

Model description taken from:

**Roldin P.¹, Swietlicki E. , Schurgers G. , Arneth A. and others?
Development and evaluation of the aerosol dynamic and gas
phase chemistry model ADCHEM ...**

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¹Division of Nuclear Physics, Lund University, 221 00, Lund, Sweden

“ADCHEM can be divided into three sub-models:

- 1. an atmospheric aerosol dynamics and particle chemistry model*
- 2. a chemical gas phase model*
- 3. a radiative transfer model*

The aerosol dynamic model in ADCHEM is a sectional model which discretizes the particle number size distribution into finite size bins. The particles are assumed to be internally mixed which means that particles of the same size have the same composition. The model includes Brownian coagulation, dry deposition, wet deposition, in-cloud processing, condensation, evaporation, primary particle emissions, homogeneous nucleation and dispersion in the vertical (1-D model) and horizontal direction (2-D model) perpendicular to the air mass trajectory path. The model treats both organic and inorganic particle chemistry with sulfate, nitrate, ammonium, sodium, chloride, non water soluble minerals (metal oxides/hydroxides), Elemental Carbon (EC), Primary Organic Aerosol (POA), Anthropogenic and Biogenic Secondary Organic Aerosol (ASOA and BSOA), and in-cloud processing of the aerosol particles, including dissolution of sulfur dioxide and hydrogen peroxide into the particle water phase. SOA are formed by condensation of oxidation products of α -pinene, β -pinene, Δ^3 -carene, D-limonene, isoprene, benzene, toluene and xylene. The aerosol dynamics and particle chemistry model is coupled to the gas phase chemistry model through the condensation and evaporation processes.

The gas phase chemistry model calculates the gas phase concentrations of 63 different species, using 119 different chemical reactions.

The actinic flux used to calculate the photochemical reaction rates, is derived with the radiative transfer model. This model uses a quadrature two-stream approximation scheme, where the radiative fluxes are approximated with one upward and one downward flux component. The model can be used to calculate the radiative transfer in a vertically inhomogeneous atmosphere with clouds and aerosol particles (Toon et al., 1989).

Atmospheric diffusion

As default the model domain consists of 20 vertical grid cells and 20 horizontal grid cells. The vertical and horizontal grid resolution is 100 m and 1000 m, respectively. The 2-D model solves the atmospheric diffusion equation (eq. (1)) in the vertical and horizontal direction perpendicular to the air mass trajectory. Dry deposition and emissions of primary particles in the surface layer are treated separately, and are not included in the boundary conditions for the atmospheric diffusion equation. The reason for this is to make the model as fast as possible. Instead of solving the 2-D atmospheric diffusion equation for each particle size bin for 13 different compounds, and each gas phase species (63 compounds), the model solves the atmospheric diffusion equation once for each grid cell. For the 20x20 grid, this means that the diffusion equation has to be solved 400 times in each time step. Equation 1 is solved 400 times by introducing an inert species with initial concentration equal to 1, in one new single grid cell at the time. In all other grid cells the concentration is set to zero. After one time step a new concentration matrix of the inert species is received, which describes the mixing of the air between the grid cell with initial concentration equal to 1 and the surrounding grid cells. If the time step used is short enough the atmospheric diffusion equation does not have to be solved for the whole grid, but rather for the grid cells closest to the grid cell with an initial concentration equal to 1. This way the simulation time can be decreased drastically.

$$1) \quad \frac{dc}{dt} = \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial c}{\partial z} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial c}{\partial y} \right)$$

K_{zz} and K_{yy} in equation 1 are the eddy diffusivities (turbulent diffusivities) in the vertical and horizontal direction, respectively. c is the concentration of any arbitrary species. The eddy diffusivities are calculated for stable, neutral and unstable

atmospheric conditions using the representations from Businger and Arya, 1974, Myrup and Ranzieri, 1976 and Tirabassi and Rizza, 1997. As upper boundary condition the concentration gradient $\partial c / \partial z$ was set to 10^{-3} m^{-1} to account for the generally decreasing gas and particle concentrations above the model domain (2000 m a.g.l.).

Aerosol dynamics

Each aerosol dynamic process is included as a separate process in the model, using operator splitting. As default the model solves all aerosol dynamic processes with a time interval of 60 seconds. However, if treating NH_3 condensation and evaporation as a dynamic process the model solves the condensation/evaporation equation with a time interval of only a few seconds. For most applications gas and particle phase concentrations of NH_3 (NH_4^+) can be calculated assuming equilibrium between gas and particles, as long as the mass transfer of HNO_3 , HCl and H_2SO_4 is treated as an dynamic process (ch 17 in Jacobson, 2005).

Size distribution structures

In ADCHEM the changes in the size distributions upon condensation/evaporation or coagulation are solved with the full-stationary, full-moving or moving-center structures which all have different advantages and disadvantages. All these methods are mass conserving. For a description of the methods see chapter 13 in Jacobson, 2005.

Condensation and evaporation

The model considers condensation or evaporation of sulfuric acid, ammonia, nitric acid, hydrochloride acid and oxidation products of different organic compounds (X_i). This is performed by solving the condensation/evaporation equation (eq. (2)). The condensation and evaporation is solved by first calculating the growth of all particles, in each size bin separately using mass conserving and unconditionally stable analytic prediction of condensation (APC) and predictor of nonequilibrium growth (PNG) schemes developed and described by Jacobson, 2005, and then using either the full-stationary, full-moving or moving-center structure to give the full size distribution. The APC scheme is used for condensation/evaporation of organics, sulfuric acid and HCl , HNO_3 forming solid salts. For HCl and HNO_3 dissolution in the particle water,

the PNG scheme is used instead. In this scheme NH_3 condensation/evaporation can either be treated as a dynamic process similar to the HCl and HNO_3 mass transfer or as an equilibrium process solved after the mass transfer of HNO_3 and HCl has been solved. Treating the NH_3 mass transfer as an equilibrium process enables the model to take long time steps (minutes) when solving the condensation/evaporation process (ch 17 in Jacobson, 2005).

$$2) \quad \frac{\partial n_D(D_p, t)}{\partial t} = -\frac{\partial}{\partial D_p} [I_D(D_p, t)n_D(D_p, t)]$$

$$I_{D_i}(D_p, t) = \frac{dD_p}{dt} = \frac{4D_i M_i}{RTD_p \rho_{p_i}} f_i(Kn_i, \alpha_i)(p_{i\infty} - p_{i_s})$$

$$f_i(Kn_i, \alpha_i) = \frac{0.75\alpha_i(1 - Kn_i)}{Kn_i^2 + Kn_i + 0.283Kn_i\alpha_i + 0.75\alpha_i}$$

In equation 2, $I_{D,i}$ is the diameter growth rate and f_i is the Fuchs-Sutugin correction factor in the transition region. D_p , t , n_D , T , R , ρ_{p_i} , Kn_i , M_i , α_i , $p_{i\infty}$ and p_{i_s} are the particle diameter, time, number distribution, temperature, ideal gas constant, particle density of species i , non-dimensional Knudsen number, molar mass, mass accommodation coefficient, partial pressure and saturation vapor pressure of species i . The mass accommodation coefficients for HNO_3 , NH_3 , H_2SO_4 , HCl, SO_2 , H_2O_2 and organic vapors were set to 0.2, 0.1, 1.0, 0.2, 0.11, 0.23 and 1.0 respectively. For the inorganic compounds the mass accommodation coefficients are approximately (within a factor of 2) the values recommended in Sander et al., 2006 over liquid water at temperatures between about 260-300 K. Usually it is assumed that the saturation vapor pressure of sulfuric acid is zero (Korhonen, 2004a and Pirjola and Kulmala, 1998). The saturation vapor pressure for all condensable organic compounds was set to zero when using species specific organic mass yields according to the two-product model (see section 2.4). While if using the volatility basis set (VBS) approach (Donahue et al., 2006), the VBS account for the vapor pressure of each volatility class (see section 2.4), which allows the organic vapors to be transported to and from the particle surfaces. The saturation vapor concentrations of ammonia, nitric acid and hydrochloride acid and the equilibrium concentration of sulfuric acid and hydrogen peroxide are calculated using a thermodynamic model described in section 2.2.7. The

reaction between the hydrogen peroxide and sulfuric acid in the particle water phase gives molar condensation growth rates of sulfuric acid (equation 6, section 2.2.7).

The condensable organic compounds (X_i) are formed from oxidation of monoterpenes, isoprene, benzene, toluene and xylene by OH, O_3 or NO_3 . Oxidation products of volatile organic compounds (VOC) can in many cases be the main contributor to the condensation growth rate (Komppula et al., 2006, Korhonen, 2004a, Boy et al., 2006, Tunved et al., 2006 and Kulmala et al., 2004).

Coagulation

If using the full-stationary or moving-center structure when calculating how the particle size distribution changes by Brownian coagulation so called splitting has to be used. With the splitting procedure it is assumed that only a fraction of the particles in one size bin will grow to the next size bin, while the rest of the particles will not grow at all (Korhonen, 2004b). This leads to numerical diffusion which makes the particle size distribution wider and lower the peak concentration (Korhonen, 2004b). This is since splitting make some particles grow more than in the reality, while others will not grow at all. The numerical diffusion due to coagulation is however limited since only the newly formed particles by coagulation are partitioned between the fixed size bins. The numerical diffusion can be decreased by increasing the number of size bins (Korhonen, 2004b).

Dry and wet deposition of particles

The dry deposition velocities for the different particle size bins are calculated using a resistance model based on the model by Slinn, 1982, and modified by Zhang et al., 2001. The particle transport is governed by three resistances in series, the surface layer resistance (r_a), the quasi-laminar layer resistance (r_b) and the surface resistance or canopy resistance (r_c). The dry deposition velocity for larger particles also depend on the settling velocity (v_s). If particle losses due to impaction, interception and diffusion are considered to take place in the quasi-laminar layer, the surface resistance can be neglected (Seinfeld and Pandis, ch. 19, 2006).

The wet deposition rate (s^{-1}) of different particle sizes are calculated according to the parameterization by Laakso et al., 2003, derived from 6 years of measurements at Hyytiälä field station in Southern Finland. The only input to the wet deposition parameterization apart from the particle diameter is the rainfall intensity

in mm h^{-1} . Wet deposition removal of particles is considered for all grid cells below the estimated cloud base.

Primary particle emissions

Primary particle emissions in the surface layer are treated as a separate process before the atmospheric diffusion equation is solved. Primary particle emissions included in the model are:

- 1) Marine aerosol emissions
- 2) Non-industrial combustion
- 3) Road traffic emissions
- 4) Ship emissions

The marine aerosol emissions are calculated using the emission parameterization from Mårtensson et al., 2003. The marine particle chemical composition is assumed to be composed of sodium chloride (NaCl) and POA, with NaCl dominating in the coarse mode and POA dominating in the nucleation and Aitken mode, according to the size resolved chemical analysis of Marine aerosol particles at Mace Head during the biological active period (spring, summer and autumn) (O'Dowd et al., 2004).

Inorganic particle chemistry and particle water content

The aerosol dynamics and particle chemistry model includes an inorganic thermodynamic particle chemistry model. The main purpose of the model is to calculate the saturation vapor pressures (concentrations) of hydrochloride acid, nitric acid and ammonia, and equilibrium concentrations of sulfur dioxide and hydrogen peroxide in the particle or cloud droplet water. In the model it is assumed that the inorganic aerosol particle phase is a pure aqueous solution, even if the relative humidity (RH) in the atmosphere is low. However, if the product of the saturation vapor pressure of ammonia and nitric acid is lower above a solid ammonium nitrate salt surface than above the aqueous solution, the saturation vapor pressures for ammonia and nitric acid above the solid salt surface is used instead of the saturation vapor pressures above the liquid surface. This method of calculating the saturation vapor pressures for ammonia and nitric acid was adopted from Zhang and Wexler, 2008.

From the modeled particle mole fraction of ammonium, chloride, sodium, nitrate and sulfate an approximated particle salt composition is estimated for each particle size bin according an explicit scheme.

Molalities of single salts (m_i^0), for NH_4NO_3 , HNO_3 , $(\text{NH}_4)_2\text{SO}_4$, NH_4HSO_4 , H_2SO_4 , NaHSO_4 , $(\text{Na})_2\text{SO}_4$, NaCl and HCl are calculated according to parameterizations from Table B.10 in Jacobson, 2005. These parameterizations are high order polynomials as functions of the water activity (a_w). The water mass content (W) in the inorganic particle fraction in each particle size bin is derived using the Zdanovskii-Stokes-Robinson (ZSR) model (Stokes and Robinson, 1966).

The inorganic and organic growth factor (Gf_i and Gf_o) are given by equation 3 and 4 respectively. $V_{p,\text{salt}}$ is the dry particle volume of water soluble inorganic salts and ρ_{water} is the density of water. Using equation 4, the organic growth factor is 1.2 when the water activity is equal to 0.9.

$$3) \quad Gf_i = \left(\frac{V_{p,\text{salt}} + W/\rho_{\text{water}}}{W/\rho_{\text{water}}} \right)^{1/3}$$

$$4) \quad Gf_o = \left(1 + 0.081 \frac{a_w}{(1 - a_w)} \right)^{1/3}$$

Once the water content in the inorganic particle phase has been calculated it is possible to determine the molality of different ions in the water phase. The mean binary solute activity coefficients of each salt in the particle water phase are calculated with the model described by Jacobson, 2005 ch. 17. From these binary activity coefficients the mean mixed solute activity coefficients are derived using Bromley's method (Bromley, 1973). Next step in is to determine the hydrogen ion concentration in the particle water phase. This is performed by solving an ion balance equation. Finally the saturation vapor pressures (concentrations) of ammonia, nitric acid and hydrochloride acid and the equilibrium concentrations of sulfuric acid, and hydrogen peroxide can be determined using the derived hydrogen ion concentration and the mean mixed solute activity coefficients. The saturation vapor concentrations are used when solving the condensation/evaporation equation (section 2.2.1). The condensation growth rate due to sulfuric acid production, from the reaction between

sulfur dioxide and hydrogen peroxide in the particle water phase, is calculated using equation 5 (Seinfeld and Pandis, ch. 7, 2006).

$$5) \frac{d[S(VI)]}{dt} = \frac{W \cdot k_{S(IV)} \cdot [H_2O_2] \gamma_{H_2O_2} [HSO_3^-] \gamma_{HSO_3^-} [H^+] \gamma_H}{(1 + K_{S(IV)} [H^+] \gamma_H)} \quad (\text{moles / s})$$

Gas phase model

The chemical kinetic code is solved for all grid cells using MatLabs ode15s solver for stiff ordinary differential equations. This solver uses an adaptive time step length according to the specified error tolerance. For most species considered the loss rate only takes into account chemical losses due to reactions with other species and dry deposition losses. For the condensable organic compounds (X_i), sulfuric acid, nitric acid, ammonia, sulfur dioxide, hydrogen peroxide and hydrochloride acid the differential equations also include terms for condensation and evaporation onto or from the particle surfaces. For sulfuric acid the loss rate also consider losses due to uptake of molecules in homogeneous nucleation clusters. The condensation and evaporation of gases onto or from the particles couples the chemical model to the aerosol dynamics model. Most of the chemical reactions are taken from the kinetic code used in the chemical model by Pirjola and Kulmala, 1998 (originally from EMEP). Some new reactions, mainly concerning the oxidation of benzene, toluene and xylene are also included in the kinetic code. The chemical reaction rates were updated for those of the reactions where new reaction rates were found in the literature (Sander et al., 2006, Seinfeld and Pandis, 2006 and Atkinson et al., 2004). Pirjola and Kulmala, 1998 included DMS emissions from the ocean in their model. Reactions involving DMS were however not considered in the chemical kinetic code used in this work. All natural emission of DMS from the oceans is instead assumed to be sulfur dioxide according to Simpson et al., 2003.

The photochemical reactions depend on the spectral actinic flux (photons $\text{cm}^{-2} \text{s}^{-1} \text{nm}^{-1}$). The actinic flux is the flux of photons from all directions into a volume of air (Seinfeld and Pandis ch. 4, 2006). The actinic flux is calculated using the radiative transfer model described in section 2.5. The photolysis rates are directly proportional to the actinic flux incident on a volume of air (Cotte et al., 1997). The wavelength (λ) dependent absorption cross sections (σ) and quantum yields (Q) for the different

gases undergoing photochemical reactions were found in Sander et al., 2006. Equation 6 below gives the photochemical reaction rates for species A.

$$6) \quad j_A = \sum_i \sigma_A(\lambda_i, T) Q(\lambda_i, T) F(\lambda_i) \Delta\lambda_i$$

Dry deposition and wet deposition of gases

The dry deposition velocity of gases can be described by a similar resistance model as the one described in appendix E for particles. As for the particles the dry deposition velocity of gases depends on an aerodynamic resistance (r_a) and a quasi-laminar resistance (r_b) in series. For gases the surface resistance (r_c), is also needed. The surface resistance depends on the surface structure as well as the reactivity of the gas (Seinfeld and Pandis ch. 19, 2006).

The below cloud scavenging of SO_2 , HNO_3 , NH_3 , H_2O_2 and $HCHO$ are described by the parameterization used in Simpson et al., 2003. For all other gases the below cloud scavenging is assumed to be an insignificant loss mechanism.

Species specific SOA yields and source specific 2D-VBSs

The organic aerosol formation in ADCHEM can either be modeled with the traditional two product model approach (Odum et al., 1996), or the recently proposed VBS approach (Donahue et al., 2006 and Robinson et al., 2007). The VBS scheme lumps all organic species in to different bins according to their volatility (given by their saturation concentration (C^*), at 298 K) (Robinson et al., 2007).

Lately, Jimenez et al., 2009 developed a 2D-VBS method which apart from classifying the organic compounds according to their volatility also includes the second dimension, oxygen to carbon ratio (O/C-ratio). This 2D-VBS method is implemented in ADCHEM, with a few modifications.

Radiative transfer model

The radiative transfer model is mainly used to calculate photolysis rate coefficients for the gas phase chemistry model and to estimate the presence of clouds. The radiative transfer model uses the quadrature two-stream approximation scheme, where the radiative fluxes are approximated with an upward and downward flux component. The phase function and the angular integral of the intensity field are

approximated using the asymmetry parameter (g) and single scattering albedo (w_0). The model can be used to calculate the radiative transfer in a vertically inhomogeneous atmosphere with clouds and aerosols (Toon et al., 1989). The asymmetry parameter and single scattering albedo for aerosol particles and cloud drops is calculated using a Mie-theory model.

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