Wet Deposition in SILAM

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Outline:

- SILAM briefly
- WD in SILAM old vs. new
- Mechanistic WD
- Special case: SO2
- Improvements due to new scheme
- Conclusions



SILAM v.5: outlook

Modules

- 8 chemical and physical transformation modules (6 open for operational use),
- 6 source terms (all open),
- 2 aerosol dynamics (one open)
- 3D- and 4D- Var
- Domains: from global to betameso scale (~1km resolution)
- Meteo input:
- ECMWF
- HIRLAM, AROME, HIRHAM, ECHAM, and any other who can write GRIB-1 or GRIB-2
- WRF



Wet deposition



FIGURE 20.1 Conceptual framework of wet deposition processes.

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Wet deposition in SILAM

Operational SILAM:

- Precipitation rate from meteo
- Prescribed cloud height
- Constant precip. below cloud
- Prescribed scavenging coefficients (in- or belowcloud, rain or snow)
- Species-dependent scaling



New scheme:

- Meteo input for rain/snow profiles:
 - Precipitation rates
 - Cloud water content
 - Cloud fraction
- Equilibrium in clouds
- Fraction of cloud precipitating
- Solubilities
- Simple dissociation chemistry (SO₂)

Basic concepts

For *most* chemicals in-water equilibrium CNC is proportional to in-air concentration

- can define "Equivalent volume" of water: in-water-mass / in-air-CNC in equilibrium
- flux \propto conc. difference
- resistance: $R = \Delta CNC/F$
- exchange is a relaxation process

Exchange is driven by:

- equilibrium mass fractioning
- exchange time scales



Mechanistic Wet Deposition

Air-water relaxation

- In-cloud equilibrium
- Rainout $\tau = \text{CWC}/R$
- Washout relaxations:
 - droplet CNC to air
 - in-air to incoming rain













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Sub-cloud scavenging efficiency

10 Collector Droplet $D_p/2 = 0.1 \text{ mm}$ 10 Ε 10 mm 10 10-5 10-3 10-2 10-1 10 Collected Particle Radius, d_p/2, µm

Seinfeld & Pandis (2006)

FIGURE 20.6 Semiempirical correlation for the collection efficiency E of two drops (Slinn 1983) as a function of the collected particle size. The collected particle is assumed to have unit density.

- ► Diffusion *D*
- Interception d_p
- ▶ Impaction τ_p
- Accumulation around $1~\mu{
 m m}$
- Diffusion for gases



Gas solubility

- Henry factor mole/(I Pa) says how much of dissolved gas is in equilibrium with 1 Pa of partial pressure
- Temperature-dependent
- Henry factor does not say "how much stuff can get into droplet at given in-air concentration"
- Reason: dissociation
- Effective Henry coefficient helps helps sometimes

For SO_2 situation even worse...



$\mathrm{SO}_2{:}\xspace$ how NOT to

Blind use of Henry constant from manuals.



SO_2 solubility

Solubility depends on "background" pH of water and on SO_2 itself.

No linear models work! (incl. scavenging coefficients)

In polluted regions $\sim 1 \mu mol/m^3$







Gas solubility (cont.)

The effective Henry factor for SO_2 depends on pH, in particular on the amount of dissolved SO_2

$$[\mathrm{S(IV)}] = [\mathrm{SO}_2] \left(1 + \frac{\mathcal{K}_{S1}}{[\mathrm{H}^+]}\right)$$

Result: Solubility concept does not apply.

Operational SILAM: Saturation of SO2 in rain water.

New scheme – approximate electro-neutrality:

 $[\mathrm{H^+}]\simeq [\mathsf{Strong}\ \mathsf{Acids}] + [\mathrm{HSO}_3^-] - [\mathrm{NH}_4^+], \quad [\mathrm{HSO}_3^-]\simeq [\mathrm{S(IV)}].$



- ▶ SO2 last species to scavenge
- In-water acids and ammonia are known
- Effective equilibrium solubility for given amount of water and SO2 in cell, and given acids in rain.
- Same linear algorithm is asymptotically right



Improvement



0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
		0	LD	R١	ΛS	Bia	is	Corr		NEW	F	RMS	В	ias	Corr.
95tl	h			11.	30	1.4	6	0.58	3		1	1.16	1.	.82	0.64
Mean			3.	.94 -1.23		3	0.26			3.84		-0	.90	0.31	
Med	dian			2.	97	-0.8	7	0.27	7			2.94	-0	.59	0.32

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Example:

- heavy rain in half of grid cell
- ▶ rain scavenges 99% per time step
- little wind

Question:

How much stuff will be left in air after two time steps?







- ▶ WD scheme based on relaxation
- Incloud and subcloud
- Dissociation must be accounted for SO2
- Substantial improvement of SO2 concentrations
- Subgrid effects need to be accounted for

