An exploration of dry deposition research by FOI - with emphases on winter conditions

ADMLC October 4, 2023 Harwell, UK Oscar Björnham, FOI



Foto: Försvarsmakten/David Gemes



Dry deposition modelling at FOI





Dry deposition modelling General model used by FOI

Traditional resistance model

- Aerodynamic, R_a
- Sub-layer resistance, R_b
- Surface/canopy resistance, R_c
- Large set of partial resistances and parameters

Gas and particles treated differently Particles have

- Settling velocity
- R_c=0
- No influence of leaf bioactivity



Current model development Terrain

- Topography
- Roughness
- Vegetation/ground types
 - Deposition







Ground types

- Land Use Classes (LUC)
 - FOI uses 26 classes
 - IGBP uses 17 classes
 - Zhang uses 15 classes
 - Transformation required between sets of LUC
 - LUC provides estimates of
 - LAI
 - Roughness
 - Resistances
- Leaf Area Index (LAI)
 - Area leafs (one-sided) relative to ground area
 - Seasonal dependent

IGBP LUC

Evergreen Needleleaf Forest	Grasslands
Evergreen Broadleaf Forest	Permanent Wetlands
Deciduous Needleleaf Forest	Croplands
Deciduous Broadleaf Forest	Urban and Built-Up
Mixed Forest	Cropland/Natural Vegetation Mosaic
Closed Shrublands	Snow and Ice
Open Shrublands	Barren or Sparsely Vegetated
Woody Savannas	Water Bodies
Savannas	



Surface resistance, R_c Substances

 SO_2 and O_3 used as scaling factors [1]

- α– parameter : Aqueous solubility (SO₂)
- β -parameter : Aqueous oxidizing capacity (O₃)
- They operate in parallel

1. Zhang, L., et al., *Modelling gaseous dry deposition in AURAMS: a unified regional airquality modelling system.* Atmospheric Environment, 2002. **36**(3): p. 537-560.



Implementation

The method provides continuous flow, i.e. peeling of model particles.

Concentration is unknown for independent model particles. Wilson's method provides a solution for this by introducing a stochastic process [1].

$$\frac{1-R}{1+R} = \sqrt{\frac{\pi}{2}} \frac{v_d}{\sigma_w} \qquad \text{std for vertical vel.}$$
 reflection prob.

1. Wilson, J., F. Ferrandino, and G. Thurtell, *A relationship between deposition velocity and trajectory reflection probability for use in stochastic Lagrangian dispersion models*. Agricultural and forest meteorology, 1989. **47**(2-4): p. 139-154.



UPELLO FOI's new particle model

- Uses Venkatram [1] for deposition
 - Mass consistent
 - Allows for deposition in all directions



1. Venkatram, A. and J. Pleim, *The electrical analogy does not apply to modeling dry deposition of particles.* Atmospheric Environment, 1999. **33**(18): p. 3075-3076.



Refined model

- Resolving the domain close to the surface
- Idea is to make use of CFD-information better
- Numerical demanding



Henry, C., J. P. Minier and G. Lefevre, 2012: Towards a description of particulate fouling: From single particle deposition to clogging. Adv Colloid Interfac **185**, 34-76. Weil, J. C., P. P. Sullivan and C. H. Moeng, 2004: The use of large-eddy simulations in Lagrangian particle dispersion models. J Atmos Sci **61**, 2877-2887.



Some considerations

- In principal, the resistance model, LUC and substance parameters $\alpha \& \beta$ provide information and methods to calculate v_d.
- Problem with different sets of LUC
 - Incorporate NWS and satellite imagery?
- How accurate are the α & β parameters?
- How to use deposition modelling within a forest?
- Does the model handle the atmospheric stability accurately?
- There is little published data on CWA
- Stochastic or peeling deposition?
- How to incorporate saturation effects?





Deposition work at FOI



FOI trials

- Flow exchange and adsorption in buildings of sarin, NH₃ and Cl₂ and simulants for VX experimentally [1]
 - Effects of different wall covers and carpets
 - Unpainted concrete showed high adsorption for nerve agents

- Primary Contamination A Field trial [2]
 - Low contamination of person compared to ground



- 1. Karlsson, E. and T. Berglund, *Inläckning, adsorption och återgivning av giftig gas i vanliga byggnader och skyddsrum.* 1994, Swedish Defence Research Agency.
- 2. Koch, B., et al., *Primär Kontaminering Ett Fältförsök*. 1988: Swedish Defence Research Agency.



Meteorological impact on dry deposition of gases

L. Jonsson et al. / Journal of Hazardous Materials A124 (2005) 1-18

Investigation by models

- Evaluation of the influence of the weather on the dry deposition [1]
- Particulate dry deposition in urban settings [2]
 - u* strongly influence v_d



- 1. Jonsson, L., E. Karlsson, and L. Thaning, *Toxic gas clouds: Effects and implications of dry deposition on concentration.* Journal of hazardous materials, 2005. **124**(1-3): p. 1-18.
- 2. Jonsson, L., E. Karlsson, and P. Jönsson, *Aspects of particulate dry deposition in the urban environment.* Journal of Hazardous Materials, 2008. **153**(1–2): p. 229-243.



Inverse modelling Including deposition

Deposition poses a hard problem Methodology development [1]



1. Persson, L. and J. Burman, *Torr- och våtdeposition i ajdungerade linjära konvektionsdiffusionsmodeller*. 2017, Swedish Defence Research Agency.





Winter conditions



Vords for snow of different type





Pulversnö Rensartäcke Skare Skarsnö Sockersnö Snörök Spårsnö Sursnö Trindsnö Tösnö Upplega **Yrsnö** Snöblask **Snödrev Snöflinga** Snöglopp **Snölega** Snömodd **Snöras** Snöregn Snöyra

Snow and ice

Snow is a type of ice, they differ due to different creation processes pH of 5 - 6 Density 10 - 400 kg/m³ Snow water equivalent (SWE) or snow to liquid ratio (SLR) is important







Snow content

- Solid ice crystals
- Liquid water
- Air
- Particles
- Pollutants
- Insects
- Deposited substances
- ...





Seasons

Winter with snow

- Snow/ice surfaces
- Low LAI
- Low biological activity
- Meteorology
 - Atmospheric stability
- High anthropogenic emissions
- Low natural emissions





Measurements in the literature Deposition in winter conditions

Substances

- Ozone
- Sulfur dioxide
- NO_x
- Not much on CW

Main findings

Low deposition velocities, v_d v_d 5-10 times higher to vegetation than snow v_d for veg. much lower in winter than in summer

Temperature dependency v_d for snow increases strongly with temperature There is a 10 nm water layer on snow close to 0°C Wet snow acts as water Water content dependency

Snow "age" dependency Saturation effects may be present SO_2 has a v_d to snow of ~ 0.04-0.6 cm/s

Understudied subject, mainly quite old experiments All reported data is not consistent, i.e. there are uncertainties



A model for gas-snow interaction

M.P. Valdez, R.C. Bales, D.A. Stanley, G.A. Dawson Gaseous deposition to snow: 1. Experimental study of SO₂ and NO₂ deposition, J. Geophys. Res. 92 (1987) 9779

R.C. Bales, M.P. Valdez, G.A. Dawson Gaseous deposition to snow: 2. Physical-chemical model for SO₂ deposition, J. Geophys. Res. 92 (1987) 9789



Journal of Hazardous Materials 60 (1998) 227-245

Dry deposition and desorption of toxic gases to and

from snow surfaces

Edvard Karlsson *, Susanne Nyholm National Defence Research Establishment, NBC Department, 5-001 82 Umed, Sweden Reserved 28 October 1997; revised 10 February 1998; accepted 13 February 1998

Abstract

A model describing toxic gas deposition to and desorption from a snow surface is presented. The model is based on the assumption that the deposition is caused by an adsorption of the toxic gas to small amounts of liquid water, which exist in the snow at temperatures equal to or below

Abbreviations: A_{c} , area of the walls of the test chamber, m^{2} ; A_{s} , area of the snow cover in the test chamber, m^2 ; a, constant in Eq. (18) for r_m ; c_g , gas concentration, kg m⁻³; c_g , saturated gas concentration, kg m⁻³; c_i , solution concentration, kg m⁻³; c_i , total concentration kg m⁻³; E, turbulent kinetic energy of the air in the test chamber, $m^2 s^{-2}$; F, flux of agent (vertical), kg $m^{-2} s^{-1}$; $H = c_m / 5$, Henry's law constant in In the set of characteristic structures of the set of molecular vanour diffusion coefficient in the pores of the mow, m²s⁻¹: K?, molecular liquid diffusion coefficient in the pores of the snow, m2 s-1; K4, effective diffusion coefficient in the pores of the snow m²s⁻¹; *l*, distance between transmitters and receivers in ultrasonic turbulence instrument, m; *L*, Obukov's length, m; q, typical turbulent velocity in the test chamber, m s⁻¹; R_g , partition coefficient relating total concentration to gas phase concentration; R1, partition coefficient relating total concentration to solution concentration; r, aerodynamic resistance depending on the atmospheric turbulent transfer, s m ; r_m, molecular resistance in the atmospheric viscous sub-layer, s m⁻¹; r, surface resistance of the snow depending on the flux into the inow layer, s m⁻¹; r_i^{m} , model calculated surface resistance, s m⁻¹; r_i^{mp} , experimentally measured surface resistance, s m⁻¹; S, agent solubility in water, kg m⁻³; t, time, s; w_{+} , friction velocity, m s^{-1} ; v_d , dry deposition velocity, m s^{-1} ; v_d , dry deposition velocity onto the walls of the test chamber, m s^{-1} ; v_{2}^{aup} , measured dry deposition velocity onto snow, m s⁻¹; Vol, volume of test chamber, m³; V_{w} , convective velocity (vertical) of the liquid water, m s⁻¹; F_a, effective convective velocity (vertical) of the liquid water, m s"; x, function in expression for \$\$\psi_m\$; z, height, m; z_0, roughness height, m; z_1, reference height for gas concentration in the atmosphere, m; z2, reference height for wind velocity in the atmosphere, m; \$\Delta t\$, time interval when determining $v_{1}^{(qq)}$, s; ε , total porosity, $m^{3} m^{-3}$; ϕ , fractional volume of the now pack that is liquid water, $m^{3} m^{-3}$; μ , first order degradation coefficient, s^{-1} ; θ , fractional volume of the now pack that is air, m³ m⁻³; ν , kinematic viscosity of the air, m²s⁻¹; Ψ_{ν} , function in Eq. (17) for r_{ν} ; $\Psi_{\mu\nu}$, function in Eq. (19) for w.

Corresponding author. E-mail: karlsson@ume foa se

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Comparison with experiments on GB

- Saturation is captured by Henry's law
- Temperature dependence is captured by the amount of water on top of the snow
- Decreased deposition with time
- Decreased deposition with decreasing temperature
- Deposition increase with snow age (density)
- Desorption might overtake deposition
- Desorption decrease with time
- Model overpredicts the surface resistance



Thank You