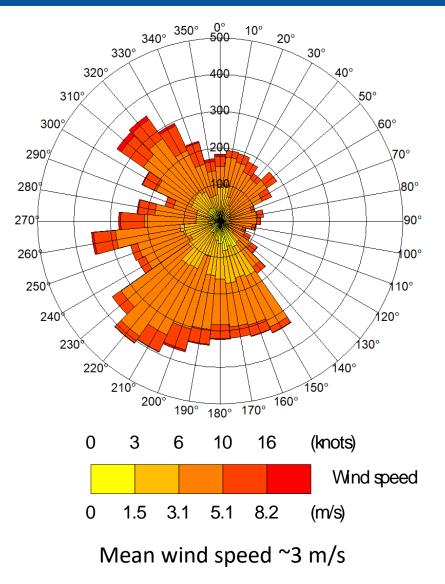
Evaluation study: Modelling approach

- Total Copper emissions reported in NAEI relatively unchanged from 1990 – 2019/20
- Dominant emission sectors: road traffic (non-exhaust) and production process
- NAEI gridded copper emission from 2019 used in modelling
- Industrial sector assigned 50 m depth, all other emissions 10 m depth, grid of 1 km x 1 km volume sources
- Model: ADMS-Urban version 5.0.1



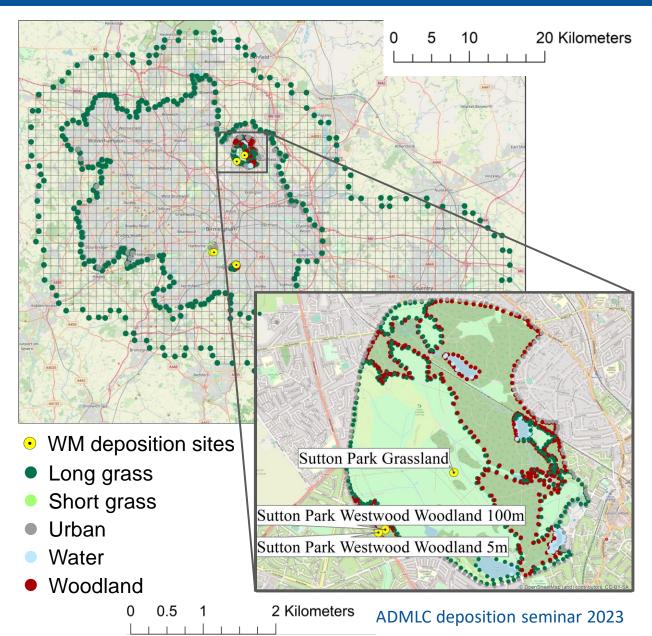
Evaluation study: Modelling approach

- Measured meteorological data from Birmingham Elmdon for 2016
- Met site roughness 0.5 m, dispersion site roughness 1.0 m
- Rural measurements of Copper aerosol from Automatic Urban and Rural Network (AURN) showed generally very low concentrations, no background concentrations applied
- New pollutant defined for copper particles with 2.5 μm diameter and 8940 kg/m³ density
- Time-variation of emissions based on previous analysis of West Midlands traffic flows (Zhong et al., 2021)



Evaluation study: modelling approach

- Spatially varying dry deposition velocity file defined based on land use
- Manual creation of points around borders of grassland (short and long), forest, water and urban areas
- ADMS uses deposition properties from nearest point in file
- Wet deposition run with default ADMS precipitation-dependent parameters (spatially uniform rainfall)



Evaluation study: Calculation of deposition velocities

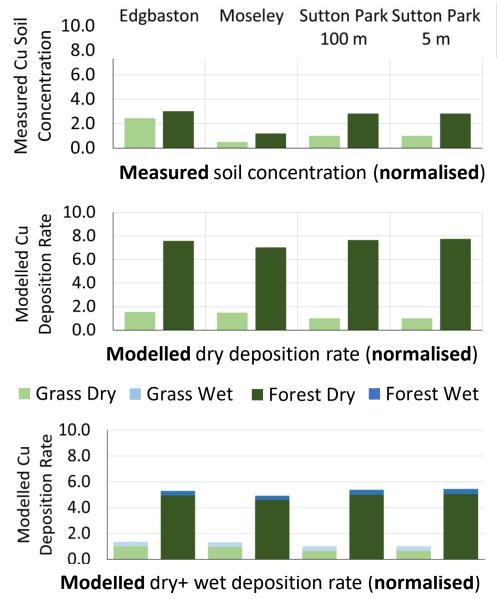
- Dominant land use approach to spatial variation of deposition velocity
- Vegetation:
 - Deposition velocity per unit leaf area from Nowak et al. (2013) as used in iTreeEco, value for 3 m/s average wind speed
 - Average Leaf area index (LAI) for forest derived from UK measurements in lio and Ito (2014) Global database of LAI in Woody Plant Species (ORNL DAAC)
 - LAI for grassland based on grass length from Byrne et al. (2005), lower values for 'new' grassland used as WM sites are not intensively managed
- Urban (impermeable surfaces): deposition velocity value from Giardina et al. (2019) for 2.5 μm diameter particles
- Water: deposition velocity value from Emerson et al. (2020) for 2.5 μm diameter particles

| Land use | Deposition velocity (m/s) |
|-------------|---------------------------|
| Woodland | 0.008059 |
| Long Grass | 0.000563 |
| Urban | 0.0005 |
| Short grass | 0.000225 |
| Water | 0.0001 |

Evaluation study: deposition analysis

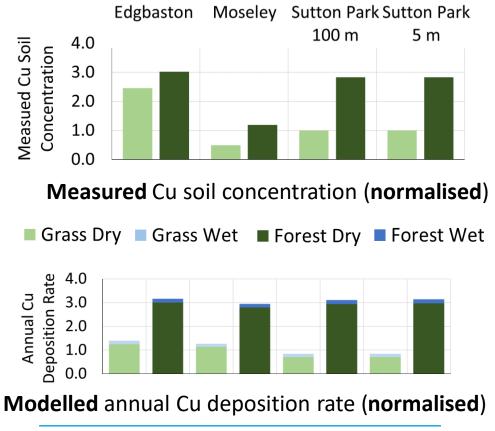
- Normalised measured soil concentrations and modelled deposition rates using Sutton Park grassland deposition
- Compare the relative increase in deposition in the forest relative to grassland sites
- Base run with dry deposition only: ADMS over-estimated increase in deposition for forest sites
- Including wet deposition reduces modelled forest/grassland ratio but this is still overestimated compared to measurements

CFRC



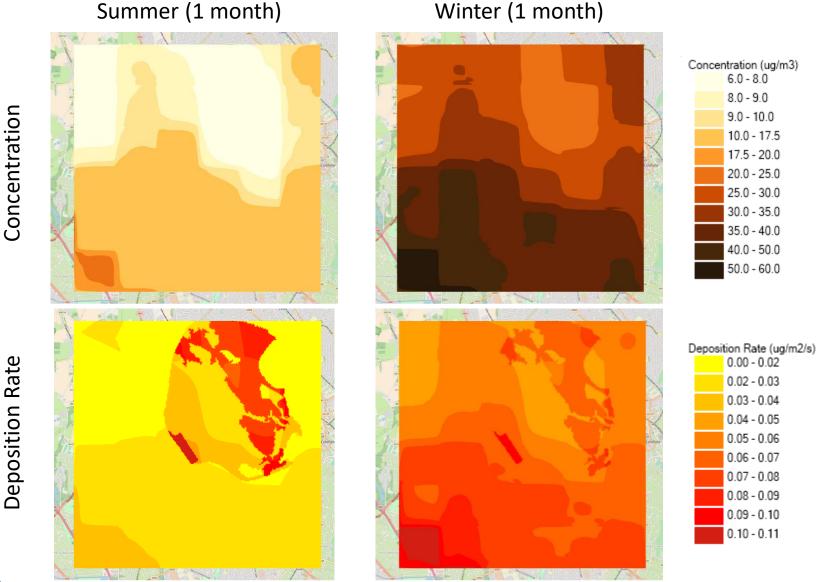
Evaluation study: deposition analysis

- ADMS temporal variation of deposition parameters is spatially uniform
- Take into account differences in summer/winter LAI for deciduous/mixed forest (van den Hurk et al., 2002)
- Created separate summer/winter .din files for leaf-on (May – November) and leaf-off periods (January-April, December)
- Deposition ratios between forest and grassland more comparable to measurements



| Land use | Deposition velocity (m/s) | | |
|-------------|---------------------------|---------|--|
| Lanu use | Winter | Summer | |
| Woodland | 0.00153 | 0.01002 | |
| Long Grass | 0.000465 | 0.00261 | |
| Short grass | 0.000615 | 0.00267 | |

Spatial variation of concentration & deposition



Concentration

CERC

•••• 0.5 km

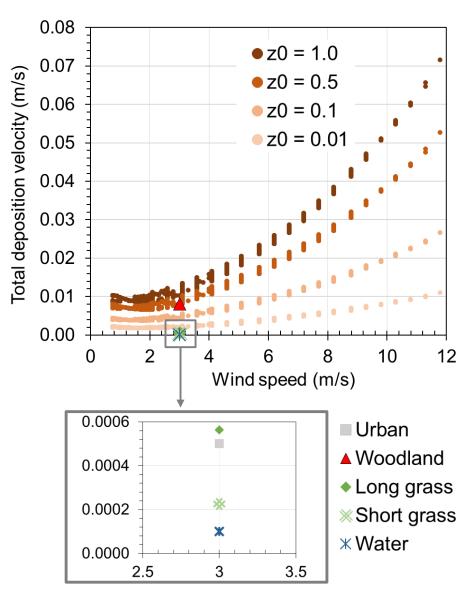
Modelling sensitivities: deposition and wind speed

How significant is the variation of deposition velocity with wind speed?

- ADMS calculates deposition velocity dependent on local wind speed and roughness length
- Increasing roughness length increases deposition velocity

CERC

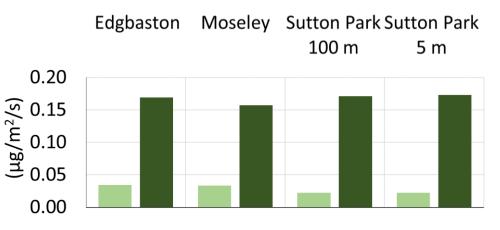
- Non-linear increase in deposition velocity with wind speed
 - Annual deposition values based on non-woodland land use are lower than values for the average wind speed and roughness length



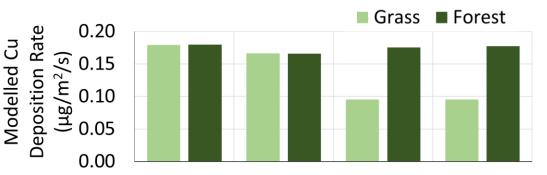
Modelling sensitivities: ADMS deposition velocity

Modelled Cu Deposition Rate

- Is the spatial variation or temporal variation of deposition velocity more significant?
- Using ADMS deposition velocity (spatially uniform, varying with wind speed) increases dry deposition at grassland sites compared to land use based deposition velocity (spatially varying, temporally uniform)
- Woodland deposition similar for both types of deposition velocity



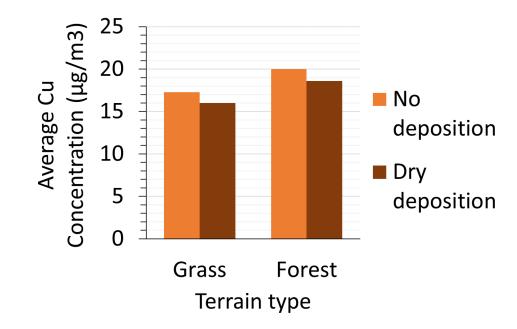
Spatially varying, land-use based dry deposition rate (**absolute**)



Spatially uniform, wind speed dependent dry deposition rate (**absolute**), roughness length 1 m

Modelling sensitivities: Concentration comparison

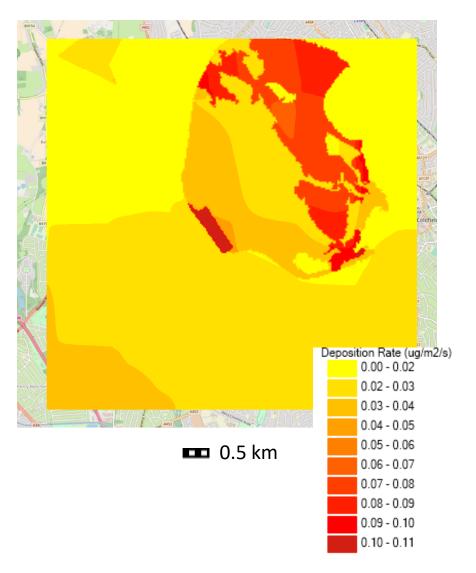
- How much are ambient annual average Copper concentrations affected by particulate deposition?
- Concentrations reduced by 7.24 – 7.54 %, little difference between grass/forest sites



| Average Cu Concentration (μ g/m ³) | | | | | |
|---|--------|---------|------------------------------|--|--|
| Terrain type | No dep | Dry Dep | Percentage difference (%) | | |
| Grass | 17.27 | 16.01 | -7.54 | | |
| Forest | 20.02 | 18.62 | -7.24 | | |

Summary

- Limited data availability for evaluation of deposition modelling
- Evaluation compared long term ratios of deposited particulates with annual average modelled deposition
 - Similar overall deposition for woodland from land use and wind speed dependent approaches; consistent with measured deposition
 - Spatially varying deposition allows exploration of vegetation effects; except close to sources this results in greater spatial variability in deposition than concentration gradients
 - Seasonal variation of vegetation properties can be significant for deposition



References & Acknowledgement

References

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Acknowledgement

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