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Polar Stratospheric Clouds

Microphysical and optical models

Addendum

By

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Polar Stratospheric Clouds
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The PSC model is continuously being updated with new experimental data and microphysical processes. This addendum describes those changes made to the model since the publication of Scientific Report 00-06 (Larsen, 2000).

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Updated homogeneous freezing rates have been applied in the latest model versions.

At 3-4 K below T_{ice}, freezing of ice out of STS become possible. The model applies homogeneous volume-proportional ice freezing rates, derived from experimental data, as given by *Koop et al.* [2000]. The much slower homogeneous surface-proportional freezing of NAD out of solution at temperatures between T_{NAT} and T_{ice} [*Tabazadeh et al.*, 2002] is also included in the model, assuming an instant conversion to stable NAT after freezing. The freezing rate for the two processes are illustrated in Figure 3.4.1 below, calculated for different particle sizes. The left-hand side of Figure 3.4.1 shows the ice freezing rates. Assuming a critical freezing rate of 1 s^{-1}, the ice freezing occurs in a very narrow temperature interval of 0.1-0.2 K at temperatures roughly 3 K below T_{ice} at an H_2O/ice saturation ratio around 1.7. In comparison with ice freezing, the NAD homogeneous freezing rates peak a few K above T_{ice} at HNO_3/NAT saturation ratios around 30 with much lower freezing rates and a more pronounced size dependence. The NAD freezing rates and saturation ratios shown in Figure 3.4.1 have been calculated for equilibrium STS compositions at decreasing temperatures, taking account of the uptake of HNO_3 and H_2O in the STS.

It should be noticed that to simulate a partial ice freezing of only the larger particles in a size distribution, temperature histories would be needed with an accuracy of a tenth of a degree (which is unrealistic in any meteorological model). It should also be noted that once a fraction of the large-size end of the distribution is frozen into ice particles, fast condensation of water vapor to these particles will decrease the partial water pressure towards equilibrium with ice and thereby require even lower temperatures to freeze the remaining smaller particles. This will cause a substantial broadening of the temperature interval in which freezing of the full range of particles may take place. Therefore accurate cooling rates are also required. The NAD freezing will be much more size selective than ice freezing.

Comparison between observations and model simulations of the formation of solid particles in synoptic Arctic PSCs led Larsen et al. (2004) to conclude that the homogeneous surface-proportional freezing rates of NAD out of solution at temperatures between T_{NAT} and T_{ice} [*Tabazadeh et al.*, 2002] were too high, recommending that the freezing rates be reduced by a factor 20 (i.e. multiplied by an adjustment factor of 0.05). The PSCBOX model currently takes this adjustment factor as a free parameter in the model code.
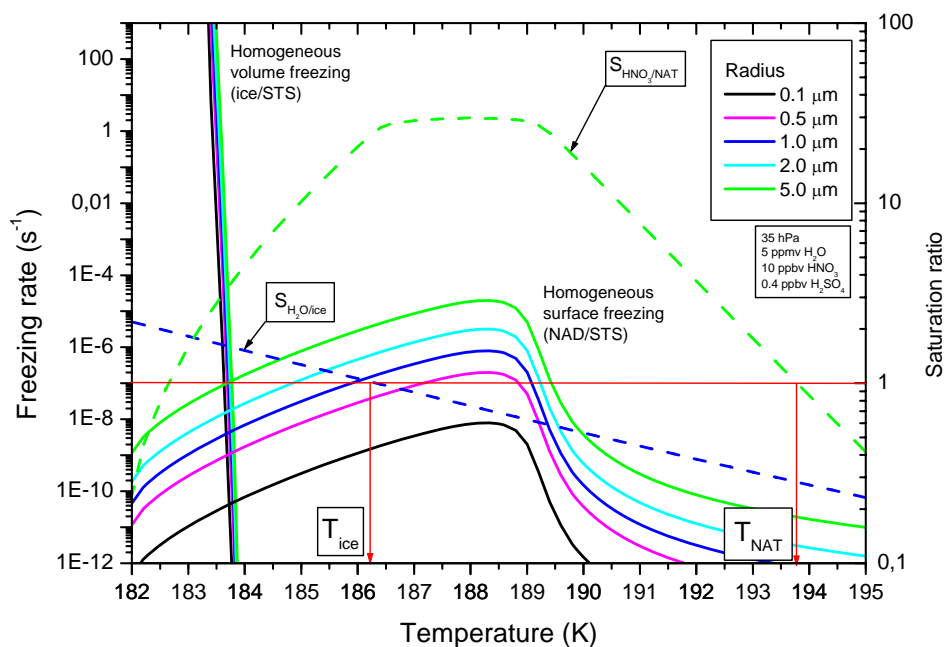
Figure 3.4.1 Homogeneous volume-proportional freezing rates of ice (nearly vertical solid color-coded curves in the left-hand side of the diagram) [*Koop et al.*, 2000] and surface proportional NAD (solid color-coded curves) [*Tabazadeh et al.,* 2002] in STS solution for different particle sizes as indicated in the legend. The NAT freezing rates are calculated for STS equilibrium compositions as function of temperature, assuming 10 ppbv HNO_3, 5 ppmv H_2O, and 0.4 ppbv H_2SO_4 at 35 hPa pressure altitude (no adjustment factors applied, cf. text). The partial pressure of HNO_3 is reduced at lower temperatures, corresponding to the uptake in STS, giving rise to a maximum in the saturation ratio over NAT. T_{NAT} and T_{ice} are indicated corresponding to saturation ratios (dashed curves) over NAT ($S_{HNO3/NAT}$) and ice ($S_{H2O/ice}$) equal to 1.

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Figure 3.8
Notice that the correct unit on the particle radius axis in μm.

As a supplement to Figure 3.8, Figure 3.8.1 below shows the time to grow/evaporate PSC particles to double/half sizes.

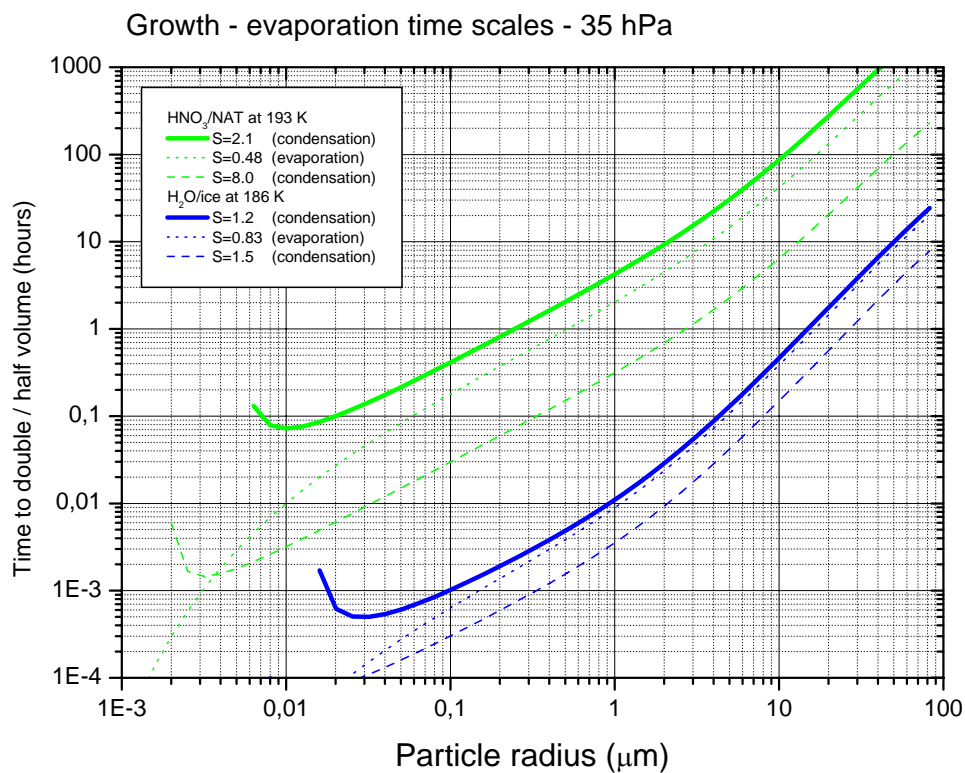Growth - evaporation time scales - 35 hPa

Figure 3.8.1 Time to grow (solid curves) or evaporate (dashed curves) NAT (green) and ice (blue) particles to double, half sizes respectively, calculated at the same atmospheric conditions as in Figure 3.8.

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Diffusion coefficient of HNO₃ in air (Dₙ).

$$D_n = 0.559\, D_w$$

where D_w is the diffusion coefficient of water vapor in air, calculated from *Pruppacher & Klett* [1997, formula 13-3] as function of air temperature and pressure.

The coefficient of proportionality, 0.559 is calculated as follows (suffix *n* refers to HNO₃, *w* to H₂O and *a* to air molecules):

$D_n = \dfrac{v_{th,n} l_n}{3}$ where $v_{th,n}$ is the thermal speed of HNO₃ and l_n is the mean free path of HNO₃ [e.g. *Turco et al.*, 1989, formula 8].

$v_{th,n} = \sqrt{\dfrac{8RT}{\pi M_n}}$ where R is the universal gas constant, T is the air temperature, and M_n

is the molar mass of HNO₃ [*Pruppacher & Klett,* 1997, formula 5-49]. Similar formula for air molecules, i.e.

$$v_{th,n} = \left(\frac{M_a}{M_n}\right)^{1/2} v_{th,a}$$

$l_n = \dfrac{4(M_a + M_n)^{1/2}}{\pi n (d_a + d_n)^2 M_a^{1/2}}$ where n is the number density of air molecules, and d is the

molecular diameter [*Hamill et al.*, 1977, formula 6], i.e.

$$\frac{l_n}{l_a} = \frac{2\sqrt{2}(M_a + M_n)^{1/2} d_a^{2}}{M_a^{1/2}(d_a + d_n)^2} = \Theta_n, \text{ and likewise } \frac{l_w}{l_a} = \frac{2\sqrt{2}(M_a + M_w)^{1/2} d_a^{2}}{M_a^{1/2}(d_a + d_w)^2} = \Theta_w$$

Using the above expressions

$\dfrac{D_n}{D_w} = \dfrac{v_{th,n} l_n}{v_{th,w} l_w} = \left(\dfrac{M_w}{M_n}\right)^{1/2} \dfrac{\Theta_n}{\Theta_w} = 0.559$, assuming d_a=3.65 Å, d_n=5.2 Å, and d_w=4.0 Å.

The diffusion coefficient is corrected for discontinuity effects at distances near the surfaces of the small particles smaller than the mean free path [*Pruppacher & Klett,* 1997, cp. 5].

Page 18, Figure 3.2

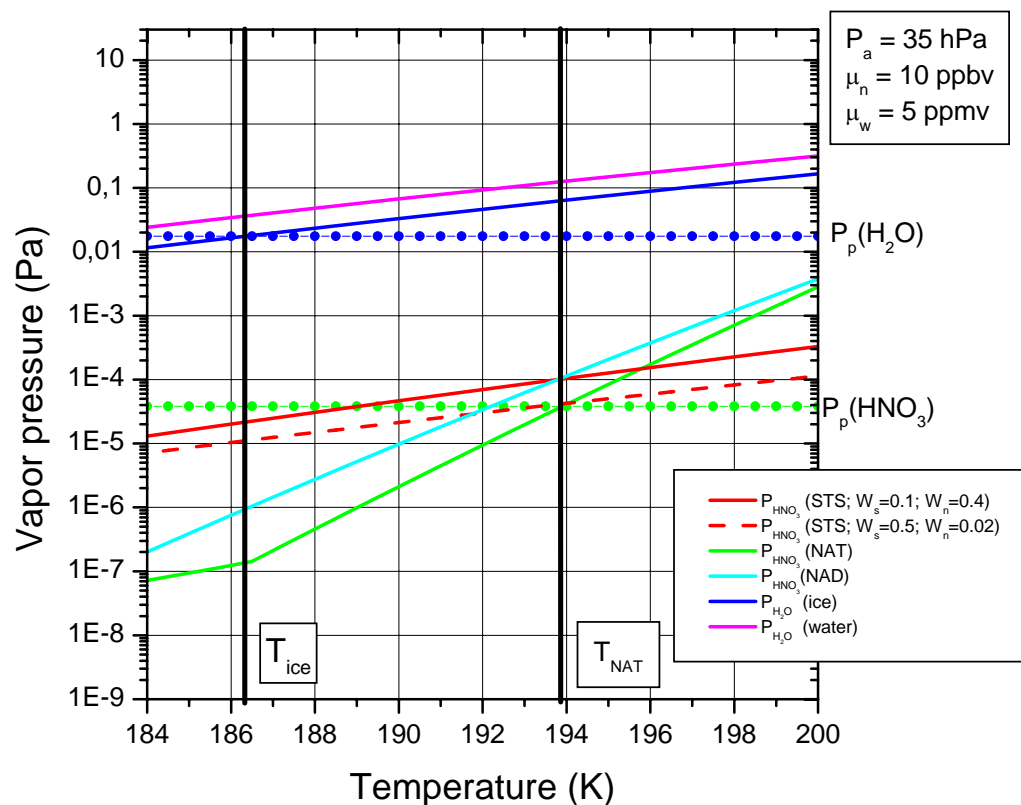The plot is supplemented with the vapor pressure of HNO_3 over nitric acid dihydrate (NAD).

Figure 3.2. Examples of HNO_3 vapor pressures over STS (red), NAT (green), and NAD (cyan) and H_2O vapor pressures over ice (blue) and water (magenta). Partial pressures of HNO_3 and H_2O at 35 hPa at typical mixing ratios of 10 ppbv HNO_3 and 5 ppmv H_2O are indicated by green and blue dot-lines.

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Further to T-matrix calculations:

The aerosol backscatter ratio R is defined as

$$R = \frac{B_a}{B_m} = \frac{\beta_a^{\text{II}} + \beta_a^{\perp}}{\beta_m^{\text{II}} + \beta_m^{\perp}} = \frac{\int\limits_0^\infty n(r)\frac{d\sigma_b}{d\Omega}dr}{n_g \frac{d\sigma}{d\Omega}_{Ray}} = \frac{\int\limits_0^\infty n(r)\frac{d\sigma_b}{d\Omega}dr}{\frac{P_a}{kT}\frac{d\sigma}{d\Omega}_{Ray}}$$

where B_a is the total particle volume backscattering coefficient, and B_m is the total molecular (Rayleigh) volume backscattering coefficient, and $\beta^{\text{II}} and \beta^{\perp}$ are the corresponding parallel and perpendicular components of the volume backscatter coefficients. $\frac{d\sigma_b}{d\Omega} and \frac{d\sigma}{d\Omega}_{Ray}$ are the particulate and molecular backscattering cross sections, n the number density of particles, n_g the number density of gas molecules, P, T, and k the air pressure, temperature and Boltzmann's constant

The backscattering differential cross section is calculated from the scattering matrix element F_{11} at 180° as

$$\frac{d\sigma_b}{d\Omega} = \frac{F_{11}Q}{4\pi}$$

where Q is the scattering cross section averaged over the uniform orientation distribution of a (non)spherical particle.

The aerosol depolarisation ratio δ_a and volume depolarisation ratio δ are defined as

$$\delta_a = \frac{\beta_a^{\perp}}{\beta_a^{\text{II}}} \qquad \text{and} \qquad \delta = \frac{\beta_a^{\perp} + \beta_m^{\perp}}{\beta_a^{\text{II}} + \beta_m^{\text{II}}}$$

The aerosol depolarisation ratio δ_a is calculated from the scattering matrix elements $F_{i,j}$ at 180° as

$$\delta_a = \frac{\int\limits_0^\infty n(r)\frac{F_{11} - F_{22}}{F_{11} + F_{22} + 2F_{12}}\frac{d\sigma_b}{d\Omega}dr}{\int\limits_0^\infty n(r)\frac{d\sigma_b}{d\Omega}dr}$$

The volume depolarisation ratio δ is related to the aerosol depolarisation ratio δ_a as

$$\delta = \frac{\delta_a\big[(R+1)\delta_m + R\big] + \delta_m}{\big[\delta_m R + R + 1 + \delta_a\big]}$$

where δ_m is the molecular depolarisation, $\delta_m = \frac{\beta_m^{\perp}}{\beta_m^{\text{II}}}$, assumed to 1.4%.

The model applies the T-matrix code of Mishchenko and Travis (1998), using a pre-calculated database of expansions of the elements of the scattering matrix in generalised spherical functions ($\alpha_1..\alpha_4$, β_1, β_2 in Mishchenko's notation). The data base spans the particle aspect ratio range 0.50 to 2.00 in steps of 0.05 and real part refractive indices in the range 1.29 to 1.61 in steps of 0.02. The model calculates the differential back scattering cross section, extinction cross section, and depolarisation for a given wavelength, angel, refractive index, and aspect ratio. The recommendations of Mishchenko for input parameter settings have been followed. The data base is calculated for volume-equivalent sizes (RAT=1D0 in Mishchenko's notation) and imaginary refractive index 1E-8. See further description in the original Mishchenko code (Mishchenko and Travis, 1998).

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The internal structure of the Eulerian model version has been changed. In the new version the number density of the four different particle type together with the condensed masses of H_2SO_4, HNO_3, and H_2O per particle of each type constitute the integration variables.

```
***************************************************************************
      SUBROUTINE PSCBOX(
***************************************************************************
             DTIME,
             THKNES,
             NBINS,TYPES,NWORK,
             TAIR,PAIR,PPWV,PPNA,
             ND,
             MCS,MCN,MCW,
             SDND,SDMCS,SDMCN,SDMCW,
             PRESENCE,SEDMNT,
             PTSIZE,WORK)

      Declaration of input/output variables:
      INTEGER NBINS,TYPES,NWORK
      REAL(KIND=4)
             DTIME,
             THKNES,
             TAIR,PAIR,PPWV,PPNA,
             ND(NBINS,TYPES),
             MCS(NBINS,TYPES),MCN(NBINS,TYPES),MCW(NBINS,TYPES),
             SDND(NBINS,TYPES),
             SDMCS(NBINS,TYPES),SDMCN(NBINS,TYPES),SDMCW(NBINS,TYPES),
             PTSIZE(NBINS,8),WORK(NBINS,NWORK)
      LOGICAL PRESENCE(TYPES),SEDMNT(TYPES)

      Input:
          DTIME:    (s)              Integration time step
          THKNES:   (m)              Vertical thickness of layer
          NBINS:                     Number of particle radii bins
          TYPES:                     Number of particle types comprehended by the model
          NWORK:                     2nd dimension of work array
          TAIR:     (K)              Ambient air temperature
          PAIR:     (Pa)             Ambient air pressure

      Input/output:
          PPWV:     (Pa)             Ambient partial pressure of water vapor
          PPNA:     (Pa)             Ambient partial pressure of nitric acid
          ND:       (par/kg air)     Number density of particles per kg of air
          MCS:      (kg/particle)    Mass of condensed sulfuric acid per particle
          MCN:      (kg/particle)    Mass of condensed nitric acid per particle
          MCW:      (kg/particle)    Mass of condensed water per particle
          SDND:      (par/m**3)      Sedimentation flow of particles in time interval
DTIME
          SDMCS:     (kg/particle)   Mass  of  condensed  sulfuric  acid  in  sedimenting
particles
          SDMCN:      (kg/particle)  Mass  of  condensed  nitric  acid  in  sedimenting
particles
          SDMCW:    (kg/particle)   Mass of condensed water in sedimenting particles
          PRESENCE:(logical)       Indicator of presence of different types of particles
          SEDMNT:   (logical)        Indicator of sedimentation of different types of
particles

      Work array:
          PTSIZE:   (m,m**2,m**3)  Particle radii, surface, volume, etc.
                                    (not to be changed)
          WORK:                    Work array (allowed to be changed)


***************************************************************************

      This subroutine calculates the particle size distributions and chemical
      compositions in an ensemble of liquid supercooled ternary solution (STS)
      stratospheric particles (type 1b PSC at low temperatures), frozen stratospheric
      sulfate aerosols, and polar stratospheric clouds (PSC) of type 1a and 2 in a
      SINGLE point in space (box) and time. Individual PSC-box models can be placed in
      grid-points of a larger model, or can be used for air parcel trajectory
```

calculations, or can be stacked to form a column model. The placement of the
box-model within a larger model (geographical/vertical) is referred to as the
location of the box-model.

At each location the PSC-box model takes as input the ambient air state
variables: temperature (TAIR), pressure (PAIR), partial pressure of water
vapor (PPWV), and partial pressure of nitric acid vapor (PPNA).

The particle size distribution of each particle type is divided into a number
of bins (NBINS) on a geometrically increasing volume scale. It is required,
that NBINS > 2. NBINS must be the same for all locations of the PSC-box model.

The number density (ND - particles per unit air mass), i.e. the
the particle size distributions, are stored in the following arrays:
ND(i,1), i=1,...NBINS   Liquid sulfate aerosols which, at low temperatures,
                             take up nitric acid and water, turning into
                             supercooled ternary solution Type 1b PSC
ND(i,2), i=1,...NBINS   Frozen sulfuric acid tetrahydrate particles (SAT)
ND(i,3), i=1,...NBINS   Nitric acid trihydrate (NAT) type 1a PSC
ND(i,4), i=1,...NBINS   Water ice type 2 PSC
ND-array element no. i holds the particles per unit air mass in the particle
radius interval spanned by bin no. i.

The subroutine calculates the differential size distribution ND(i,1)
of liquid ternary sulfuric-nitric acid solution aerosol particles,
assuming the ternary aerosols to be in equilibrium with the water and nitric
acid vapor at an arbitrary ambient atmospheric state, specified as input
(TAIR, PPWV, and PPNA).

For each type (j=1,2,3,4) of particle, the condensed masses are stored as
follows:
        condensed sulfuric acid mass per particle, MCS(i,j), i=1,...NBINS, j=1,2,3,4
        condensed nitric acid mass per particle,   MCN(i,j), i=1,...NBINS, j=1,2,3,4
        condensed water per particle,   MCW(i,j), i=1,...NBINS, j=1,2,3,4

Currently, the phase transition between liquid/solid PSCs is unknown.
The model applies homogeneous volume dependent freezing of ice in HNO3/H2O
supercooled solutions according to Koop et al. (2000). Homogeneous freezing
of NAT (NAD) in supercooled solution according to Tabazadeh et al. (2002)
can also be simulated if the common block variable TABA_COR > 0.0, set in calling
program.
Upon freezing of a STS particle all the nitric acid together with water is
deposited as nitric acid trihydrate (NAT) and all sulfuric acid together with
water
as sulfuric acid tetrahydrate (SAT). Any unbound water in hydrates are assumed to
form
ice. Upon heating an ice PSC the ice evaporates, turning into a type 1a NAT PSC.
Upon further heating the NAT will evaporate, whereby the frozen sulfate aerosol
core is released (SAT particle).

Any frozen SAT particles are assumed to melt when the air temperature
is above the SAT melting temperature. SAT melting (deliquescence) upon cooling
(Koop and Carslaw, 1996) can also be simulated if the logical parameter SAT_DELI
is be set to .TRUE. When melting a SAT paticle the number density is transferred
from the frozen to the liquid particle category and the equilibrium composition
and ternary density is recalculated.

The SAT particle may also act as nucleation center for type 1a NAT PSC formation
upon subsequent cooling, simulating preactivated SAT (Zhang et al., 1996).

HNO3 condensation on ice is included if logical parameter HNO3_ON_ICE
is set to .TRUE.

The logical input/output variables PRESENCE(j), (j=1,2,3,4) can be used
in the calling program to test whether particles of a given type are present.

The number density of particles (ND), and the masses of condensed substances
(MCS, MCN, MCW)) constitute the integration variables of the model.
When the subroutine is called, these variables must hold the
values, calculated by the routine in the previous time step (or the initial
values, cf. below). Upon exit these variables will hold the new values at a
time DTIME later. The new values are calculated by a first order explicit
Euler expression within the routine. The ambient air state variables (TAIR,
PAIR) are assumed to be constant during the time interval DTIME. In order to
perform calculations at different geographical locations and altitudes (grid
points), these variables must be defined at each point.

Nitric acid and water are taken up or released from/to the air during
condensation/evaporation. On exit new values of gas phase partial pressures
of nitric acid (PPNA) and water (PPWV) are recalculated.

The balance calculations of particle number density and masses of condensed
substance use as input the sedimentation flow of particles (SDNA).
The variables SDMCS, SDMCN, AND SDMCW hold the masses of condensed H2SO4, HNO3,
and H2O of the particles falling in from the layer above. The routine will return
as output, in the same variables, the flow to be used in the box-calculations
in the layer below.
The logical array SEDMNT(j), (j=1,2,3,4) indicate, if there is a
sedimentation flow of particles of type j from the layer above on entry,
and indicate, in the same variable, if there is a sedimentation
flow to the layer below on exit.

Thus, for the calculations in a column, the subroutine should be called
in a sequence from the top-layer to the bottom-layer. At the top layer,
the sedimentation input variables should be set equal to zero; the logical
sedimentation indicator (SEDMNT) should be set to .FALSE., and the calling
program should not change the values of these variables between calls in
the column sequence. The sedimentation variables will hold the fall out of
particles in the bottom layer after the last call of the subroutine in the
column sequence. The same array for storing the sedimentation flows and
logical indicators can be used at different locations, if the calculations
are performed column-wise.

A positive vertical extent (THKNES) of the PSC-box (vertical distance
between layers) must be given as input to the subroutine. This extent
need not be the same, neither at all locations, nor at all times.

The subroutine uses adjustable array dimensions of all arrays.
The parameter NBINS and the arrays in the argument list of the
subroutine must be set and dimensioned (cf. above) in the calling
program.

The minimum and maximum particle radius are given as parameters to
SUBROUTINE SETBIN, which must be called once before any call to PSCBOX
(cf. below). Subroutine SETBIN will store the values of the particle radius,
surface area, and volume of each bin in the array PTSIZE. This array PTSIZE
must be used at all locations, and the array must not be changed between the
calls of subroutine PSCBOX.

Subroutine PSCBOX_START can be used to initialise PSCBOX, including a call
to subroutine SETBIN. PSCBOX_START can be used to calculate initial values
of particle number density and chemical composition of a liquid stratospheric
sulfuric acid particle ensemble with an initial log-normal size distribution
(parameters given to the suboutine). Under warmer stratospheric conditions
with no PSCs this distribution could normally be used as initial values of
the PSC-box model. In addition PSCBOX_START will initialise sedimentation
variables.

The total particle surface area density of a given particle type can
be calculated by SUBROUTINE SURFCE. The condensed phase mixing ratios
of sulfuric acid, nitric acid, and water can be calculated by SUBROUTINE MIXCON.
Parameters of log-normal distribution fits to individual particle
distributions can be calculated by SUBROUTINE LGNPAR (cf. below).

The array WORK can be be used by the calling program unit between calls
of the subroutine, and the same array WORK can be used at all locations.

The PSC-box model uses a number of named common blocks, holding values
which can be also be utilised in the calling program unit:

COMMON /TAU/TAUMAX
holding the following REAL value:
TAUMAX: Inverse of minimum time constant encountered in the
             microphysical processes (1/s);
             Subroutine PSCBOX will integrate the state variables
             forward in time and return after DTIME seconds. During
             DTIME the air temperature and pressure are assumed to
             be constant. PSCBOX will try to integrate the state
             variables in one integration step of DTIME seconds;
             however, if the microphysical minimum time constants
             encountered are smaller than DTIME, the actual
             integration step will be reduced to 1/TAUMAX in order
             to make a stable integration; in this case PSCBOX will

```
                    use more than one step to integrate DTIME seconds forward.
                    A minimum time step DTMIN, defined as a parameter below,
                    is used.

        COMMON /SED/SEDI
        holding the following LOGICAL value:
        SEDI:       A logical flag to indecate, if particle sedimentation
                    calculations are to be performed by PSCBOX. This flag
                    will be set to .TRUE. initially by subroutine SETBIN;
                    however, this value can be changed to .FALSE. by the
                    calling program unit (after the call to SETBIN), if
                    sedimentation calculations are not wanted.


        COMMON /CONTRL/TEST
        holding the following INTEGER value:
        TEST:       The value of TEST indicates, if values of local
                    variables in various sub-programmes, used in the PSC-box
                    model, should be printed to a file. This facility is
                    mainly used to test the program. If TEST is equal to
                    zero, no printing will take place. TEST is initially
                    set to zero by subroutine SETBIN. If this detailed
                    (voluminous) output is needed, TEST must be set to
                    a positive value ( >= 50 ) in the calling program
                    unit, and a formatted file with unit number TEST must
                    be opened from the calling program unit. Values of
                    local variables will then be printed on file unit TEST
                    as long as TEST is non-zero. The file must also be closed
                    from the calling program unit. TEST must be >= 60 for
                    very detailed output, and 50 <= TEST < 60 for moderate
                    detailed output.


        COMMON /BINS/VR,ZERO,D1,LOGVR
        holding the following REAL values:
        VR:         VRATIO
        ZERO:       Smallest significant number density of particles
                    in a single bin (1/kg air)
        D1:         Parameter, related to VRATIO, used in log-normal dist.
        LOGVR:      ALOG(VR)

        Values in common /BINS/ are set by subroutine SETBIN, and must
        not be changed by the calling program.


        Multiplication factor for Tabazadeh freezing rates (if =0, no freezing):
        REAL TABA_CORR
        COMMON /CORRECT/TABA_CORR

        All calculations are performed in SI units.

        The entire PSC-box model is written in ANSI fortran 90.
```

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Eulerian PSCMODEL version:

```
PROGRAM PSC_MODEL_E

Main program used to run the PSCBOX model in the Eulerian-radius-space
version, i.e. using fixed size bins.
The program file PSCMODEL.FOR must be linked to PSCBOX.FOR holding the
microphysical, thermodynamical, and optical subroutines of the PSC box
model.

A few lines of code in this program must be changed, depending on
the computer (operative system) to be used and where input/output files
are stored. The statements of the program, which have to be changed, are
all preceded by a comment line, starting with 'CMP'.  All instructions in
comment lines, starting with 'CMP', should be invoked, before compiling
and running the program. Comment lines starting with 'CMP' are only found
in this main program file.

Input/Output files:
-------------------

The program uses a simple self-explaining ASCII input file, stored in
the associated input file directory. The input file can have any name
with extension '.INP'. Output file names are generated from the applied
input file name, all with extension .DAT and stored in the associated
output file directory. The input/output directories must be specified
in the main program before compiling (cf. CMP comment lines).

Time units.
-----------
The model performs all calculations internally in SI units, i.e. time in
seconds. However, other units for input/output can be required.
The units (Days, Hours, Minutes, Seconds) of the time specifications in
the input file and the tempetature table file can be set in the input file.
These units are also used for output.

Computing control:
------------------

Two numbers can be set in the input file to control the integration
of the PSC-model:
    Maximum integration step size (s)

    Integration start and stop time (Days, Hours, Minutes, Seconds);
        when the integration has reached the stop time, the program
        is terminated (in batch mode), or control is transferred to
        the interactive routine (using the interactive mode on a PC).

Output control:
---------------

A number can be set in the input file to control the frequency
of output from the PSC-model (Days, Hours, Minutes, Seconds).

Model structure:
----------------

The number of layers in the vertical direction is specified in the
input file. A maximum of MAXLAY layers can be used. If a negative
number is specified, the absolute value is used as the number of
layers, but no sedimentation of particles between the layers is
calculated. The layers are numbered from the top to the bottom,
and the top layer is no. 1.

The potential temperature THETA (K) of the bottom layer and the layer
thickness dPOT (K) (delta-potential temperature) are specified in
the input file which, together with temperature/pressure specification
in the input fili, will have the following influence:

Temperature, pressure, and potential temperature:
-------------------------------------------------
```

The temperature can be calculated from a function of time as

    TAIR(time) = RAMP-function(time)

The RAMP-function is a continuous piece-wise linear function, specified
by 4 coordinate pairs: { (ramp time i, temperature i); i=1..4 };
i.e. the graph of this function is made up of 3 straight line segments
between the 4 coordinate points. For time values less than ramp time 1,
the function is constant equal to temperature 1, and for time values
greater than ramp time 4, the function is constant equal to
temperuture 4. The 4 coordinate pairs are specified in the input file.
The same temperatur applies for all layers when using the RAMP-function.
Isentropic conditions are assumed and pressures are calculated from
temperatures and the specified potenteal temperatures in each layer.
If the RAMP temperature function is to be used, the temperature calculation
method flag in the input file must be specified as 0 (zero).

Alternatively, the temperature history may be specified individually in
each layer from a time table of the temperature. The table must be stored
in the input directory as an ASCII file with 1+NLAYER columns
(time,temp1,temp2...temp-nlayer), (Kelvin), using the above speficied time
units. Cubic spline interpolation will be used between the table entries.
Time values in the table must be strictly increasing.
The name of the temperature table file is specified in
the input file, residing in the input directory.
Isentropic conditions are assumed and pressures are calculated from
temperatures and the specified potential temperatures in each layer.
If the temperature table is to be used, the temperature calculation method
flag in the input file must be specified as 1 (one).

Finally, both temperature and pressure can be specified for each layer in
an input table file, giving 1+(2*NLAYER) columns
(time, temp1, pres1, temp2, pres2,...,temp-nlayer,pres-nlayer)(Kelvin,Pa)
The temperature calculation method flag must set to 2 (two).
In this case the specified potential temperature is ignored, but dPOT is
used to specify the top layer thickness.

If a temperature (pressure) input file is used the ramp temperature
information in the input file is ignored. If a ramp temperature function
is used the specification of temperature table file name is ignored.

The temperature calculations as described above may be overlayed
by adding a sinosoidal temperature oscillation. Amplitude (K) and period
(user units) are specified in the input file. If no oscilations are to be
used, specify amplitude AND period equal to zero. To apply a constant
temperature correction in all layers, specify the amplitude with sign,
and set the period equal to zero.

Initial values:

Initial values of water vapor (ppmv) is specified in the input file,
one value for each layer.

Initial values of nitric acid (ppbv) is specified in the input file,
one value for each layer. If a positive value is given, this value is used;
if zero is specified, an observed vertical profile of nitric acid from
LIMS-data is used, (cf. JGR 89,5125,1984), either from a northern
(positive latitude) hemisphere or southern (negative latitude) hemisphere
data set.

Initial values of the total number density of sulfuric aerosols (1/ccm)
is specified in the input file (same for all layers). If a positive value
is given, this value is used for all levels; if zero is specified, number
density is derived in consistency with SAGE I and II aerosol surface
climatology (Hitchman et al., JGR 99,20689, 1994).

Median radius and geometric standard deviation of the initial
lognormal distribution is given in the input file (same for all
altitudes).

Optical calculations:

Calculation of particle backscatter ratios, extinction coefficients and
depolarisation (Mie scattering or T-matrix) can be specified by a logical

flag in the input file. Directory of T-matric coeffients must be
specified in the main program before compiling (cf. CMP comment lines).
Wavelengths are speficied as parameters in the main programme and
must be set before compilation. The number of size bins must be large
to obtain reliable backscatter values. IF(OPTICS)-ENDIF blocks in the main
program and subroutine DUMP should also be inspected and changed according
to the actual optical parameters required.

Output on files:

Three types of ASCII output files can be created by the program:

    1:    Historical output files
    2:    Distribution output file
    3:    Vertical profile output file

The output file names are generated from the input file name (e.g.
XXXXX.INP) and stored in the specified output file directory:

HISTORICAL OUTPUT FILE is always created for each layer, named
XXXXX-Hyy.DAT, where yy is the layer number. The historical output files
hold a number of records; one record for each output time, as
specified in the input file. Each record holds the following values:

A: Time (Days, Hours, Minutes, Seconds; as specified in the input file)
B: Temperature (K)
C: Total number density of frozen sulfate particles (1/ccm)
D: Total number density of PSC 1 particles (1/ccm)
E: Total number density of PSC 2 particles (1/ccm)
F: Saturation ratio of nitric acid over NAT
G: Saturation ratio of water vapor over ice
H: Mixing ratio of water vapor (ppmv)
I: Mixing ratio of nitric acid vapor (ppbv)
J: Total (gas phase and condensed phase) mix. ratio, water (ppmv)
K: Total (gas phase and condensed phase) mix. ratio, nitric acid (ppbv)
L: Ratio of total to initial mixing ratio of water (%)
M: Ratio of total to initial mixing ratio of nitric acid (%)
N: Total volume of frozen sulfate particles (micron**3/ccm)
O: Total volume of PSC 1a particles (micron**3/ccm)
P: Total volume of PSC 2 particles (micron**3/ccm)
Q: Total volume of all particles (micron**3/ccm)
R: Total number density of PSC 1b (STS) particles (1/ccm)
S: Total volume of PSC 1b (STS) particles (micron**3/ccm)
T: Sulfuric acid weight fraction liquid PSC 1b aerosols [0;1]
U: Mean radius liquid PSC 1b aerosols (micron)
V: Median radius frozen sulfate aerosols (micron)
X: Median radius PSC 1 (micron)
Y: Median radius PSC 2 (micron)
Z: Nitric acid weight fraction liquid PSC 1b aerosols [0;1]
AA: NAT condensation temperature (K)
BB: Ice frost point temperature (K)
CC: Air pressure (hPa)
DD: Total mixing ration of sulfuric acid (ppb)
EE: Optical parameter 1
FF: Optical parameter 2
GG: Optical parameter 3
HH: Moleratio
II-UU: Cumulated size distribution
(AEROSOL_BACKSCATTER_RATIO(J,L),J=1,N_WAVE),!   (47-53)
(EXTINCTION(J,L),J=1,N_WAVE),   !   (54-60)
(DEPOL(J,L),J=1,N_WAVE)   !   (61-67)

DISTRIBUTION OUTPUT FILES are created, if a non-zero distribution-
dump-frequency is specified in the input file, or if a command
is given interactively for this (PC). The names of the distribution
output files are XXXXX-Dyy.DAT, where yy is the layer number.
The distribution output files holds a number of blocks of records.
A block is written to each distribution output file at each distribution
output time. The first record in a block holds the time (Seconds, Days or
Hours as specified in the input file). Then follows a number of records;
one record for each size bin giving the following values:

```
A:  Particle radius (micron)
B:  Differential concentration of liquid sulfate particles (1/micron ccm)
C:  Differential concentration of frozen sulfate particles (1/micron ccm)
D:  Differential concentration of PSC 1 particles (1/micron ccm)
E:  Differential concentration of PSC 2 particles (1/micron ccm)
F:  Differential concentration of all particles (1/icronm ccm)
```

A VERTICAL PROFILE OUTPUT FILE is created, if a non-zero vertical-dump-
frequency is specified in the input file, or if a command is given
interactively for this (PC). The name of the vertical profile output
files is XXXXX-V.DAT. The vertical profile output file holds a number of
blocks of records. A block is written to the vertical output
file at each vertical output time. The first record in a block holds
the time (Days or Hours; as specified in the input file). Then follows
a number of records; one record for each layer, starting from the
BOTTOM layer. Each record holds the following values:

```
A:  Altitude (km)
B:  Pressure (hPa)
C:  Temperature  (K)
D:  Total number density of frozen sulfate particles (1/ccm)
E:  Total number density of PSC 1 particles (1/ccm)
F:  Total number density of PSC 2 particles (1/ccm)
G:  Saturation ratio of nitric acid over NAT
H:  Saturation ratio of water vapor over ice
I:  Mixing ratio of water vapor (ppmv)
J:  Mixing ratio of nitric acid vapor (ppbv)
K:  Total (gas phase and condensed phase) mix. ratio, water (ppmv)
L:  Total (gas phase and condensed phase) mix. ratio, nitric acid (ppbv)
M:  Ratio of total to initial mixing ratio of water (%)
N:  Ratio of total to initial mixing ratio of nitric acid (%)
O:  Total surface area density of frozen sulfate particles (æm**2/ccm)
P:  Total surface area density of PSC 1 particles (æm**2/ccm)
Q:  Total surface area density of PSC 2 particles (æm**2/ccm)
R:  Total surface area density of all particles (æm**2/ccm)
S:  Total number density of liquid sulfate particles (1/ccm)
T:  Total surface area density of liquid sulfate particles (æm**2/ccm)
U:  Sulfuric acid weight fraction in LIQUID sulfate aerosols [0;1]
V:  Median radius liquid sulfate aerosols (æm)
X:  Median radius frozen sulfate aerosols (æm)
Y:  Median radius PSC 1 (æm)
Z:  Median radius PSC 2 (æm)
AA: Nitric acid weight fraction in LIQUID sulfate aerosols [0;1]
AB: NAT condensation temperature (K)
AC: Ice frost point temperature (K)
AD: Air pressure (hPa)
AE: Total mixing ration of sulfuric acid (ppb)
AF: Optical parameter 1
AG: Optical parameter 2
AH: Optical parameter 3
AI: Moleratio
```

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Example on input file for the Eulerian PSCMODEL version:

```
Constant cooling - heating, PSC model E version, Homogeneous freezing
-4                      Number of layers (IF < 0: no sedimentation calculations)
0.001, 100.0           Min. max. radius (MICRONS)
360.0                  Max. integration time step (seconds)
h                      Time units (H/D/M) of the following time specifications and I/O
0.0                    Integration start time (H/D/M)
96.00                  Integration stop time (H/D/M))
0.1, 0.0, 0.0          Time interval between plot/print output (H/D/M), history, vertical,
distribution
475.0, 20.0            Bottom layer potential temperature and potential temperature increment (K)
0                      Temperature calculation (0: ramp; 1: Temp table; 2: Temp/Press table)
                       Temperature/pressure history file
0.0,225.0              Ramp time 1 (H/D/M), temperature 1 (K)
48.0,180.0             Ramp time 2 (H/D/M), temperature 2 (K)
60.0,180.0             Ramp time 3 (H/D/M), temperature 3 (K)
96.0,225.0             Ramp time 4 (H/D/M), temperature 4 (K)
0.0, 0.0               Temperature sine oscillation period (H/D/M); amplitude (K)
5.0, 5.0, 5.0, 5.0     Mixing ratio water vapor in each layer, initial value (ppmv)
0.0, 0.0, 0.0, 0.0     Mixing ratio nitric acid in each layer, initial value (ppbv);  (IF 0: LIMS-
data)
10.0, 0.0              Number density sulf.aerosols (1/ccm);    (IF 0: Antarctic profile)
0.0725, 0.15           Median radius (microns)
1.86, 1.15             Geometric std. dev.
80.00                  Latitude
.t.                    Optical calculations
2                      Particle surface area (2) or volume (3)
5.0E-2                 Correction factor for homogeneous NAT nucleation
```

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