MATCH overview

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History of development

•Development started at SMHI during early/mid 1990s

•County-studies in Sweden

•Environmental assessment in Sweden (National and external contribution to Acid deposition in Sweden).

•Emergency preparedness system (Operational system running on weather forecast for European (including Swedish) nuclear power-plant accidents)

•“Climate gases” (CO_2 and CH_4) in the Arctic (Stockholm University)

•Regional studies of sulphur in Asia, Africa and Latin America (RAPIDC-I)

•Ozone chemistry

•Particle modules

MATCH documentation

- ~40 peer-reviewed scientific articles

- ~100 technical reports…

- MATCH manual available on local www-site

MATCH team at SMHI

- ~10 persons (including 2 Ph.D. students)
- Meteorologists, Chemists, Physicists, Engineers, (computers scientists)

MATCH installations

- SMHI
  - ➢ Research tool
  - ➢ Operational (emergency preparedness, environmental assessments)
  - ➢ Consultancy work (embedded in a GUI)
    - ✓ Estonia
- Stockholm University
- Tromsö (Norway)
- Finish Meteorological Institute
- Santiago, Chile
- Malaysian Meteorological Institute
- UNEP RRC-AP

Terminology (dispersion modelling)

"Eulerian model"

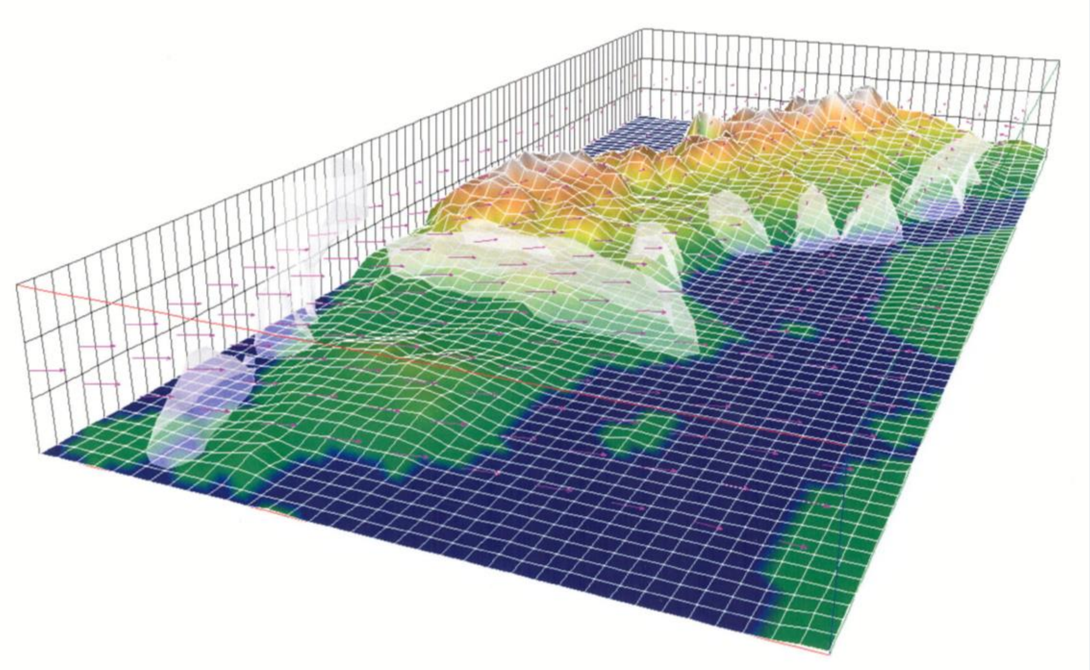
The atmosphere is divided into a large number (nx×ny×nz) of boxes. Fluxes between boxes and processes´inside boxes are taken into account.

"Off-line model"

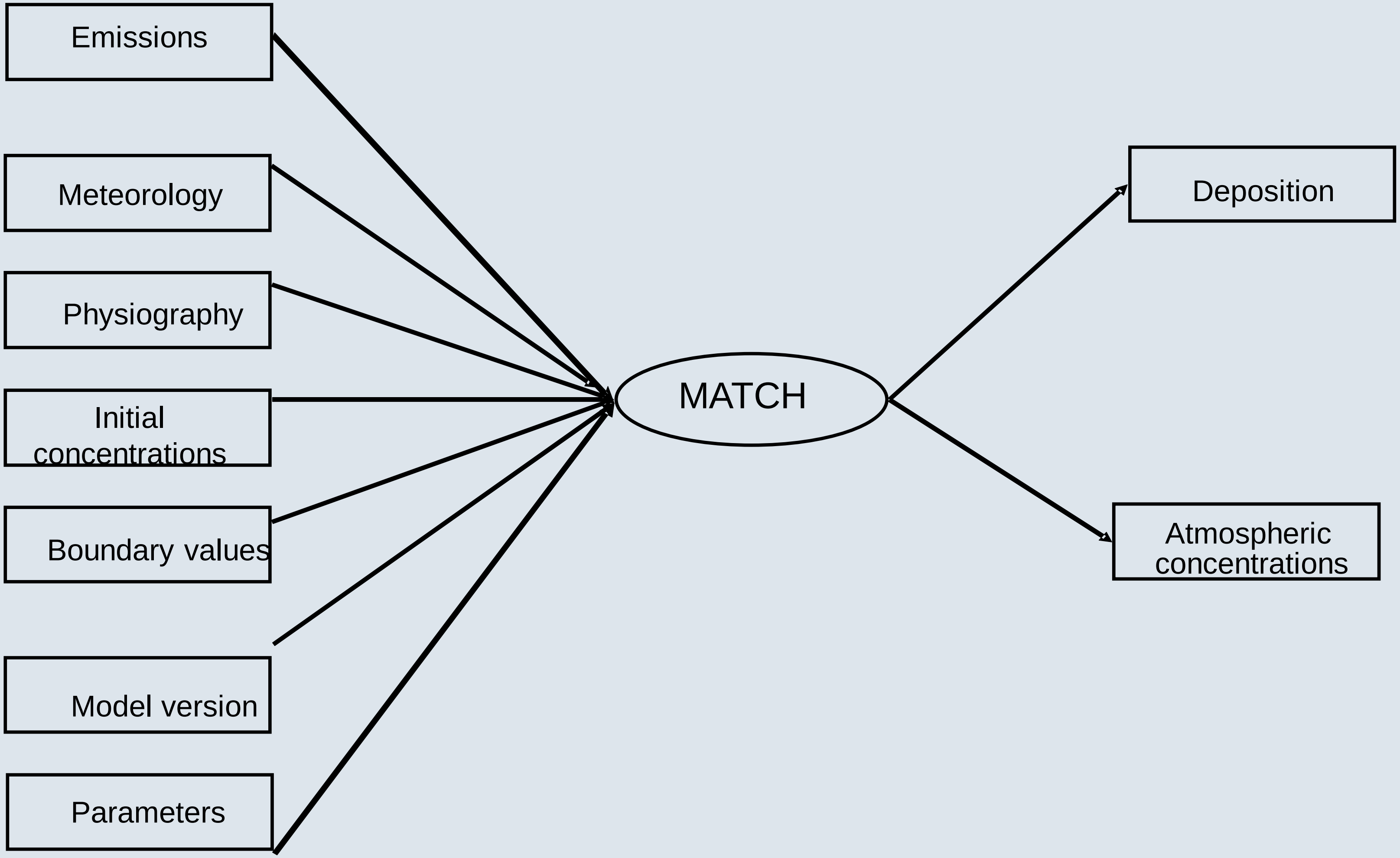
Meteorological data from an auxiliary driver. Data can be from archived meteorology or weather forecasts, or climate scenarios.

"CTM"

Chemistry Transport model; Chemical conversion, deposition and atmospheric transport and dilution described in the model.



Input / output


Emissions

Meteorology

Physiography

Initial concentrations

Boundary values

Model version

Parameters

MATCH

Deposition

Atmospheric concentrations

Processes included in MATCH

$$\text{CONC. CHANGE} = \text{EMIS} + \text{ADV}_{XY} + \text{ADV}_{Z} + \text{CONV}_{Z} + \text{TURB}_{Z} + \text{CHEM} + \text{DRYDEP} + \text{WETDEP}$$

- **At ever timestep, in every model cell, each process occur**
- **Each process is dealt with in one (or several) (fortran-) subroutines**
- **Most processes (chemistry, deposition etc.) can be described in a number of different ways (chose between a number of different schemes)**

MATCH chemistry schemes

Present chemistry options

- Inert species
- Sulphur chemistry
- Sulphur/nitrogen chemistry
- Ozone chemistry (photochemistry)
- Particles
  - Secondary Inorganic Aerosols
  - Primary emitted particles
  - Sea Salt
  - Particle growth module (under development)

No chemistry

- “Passive” transport of gases and/or particles
- Wet and Dry Deposition possible
- Examples:
  - Emergency response applications
  - Base cation (soil dust) deposition
  - Sea salt model
  - CO_2, CH_4 modelling
  - Tracer experiments (ETEX, Chernobyl)

The global sulphur cycle

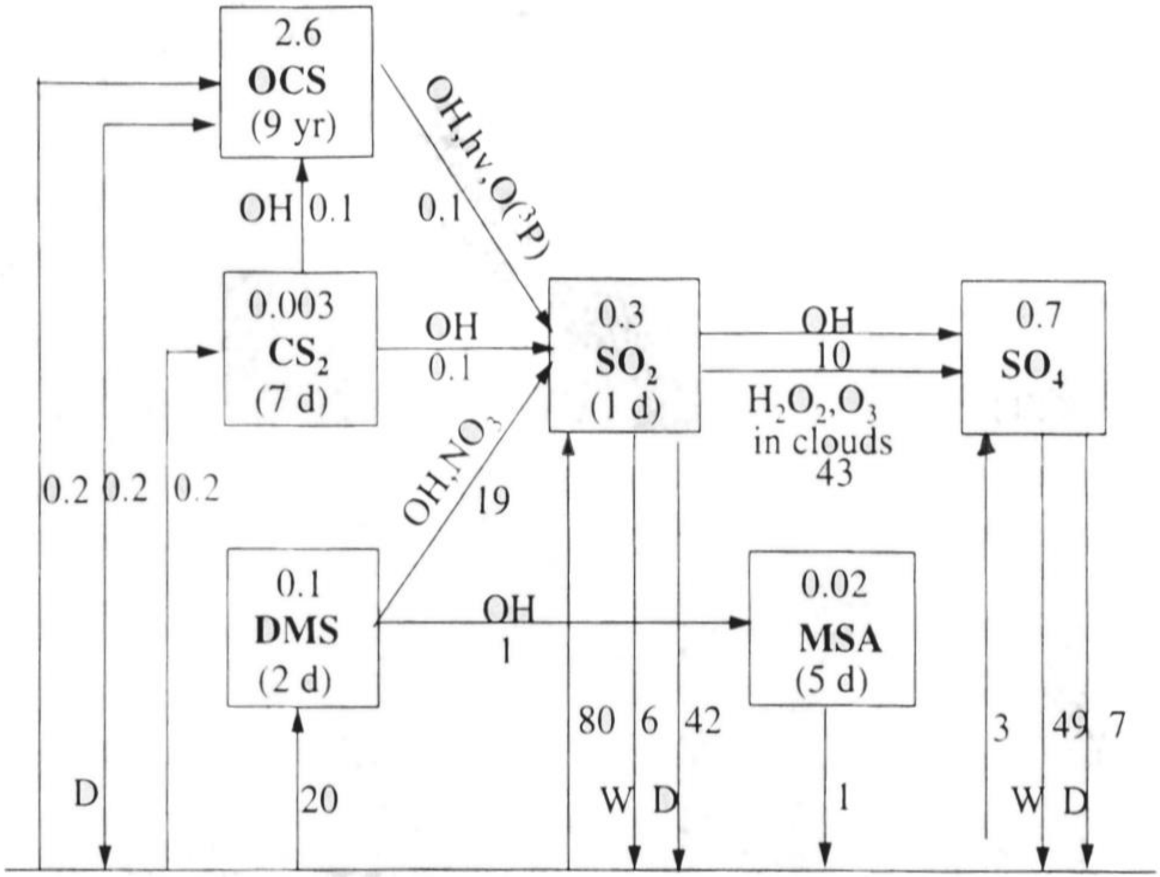


Fig. 1. The main reservoir contents (Tg S) and fluxes (Tg S/yr) in the atmospheric sulfur balance. Number in brackets refer to the residence times. The main oxidants responsible for the different oxidation processes have been indicated. D and W refer to dry and wet deposition, respectively. Data from several sources including Feichter et al. (1996), Chin et al. (1996) and Kjellström (1998).

MATCH Sulphur Chemistry Schemes

MATCH includes two different chemistry schemes aimed at studying oxidised sulphur chemistry

A simple scheme where all different SO_2 oxidation reactions are modelled using a “bulk” oxidation rate (CHEM_S_LIN)

A scheme which splits the SO_2 oxidation reactions into gas phase reactions and aqueous phase (cloud droplet) reactions (CHEM_S_FRAC)

Sulphur Chemistry Scheme (1)

Only reaction SO_2 → sulphate included

Wet and Dry Deposition included

Parameterised SO_2 oxidation rate depends on:

- **latitude**
- **season**
- **time of day**

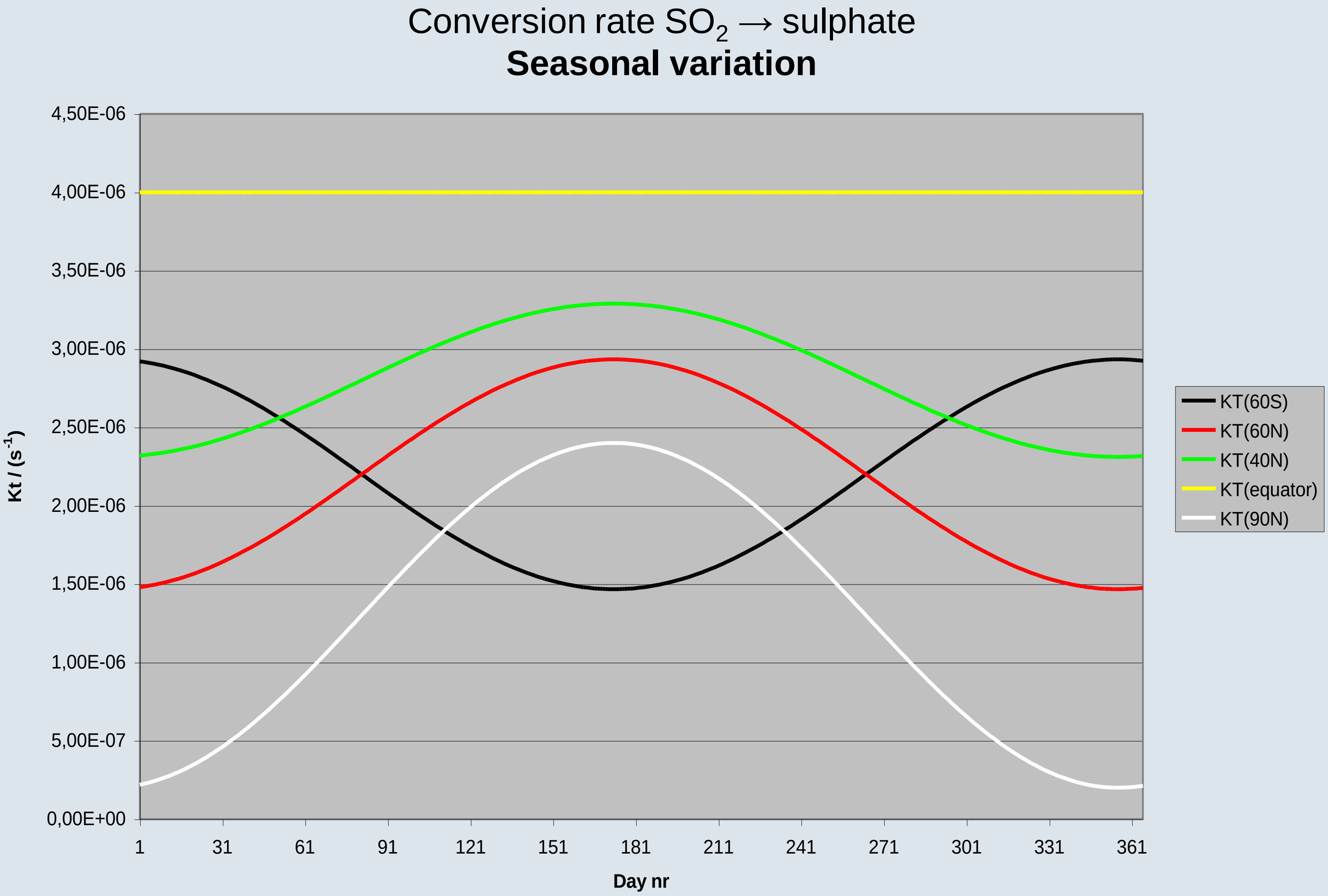
Simulates the following reactions:

$SO_2(g) + OH(g) + M \rightarrow HSO_3(g)\ [+ O_2(g)] \rightarrow SO_3(g)\ \{+ HO_2(g)\}\ [+ H_2O] \rightarrow H_2SO_4$

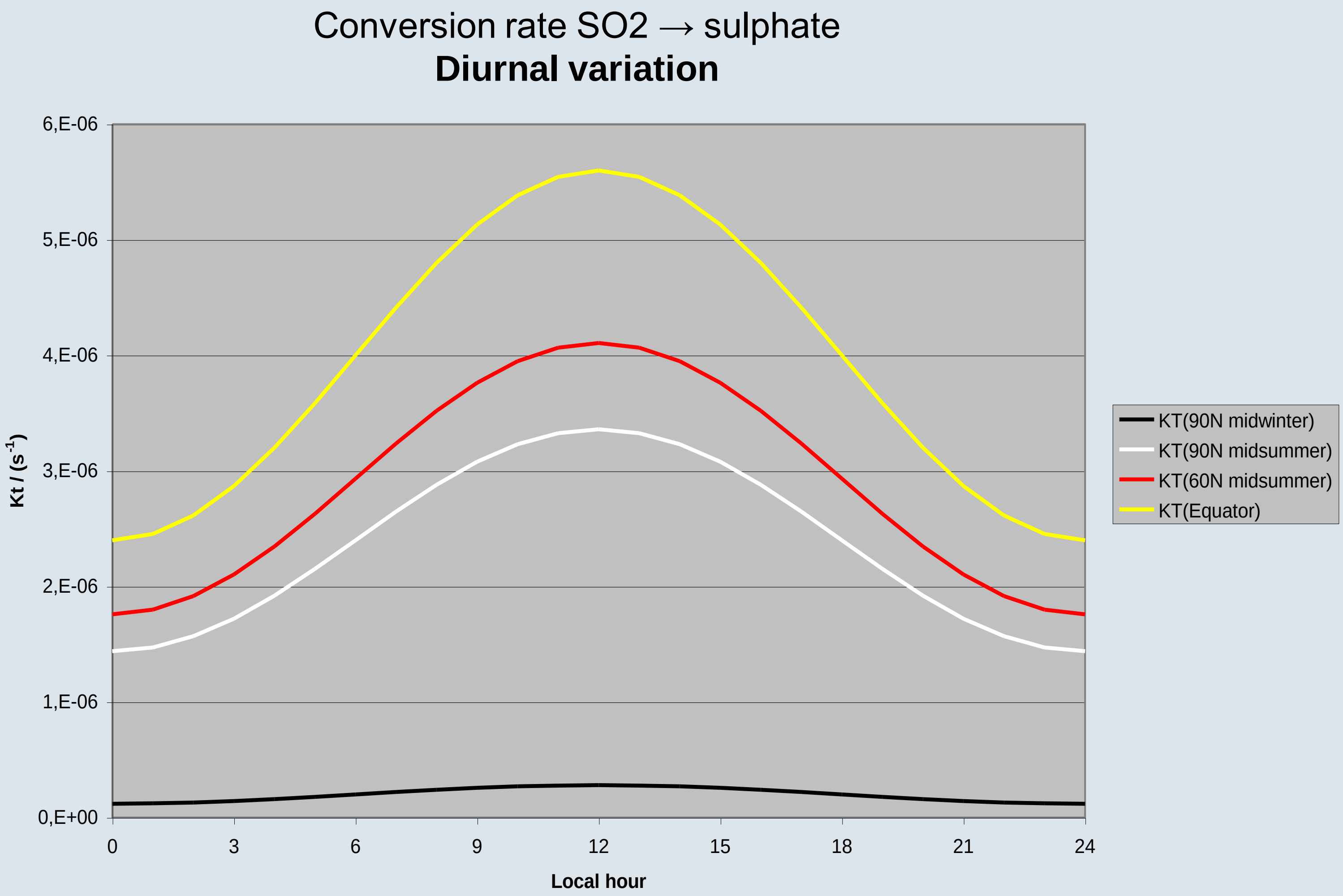
$[SO_2(g) \rightarrow SO_2(aq) \rightarrow]\ SO_2(aq) + H_2O_2(aq) \rightarrow H_2SO_4(aq)$

$[SO_2(g) + H_2O(aq) \rightarrow]\ HSO_3^-(aq) + O_3(aq) \rightarrow HSO_4^-(aq) + O_2$

Sulphur Chemistry Scheme (1)



Sulphur Chemistry Scheme (1)



Sulphur Chemistry Scheme (2)

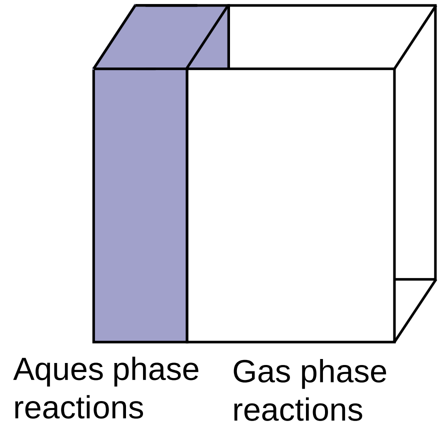
Reaction SO_2 → Sulphate split into gas phase and aqueous phase oxidation

Gas phase SO_2 oxidation rate depends on:

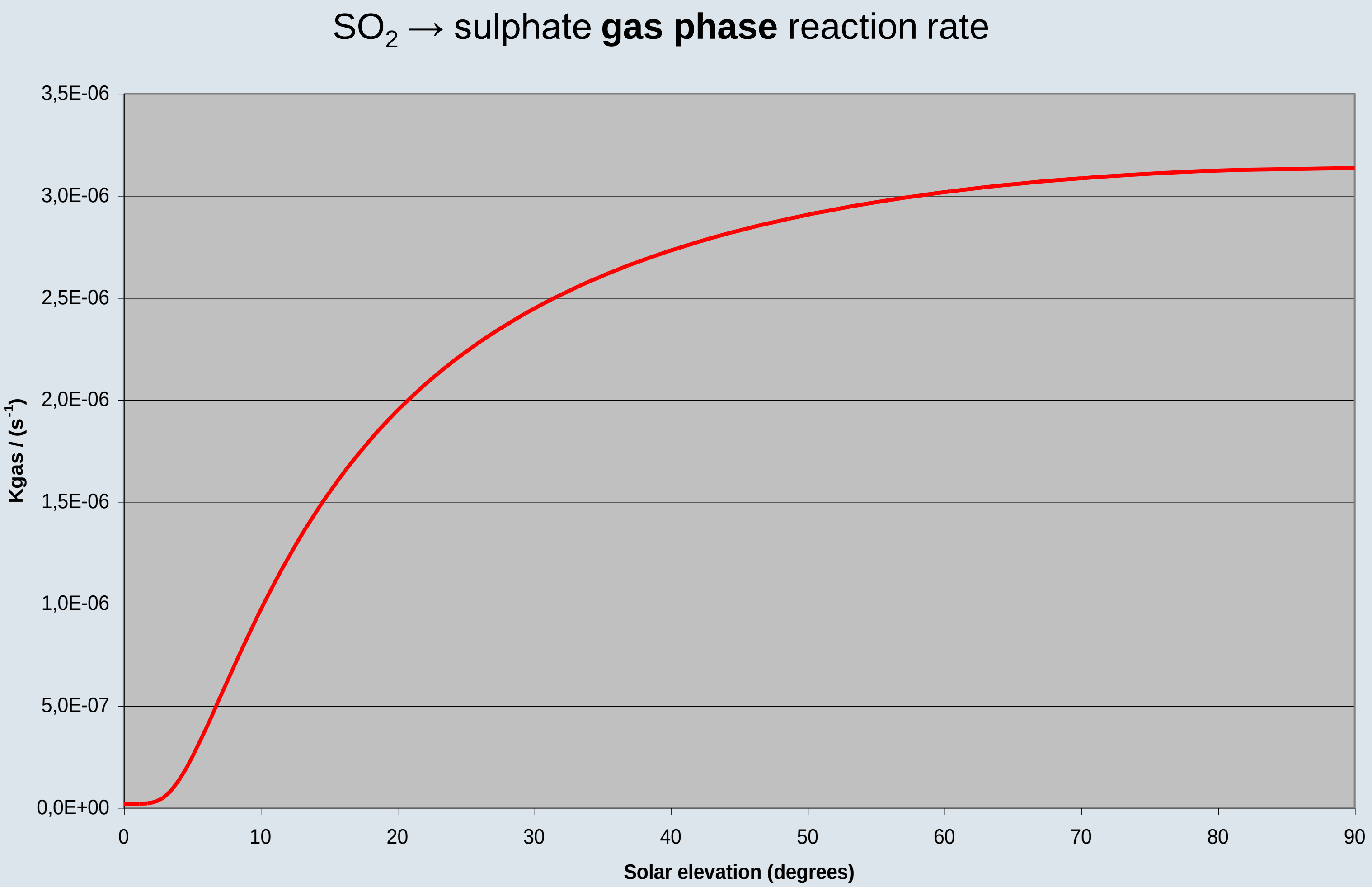
- **solar zenith angle (controls the OH concentration)**

Aqueous phase oxidation rate in cloud droplets calculated using prescribed H_2O_2 and O_3 concentrations (in the gas phase)

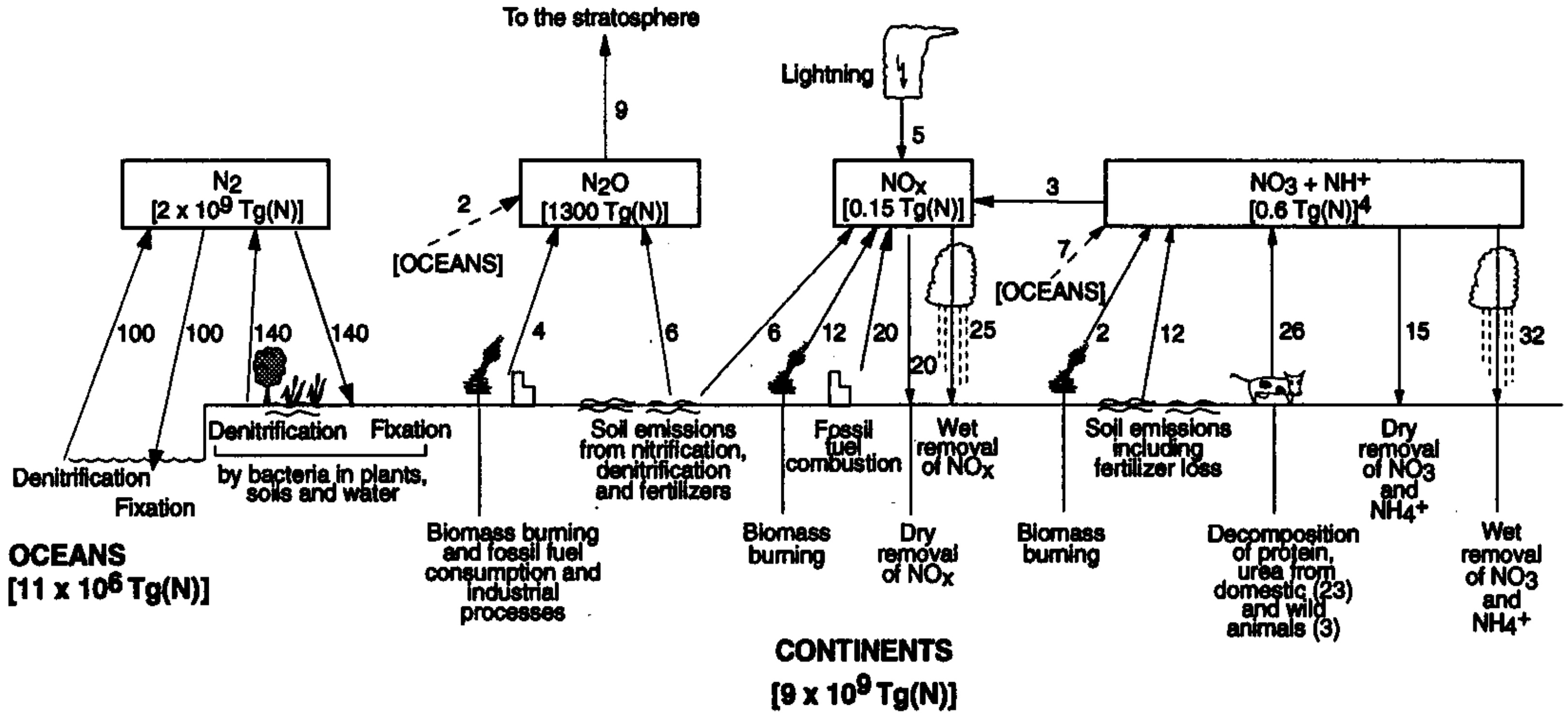
The scheme is sensitive to H_2O_2 concentrations!



Sulphur Chemistry Scheme (2)



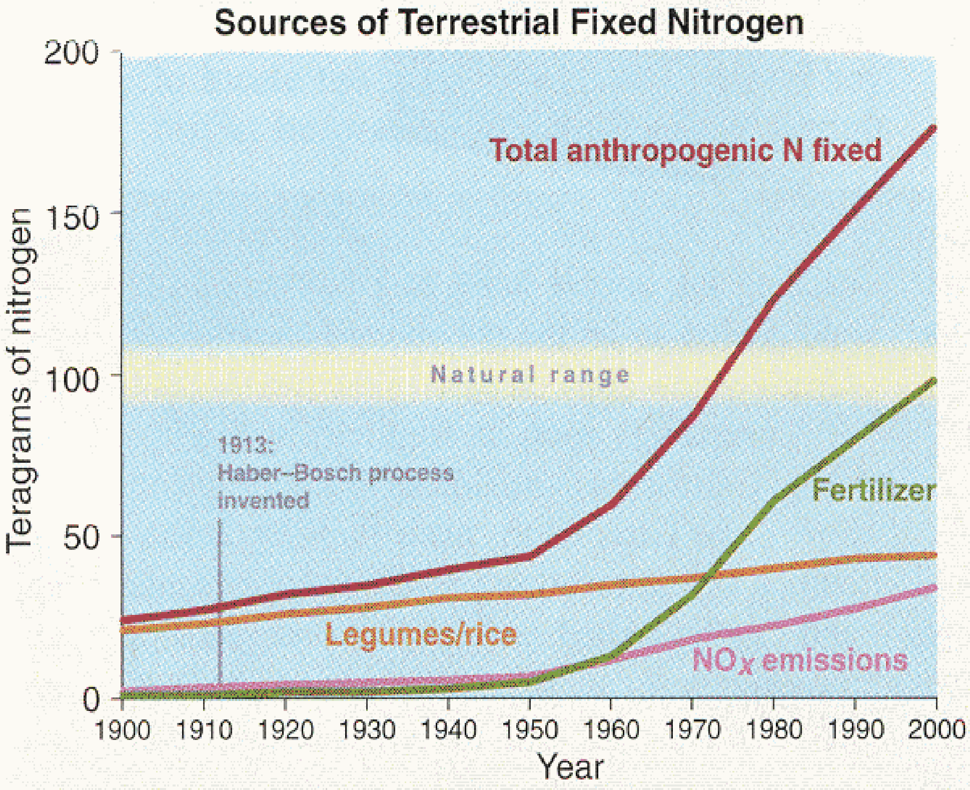
Sources and sinks for nitrogen-containing gases in the troposphere



Reservoirs and fluxes of nitrogen-containing species (Tg N year^{-1})

Nitrogen Pollution – increasing problem

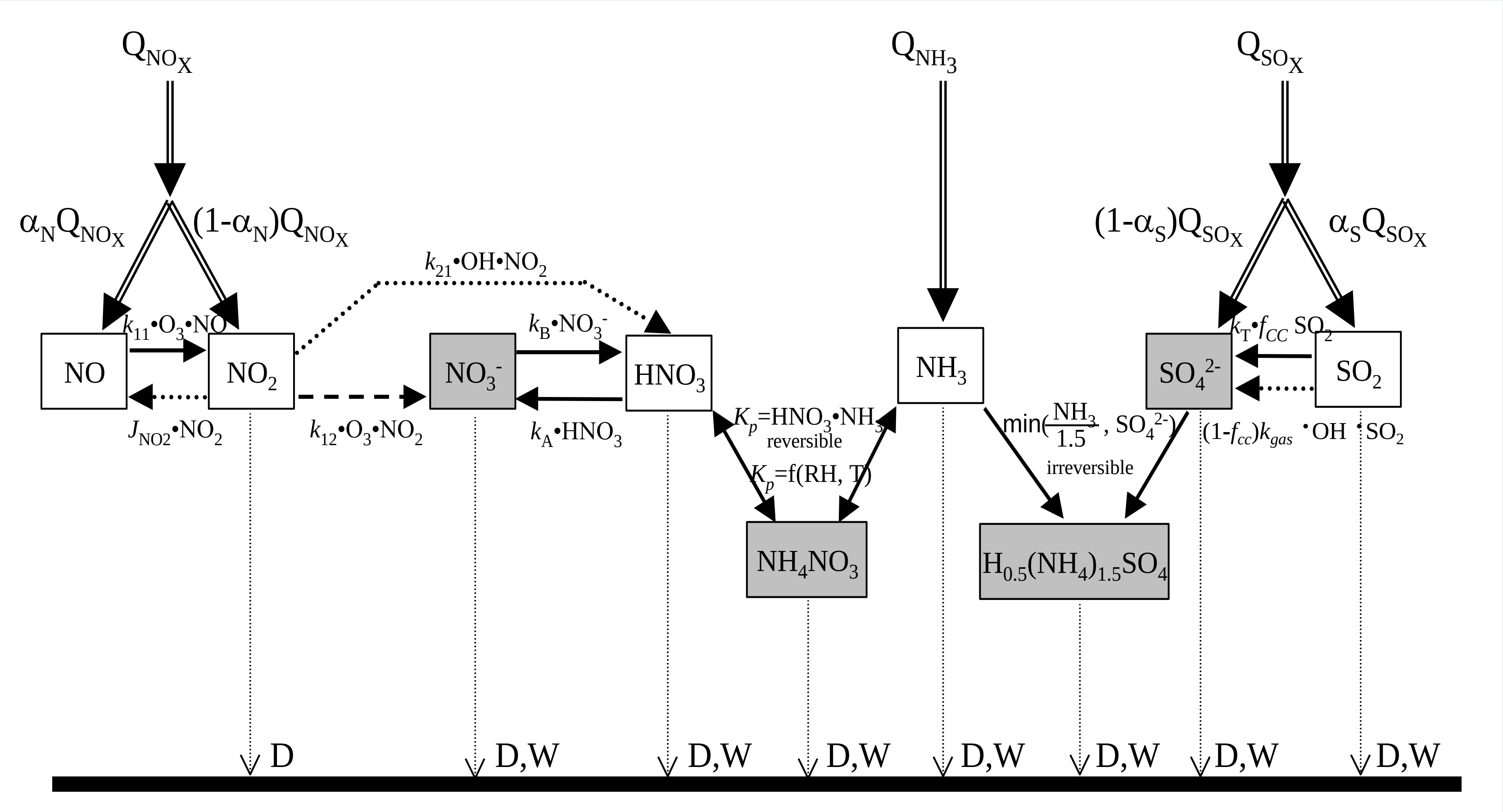
Science Vol.294 p.1268 (2001): The Other Global Pollutant: Nitrogen Proves Tough to Curb Second international Nitrogen Conference http://www.esa.org/n2001/



Overdose. Output of anthropogenic fixed nitrogen is still soaring and now far outstrips the natural terrestrial amount, leading to a host of environmental problems.

Fixed nitrogen contributes to acidification and eutrophication

Sulphur-Nitrogen Chemistry Scheme in MATCH



Sulphur-Nitrogen Chemistry Scheme

SO_2 and NO_2 gas phase oxidation:

$SO_2 + OH \rightarrow SO_4^{2-}$

$NO_2 + OH \rightarrow HNO_3$ (g)

$NO_2 + O_3 \rightarrow NO_3 \rightarrow NO_3^-$ (only night time)

Heterogeneous reactions:

HNO_3(g) $\leftrightarrow NO_3^-$ (s, aq)

SO_2 (in clouds) $\rightarrow SO_4^{2-}$

Oxidants

O_3 from other model simulations or prescribed values (based on measurements)

OH calculated from solar elevation (or from other model simulations)

Sulphur-Nitrogen Chemistry Scheme in MATCH

Ammonium chemistry:

$NH_3 + SO_4^{2-} \rightarrow \gamma NH_4HSO_4 + (1-\gamma)(NH_4)_2SO_4$

(irreversible reaction, proceeds as long as there is enough NH_3 and sulphate)

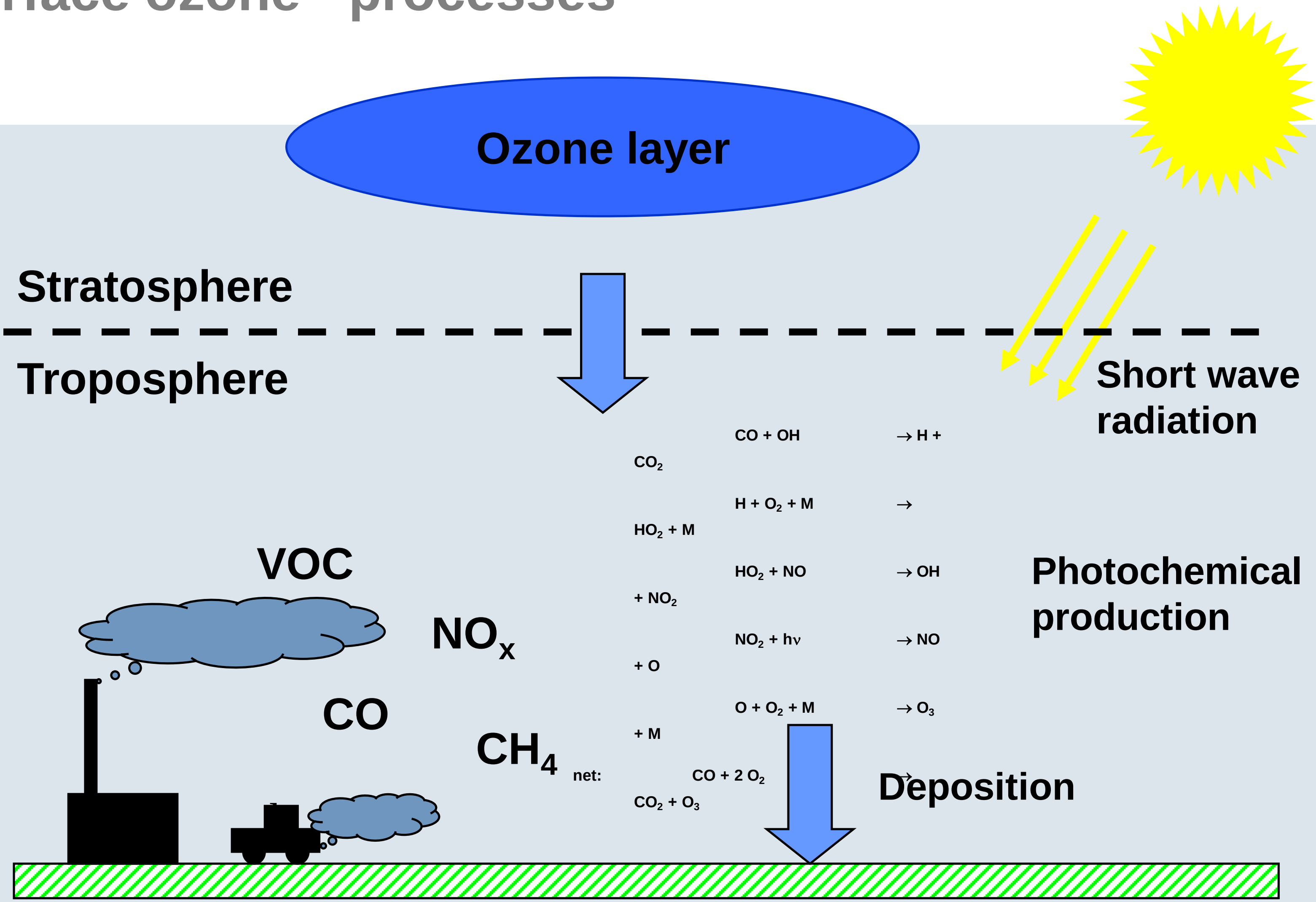
$NH_3(g) + HNO_3(g) \leftrightarrow NH_4NO_3\ (s, aq)$

(equilibrium; humidity and temperature dependent)

NO – NO_2 – O_3 steady state:

Depending on NO_X concentration and solar insolation

Surface ozone - processes



Ozone layer

Stratosphere

Troposphere

Short wave radiation

CO + OH → H +

CO_2

H + O_2 + M →

HO_2 + M

HO_2 + NO → OH

+ NO_2

NO_2 + hν → NO

+ O

O + O_2 + M → O_3

+ M

net: CO + 2 O_2 →

CO_2 + O_3

Photochemical production

Deposition

VOC

NO_x

CO

CH_4

Photochemistry Scheme in MATCH

Coupled scheme VOC: - NO_x - CO - SO_x - NH_x

Different versions exist, standard version includes

- **60 different chemical components**
- **109 thermal, gas-phase, reactions**
- **26 photolysis reactions**
- **Aqueous phase oxidation of SO_2**
- **13 (simplified) heterogeneous reactions (including NH_x chemistry)**

Modified version of the EMEP photochemistry scheme

- **Basic idea is to use a limited number of “representative” VOCs to model all emitted VOC. The selection of model VOCs is based on Photochemical Ozone Creation Potentials (POCP)**

Photochemistry Scheme

Primary Emitted VOCs

- Methane, CH_4
- Ethane, C_2H_6 (incl. Acetylene, Acetone, Trichloroethylene)
- n-Butane, n-C_4H_{10} (incl. Saturated hydocarbons, propane, butanes, pentanes, etc.)
- o-Xylene, (1,2-Dimethylbenzene), p-$CH_3C_6H_4CH_3$ (all aromatic hydrocarbons)
- Ethene, C_2H_4 (incl. some butenes and pentenes)
- Propene, C_3H_6 (incl. some butenes and pentenes)
- Methanol, CH_3OH
- Ethanol, C_2H_5OH (incl. acetates)
- Formaldehyde, HCHO
- Acetaldehyde, CH_3CHO
- Butanone, $CH_3COC_2H_5$
- Isoprene, C_5H_8

Other emissions: NO_x, CO, SO_x, NH_3

Photochemistry Scheme

Typical model split of anthropogenic NMVOC emissions

Ethane, C_2H_6	**6.7%**
n-Butane, n-C_4H_{10}	**37.1%**
o-Xylene	**24.5%**
Ethene, C_2H_4	**3.6%**
Propene, C_3H_6	**3.8%**
Methanol, CH_3OH	**1.0%**
Ethanol, C_2H_5OH	**14.0%**
Formaldehyde	**0.9%**
Acetaldehyde	**0.1%**
Butanone	**3.3%**

Biogenic emissions of isoprene (C_5H_8) calculated within MATCH. Depends on temperature, solar radiation and vegetation type. If vegetation type not available, it is also possible to input isoprene from gridded data.

Simulation time with MATCH

Model simulation time proportional to number of grid-boxes.

Model simulation time proportional to number of advected species

Model simulation time also dependent on chemistry scheme (advanced chemical scheme takes more time)

Photochemistry model very time consuming. One year simulation with photochemical model takes ~10 days on standard PCs

Deposition in the MATCH model

Deposition

Trace gases and particles are removed from the atmosphere by wet and dry deposition

Factors influencing the relative importance of dry deposition as compared to wet deposition are:

- **Gaseous or particulate form**
- **Solubility of gases and particles**
- **Precipitation amounts**
- **Terrain and surface cover type (“Land-use class”)**

Dry Deposition

Transport of gases and particulate matter from the atmosphere onto surfaces in the absence of precipitation

Important factors that governs dry deposition:

- Atmospheric turbulence
- Physical/Chemical properties of depositing species
  - Reactivity
  - Solubility
  - Size, density, shape (of particles)
- Surface properties
  - Reactivity
  - wetness
  - Smoothness
  - …

Deposition Velocity

The dry deposition flux (F_{dry}) is assumed to be proportional to the concentration (c) at some reference height **(usually 1m in MATCH)**

$$F_{dry} = -v_d\, c$$

where v_d is the *deposition velocity* (unit m/s)

Deposition Velocity (cont)

The simplest deposition schemes in MATCH use deposition velocities at 1m specified by the user.

The deposition velocities (at 1m) in this scheme may be dependent on:

- Surface type (Water, Forest, Low vegetation, No vegetation, …)
- Chemical species

Deposition Velocity (cont)

Model concentrations has to be reduced to 1 m from the middle of the lowest model layer

“Similarity theory” utilizes atmospheric stability and deposition velocity to create near-surface vertical profiles of tracer concentration

Deposition Velocity (cont)

The deposition velocity varies with time. Plants usually close the stomata at night and this will decrease the total deposition velocity for species that are taken up by vegetation.

To take into account diurnal variations in deposition, in a simple way, MATCH includes a scheme where deposition velocities (at 1m) are given as sums of constant “minimum” deposition velocities and a part which depend on the solar elevation angle

$$v_d = v_{d,min} + v_{d,stomata} f(solar\ elevation)$$

$$f(solar\ elevation)=0 \text{ at night}$$

$$f(solar\ elevation)=1 \text{ at noon}$$

$v_{d,min}$ and $v_{d,stomata}$ are species dependent

Deposition Velocity (cont)

In this deposition scheme special deposition velocities to snow covered and/or cold (T<0°C) surfaces may be used.

Deposition Velocity - Example SO_2 deposition (cm/s)

$V_{d\ sea}(SO_2) = 0.5$

$V_{d\ snow}(SO_2) = 0.06$

$V_{d\ low\ veg}(SO_2) = 0.3 + 0.5*f(sol)$

$V_{d\ forest\ nov\text{-}may}(SO_2) = 0.6 + 0.7*f(sol)$

$V_{d\ forest\ june}(SO_2) = 0.7 + 0.8*f(sol)$

$V_{d\ forest\ july}(SO_2) = 0.7 + 1.0*f(sol)$

$V_{d\ forest\ aug\text{-}sep}(SO_2) = 0.8 + 1.0*f(sol)$

$V_{d\ forest\ oct}(SO_2) = 0.7 + 0.7*f(sol)$

Deposition Velocity Particles

For gaseous species solubility and reactivity are the major factors affecting surface resistance and overall deposition velocities

For particle the most important factor is the <u>particle size</u>

Particles are transported towards the surface by similar processes as gases but are affected by

- Gravitational settling (large particles)
- Slow Brownian diffusion (for particle diameters > 0.05 µm)
- For particles > 2 µm inertial impaction relatively efficient for transport across the laminar sublayer
- Possible rebound from smooth surfaces

Deposition Velocity Particles

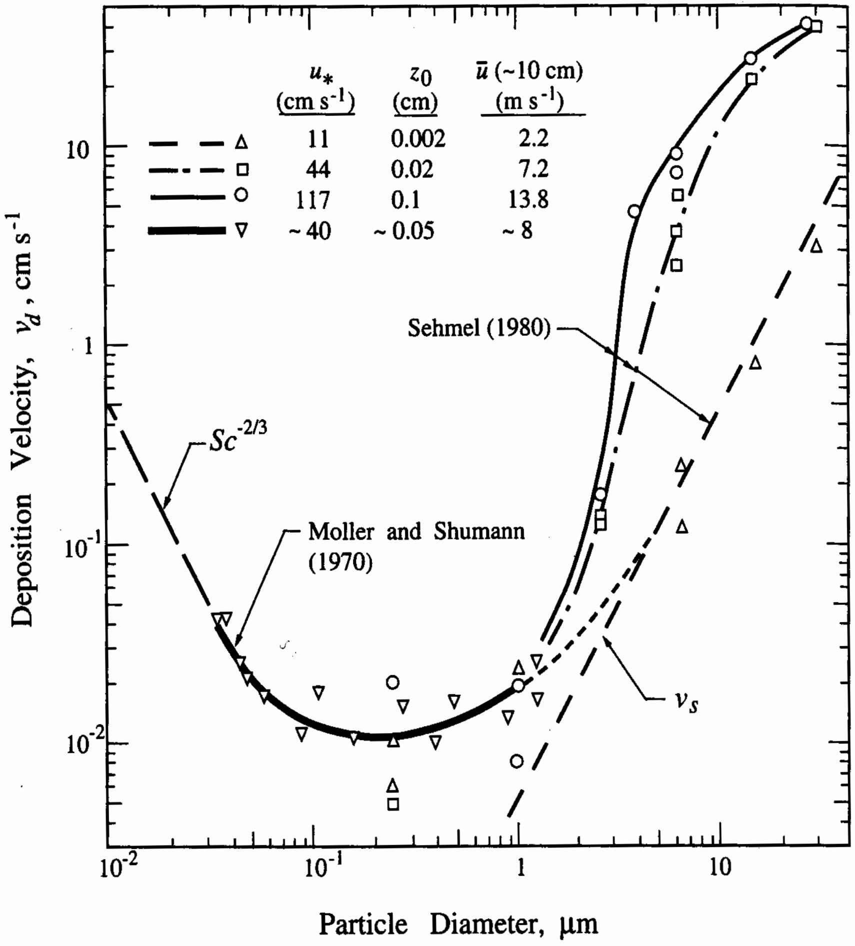


FIGURE 19.3 Particle dry deposition velocity data for deposition on a water surface in a wind tunnel (Slinn et al., 1978).

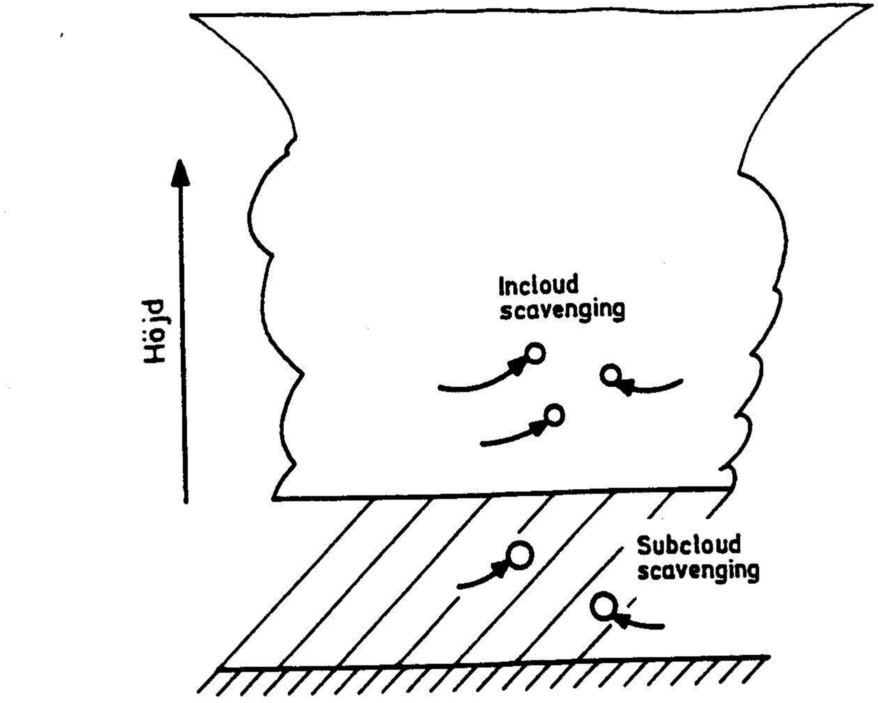
Note the low dry deposition velocities for particles in the diameter range 0.05 to 2 µm – the *accumulation* mode

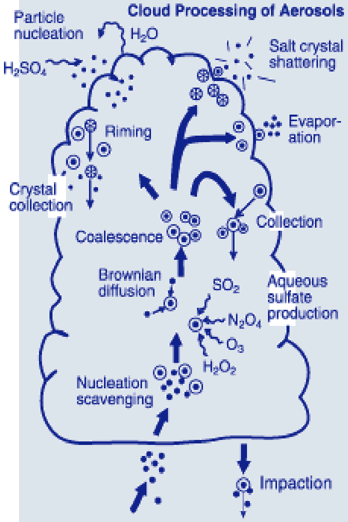
Gravitational Settling Velocity Particles

Settling velocities (at 25°C, 1atm) for particles with density 10^3 kg m^{-3}

Particle diameter (μm)	**Settling velocity (cm s^{-1})**
0.2	**0.0002**
1.0	**0.0035**
2	**0.013**
5	**0.078**
10	**0.31**
20	**1.2**
50	**7.6**

Wet Deposition - Gases and particles are scavenged in clouds and under clouds





Wet deposition modelling in MATCH ("2-dimensional")

Simple scheme using scavenging coefficients

$$\frac{dc_{i,j,k}}{dt} = -\Lambda_k c_{i,j,k} P_{surf}$$

where Λ_k is the scavenging coefficient, $c_{i,j,k}$ the concentration at level *k and* P_{surf} the surface precipitation intensity

Λ_k is a function of solubility, (precipitation intensity) *etc*. Typical Λ_k :

100×10^{-6} $s^{-1}(mm\ h^{-1})^{-1}$

Wet deposition modelling in MATCH (“3-dimensional”)

A more detailed wet deposition scheme has been implemented in MATCH for particles and some gaseous components

The scheme takes into account 3-dimensional cloud cover and cloud water content

The scheme is still under development and assumes the same lognormal distribution of the rain drop spectrum (specified by mean diameter and standard deviation for the drop size) for all clouds

Presently available in the size-resolved aerosol model and for the sulphate and ammonium-sulphate particles in the “sulphur/nitrogen” chemistry as well as for the following gases: Sulphur dioxide, ozone and hydrogen peroxide (H_2O_2)

Particle wet deposition (“3-dimensional”)

This scheme separates in-cloud scavenging from sub-cloud scavenging

All particles inside clouds are assumed to go into cloud droplets. This means that the wet deposition due to in-cloud scavenging is calculated as:

Wet deposition = (cloud cover * precipitation / cloud water content) * particle concentration

Below cloud scavenging of particles takes into account collection of particles by Brownian diffusion (important for small particles), inertial impact (important for heavy particles) and interception (important for large particles)

The total below-cloud washout coefficient, $\Lambda_{\text{below-cloud}}$, then is:

$$\Lambda_{\text{below-cloud}} = \mathit{Brownian} + \mathit{Intercept} + \mathit{Impact}$$

Boundary layer processes

-in MATCH

Vertical transport occur both through advection with the mean vertical wind and through turbulent diffusion

Near the surface of the ground is the mean vertical wind often close to zero

Still does vertical transport of tracer mass occur though the influence of turbulent eddies

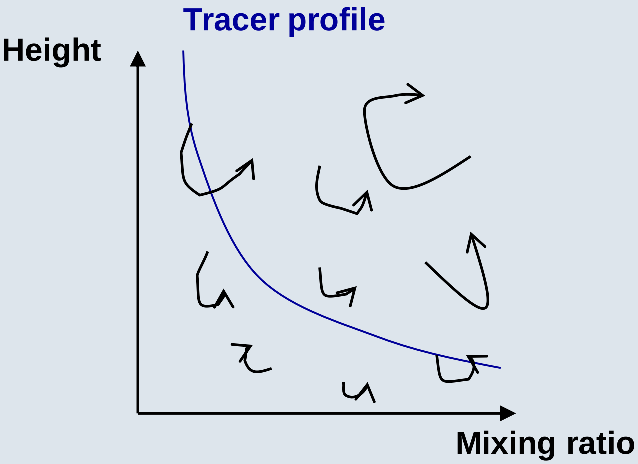
I.e. “Vertical turbulent mixing”

Turbulent transport is modelled through a diffusion analogy in MATCH:

Vertical flux proportional to turbulence and tracer gradient: $\mathrm{FLUX} \propto K_Z \times d\mu/dz$

Diffusion coefficient

Vertical tracer gradient



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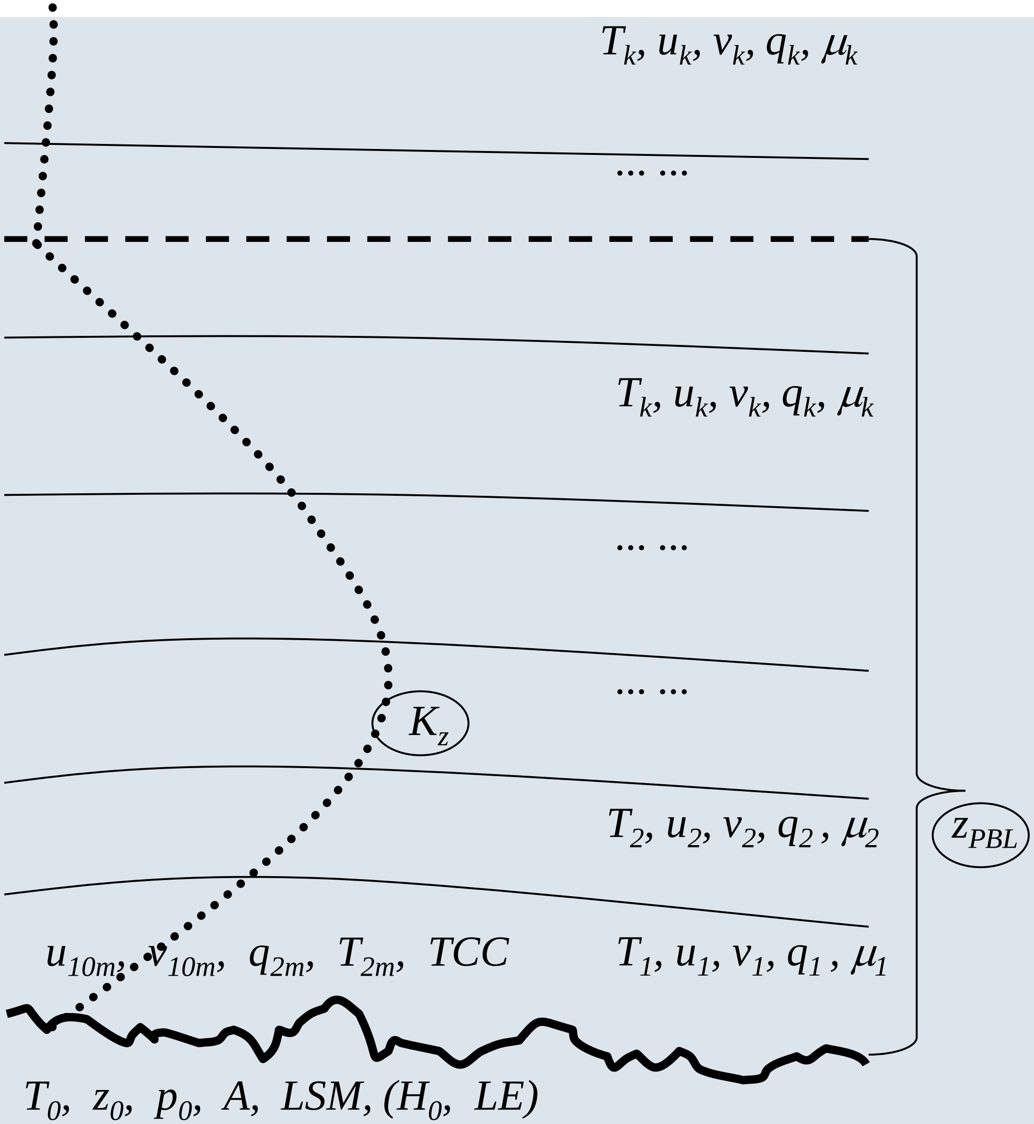
The turbulent eddies generate a net vertical flux of tracer

Near-surface turbulence calculated in MATCH based on the driving large-scale parameters



$$u_*, z_0 = f_1(u_*, z_0, |V_z|)$$

$$H_0 = f_2(z_0, T_1 - T_0, TCC, \ ...)$$

$$LE = f_3(z_0, T_1 - T_0, TCC, \ ...)$$

$$L = f_4(H_0, u_*)$$

$$z_{PBL} = f_5\left(H_0, \frac{\partial \Theta}{\partial z}, u_*\right)$$

$$K_z = f_6(z_{PBL}, H_0, L, \ ...)$$

$$\frac{\partial \mu_k}{\partial t} = f_7\left(K_z, \frac{\partial \mu_k}{\partial z}, \ ...\right)$$

Turbulence calculations

Are used for:

- **Releasing the emissions at the right height**
- **Deduce turbulent mixing during dispersion calculations**
- **Calculate near-surface (1 m) concentrations (for dry deposition calculations)**

Advection scheme

-in MATCH

MATCH utilises a mass conservative and shape preserving advection scheme

Important not to loose or create mass during simulations

Important to preserve gradients and structures during advection

Important to have an efficient (fast) advection scheme