Chemistry outlook

M. Sofiev

Chemical transformations

- Essence: oxidation of (partially) non-oxidized species released in the atmosphere

  - for many carbonaceous, terminal species is CO_2 - not reactive

- Oxidation is driven by availability of oxidants: OH, O_3, NO_3 radical and a few others, less important

- By-product of oxidation is aerosol formation: saturation vapor pressure tends to decrease with increasing oxidation degree

- Special are transformations of toxic metals and organics: oxidation often dramatically reduces toxicity. Until that happens, other reactions, e.g. methilation, can increase it and/or change the phase state
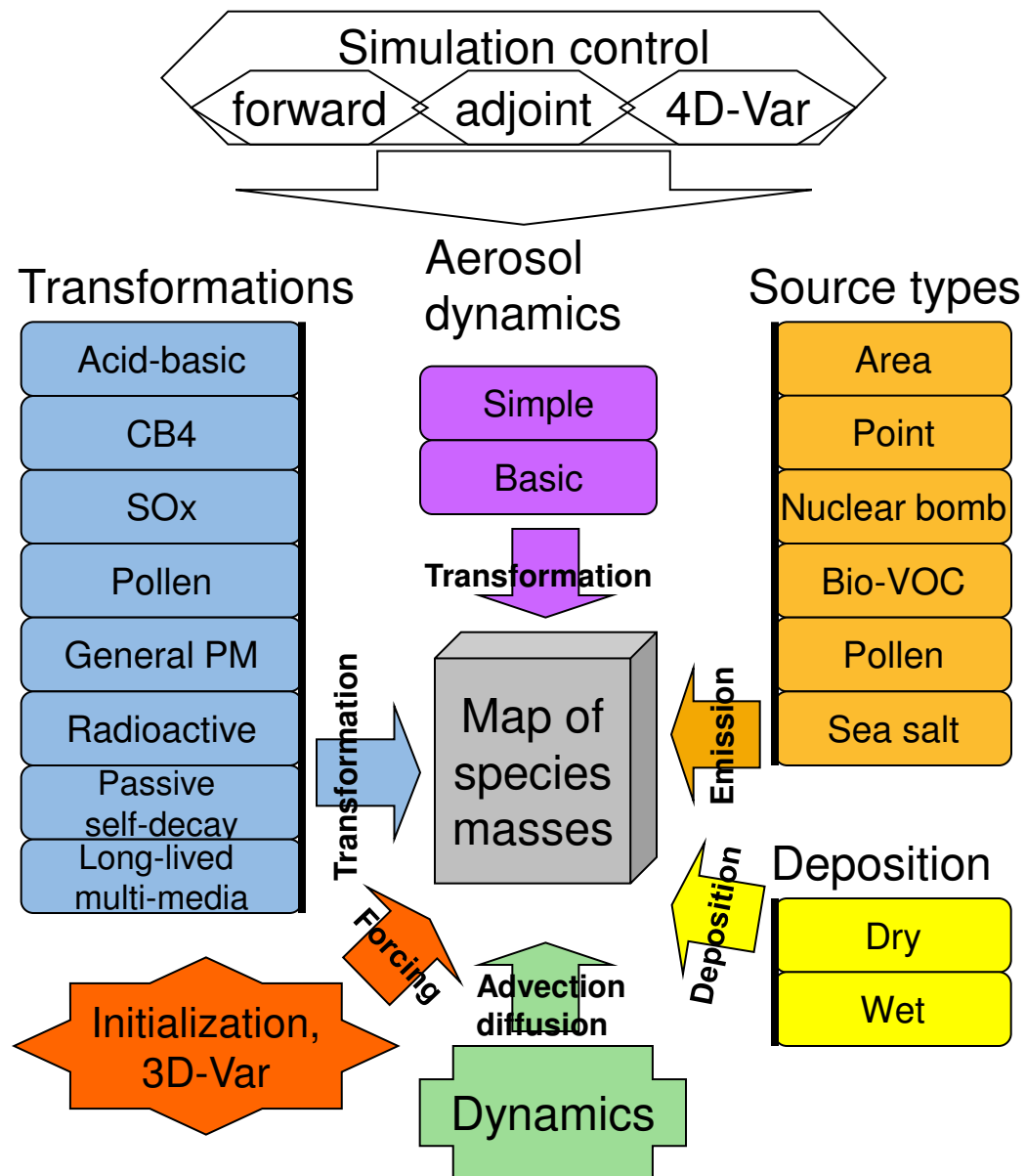
SILAM v.5: outlook

- 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
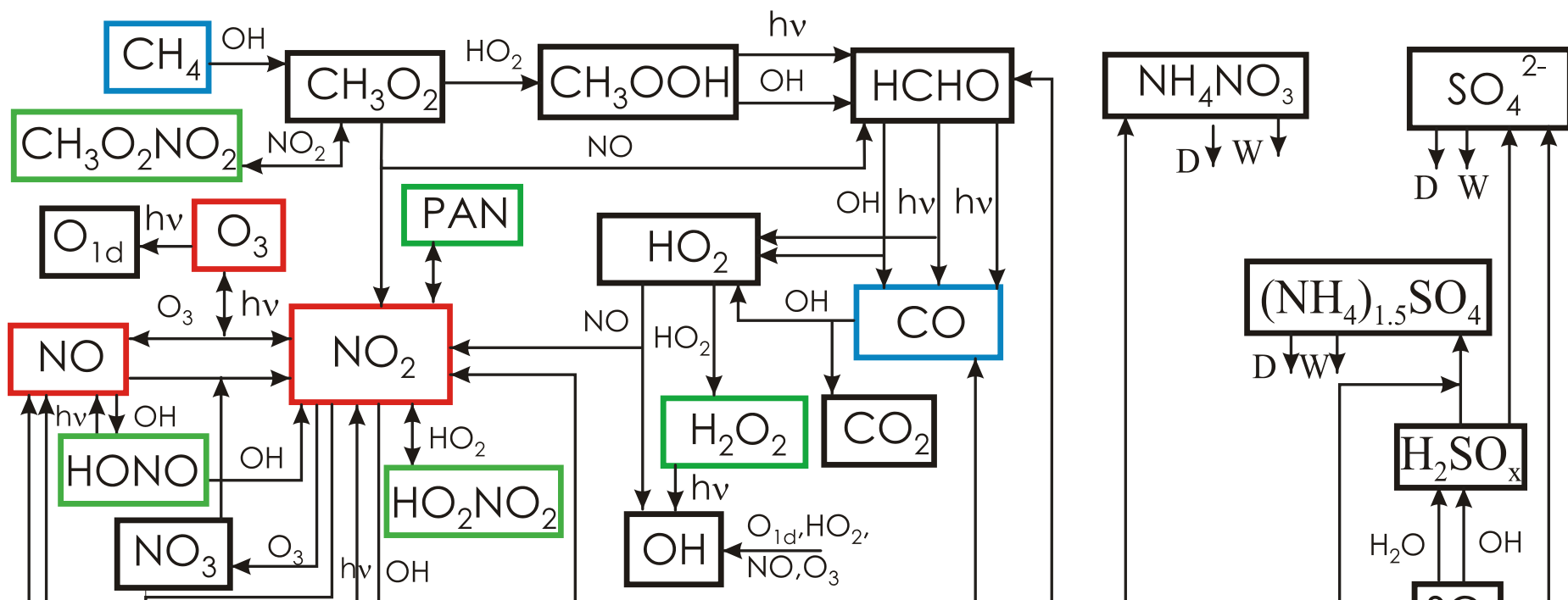- Domains: from global to beta-meso scale (~1km resolution)
- Meteo input:
  - ECMWF
  - HIRLAM, AROME, HIRHAM, ECHAM, and any other who can write GRIB-1 or GRIB-2
  - WRF

Simulation control

forward — adjoint — 4D-Var

Transformations

- Acid-basic
- CB4
- SOx
- Pollen
- General PM
- Radioactive
- Passive self-decay
- Long-lived multi-media

Aerosol dynamics

- Simple
- Basic

Transformation

Source types

- Area
- Point
- Nuclear bomb
- Bio-VOC
- Pollen
- Sea salt

Transformation

Emission

Map of species masses

Deposition

- Dry
- Wet

Forcing

Deposition

Initialization, 3D-Var

Advection diffusion

Dynamics

SILAM acid-basic chemical scheme

		SILAM	EMEP
Number of Species		29	71
Number of reactions	photochemical	12	24
	inorganic	27	21
	methane	12	11
	ethane	2	15