ATHAM

A ctive

T racer

H igh Resolution

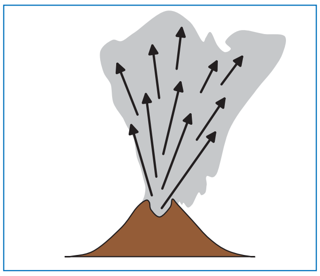
A tmospheric

Model

Hans-.F. Graf [1], Michael Herzog [2],
Josef M. Oberhuber [3], Christiane Textor[1]
Jörg Trentmann [4]

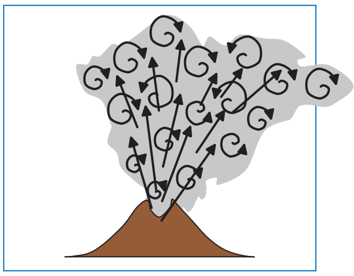
[1] Max-Planck-Institute for Meteorology, Hamburg, Germany
[2] University of Michigan, Ann Arbor, USA
[3] has been at German Climate Computing Center, Hamburg, Germany
[4] Max-Planck-Institute for Chemistry, Mainz, Germany

Processes in the plume of an explosive volcano



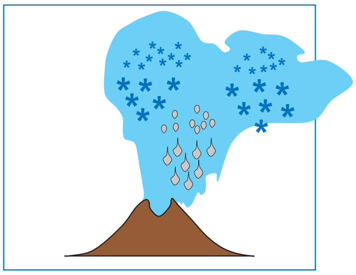
Dynamics

Advection and thermodynamics
of the gas-particle mixture



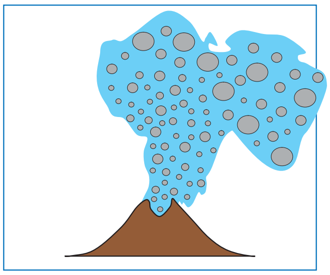
Turbulence

Entrainment of ambient air



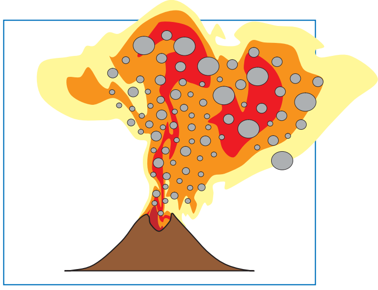
Cloud microphysics

Cloud- and precipitation processes
Release of latent heat



Aggregation of ash particles

Interaction of ash and
hydrometeors



Scavenging of volcanic gases

through hydrometeors and
aggregates

Overview

Purpose of the model
Simulation of high energy plumes with high gradients in momentum and temperature

Applications
explosive volcanic eruptions
vegetation burning
convective clouds

Scales

Spatial	mesoscale γ model (50-500 km)
Time	some hours

Model concept
complete solution of Navier Stokes equations
nonhydrostatic, includes sound waves
active tracer

Characteristics
simulation of large gradients in temperature and mass mixing ratio
high particle concentrations

Model geometry
2d axisymmetric
2d cartesian
3d cartesian

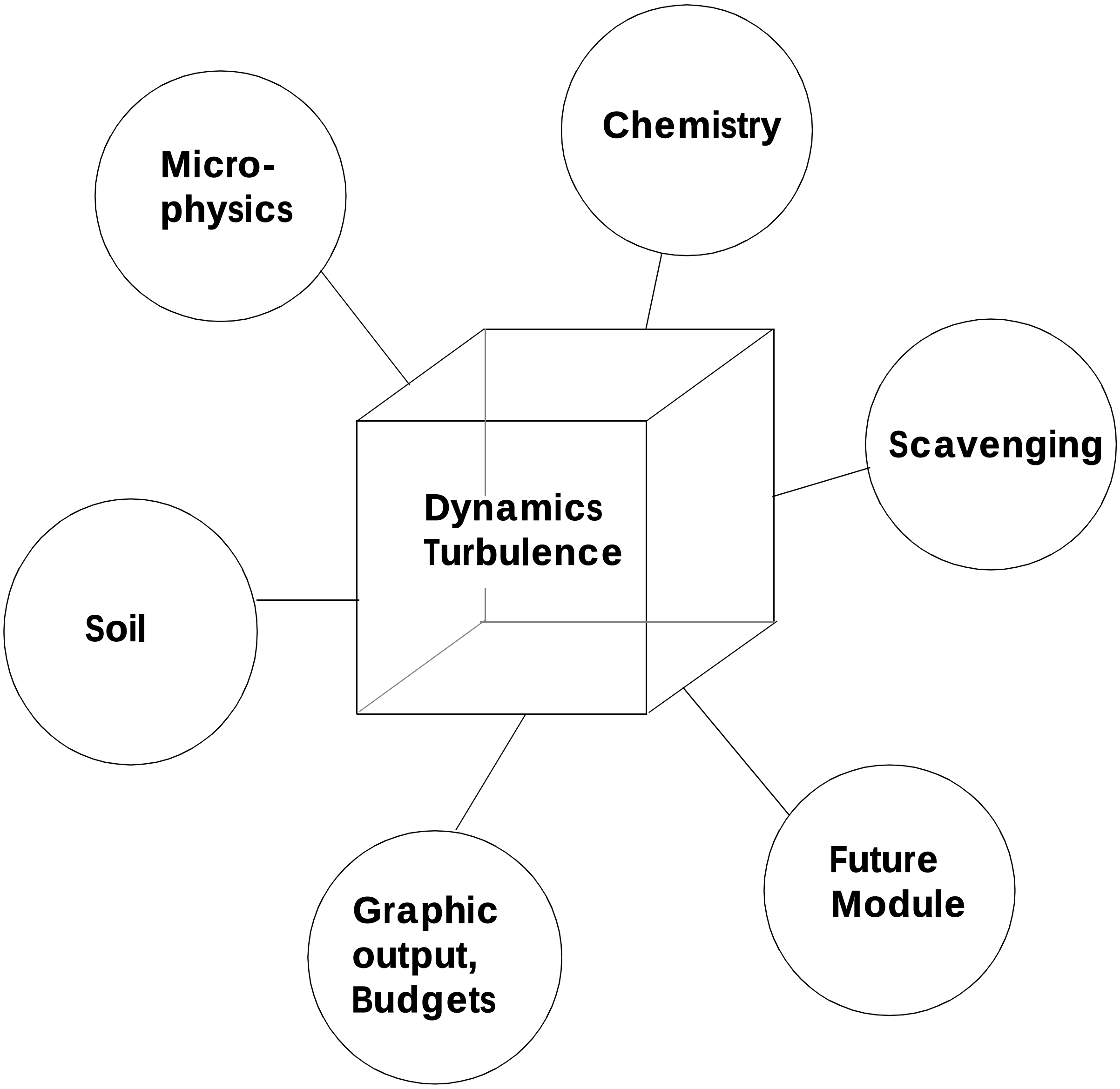
Model Grid	examples:
focusing grid	(Δx_{min}=5m, Δx_{max}=10km)
variable number of grid points	126 *126*126
variable size of model domain	200*200*50km^3)
time step is adapted according to the CFL criterion	(Δt=0.1-10 sec)

Program code of ATHAM
FORTRAN 90
one code for different model versions controlled with Flags for the Precompiler
Output files designed for GrADS
Analysis tool qview for GrADS (M. Herzog)

Modular structure
- any number of tracers can be added
- new processes are easy to include
- modules of different complexity can be exchanged

Modular structure of ATHAM

- Dynamics and turbulence are the core of the model.
- All other modules are coupled to this core by well defined interfaces.
- Modules can easily be exchanged.
- New modules can easily be added.



Modules

Dynamics	Advection and thermodynamics of the gas particle mixture Solution of the Navier-Stokes equation (Oberhuber et al. 1998, Herzog 1998)
Turbulence	Turbulent exchange coefficients for each dynamic quantity Entrainment of ambient air (Herzog 1998, Oberhuber et al. 1998)
Cloud microphysics	Complete cloud microphysics of liquid water and ice, feedback on the dynamics, Kessler-type and twomoment scheme (Graf et al. 1999, Herzog et al. 1998, Textor 2002)
Ash aggregation	Scavenging of Particles by hydrometeors Particle growth due to interaction with hydrometeors (Textor et al. 2002)
Gas scavenging	Dissolution in liquid droplets and incorporation into growing ice Kinetics of phase transfer (Textor et al. 2002) Redistribution of species contained in hydrometeors due to microphysics
Chemistry	Gas phase chemistry in the plume (Trentmann, not yet published) Calculation of photolysis frequencies (Landgraf and Crutzen, 1998).
Radiation	Absorption and scattering of terrestrial and solar radiation On-line delta-eddington scheme (Trentmann, not yet published)
Soil	Determination of the amount of settled ash particles and hydrometeors Consistent lower boundary condition for temperature and humidity

Dynamics

Concept of active Tracers

Injection of hot gas particle mixture with high vertical velocity
-> extreme acceleration and temperature anomalies

Particles occur in high concentrations, they influence the plume dynamics
-> buoyancy reduced
-> particles act as heat source for the mixture

Qualities of plume model
-> particles must be treated as active tracers independent of the gas phase
-> description of a multi-component-system

Particles in high mass fractions can no longer be treated as passive tracers with the mean flow as in usual atmospheric models, but their impact on the dynamics of the system has to be considered. In the non-hydrostatic model ATHAM, particles are treated as active tracers: they can occur in any concentration and they can influence the dynamics of the system by contributing to the mixture density, pressure and heat content. In general, the description of such a multi-component-system of gaseous, liquid and solid active tracers requires a set of dynamic and thermodynamic equations for each component including the interactions between them. However, the consideration of a higher number of grid points for investigating the mesoscale evolution of the plume, and the treatment of higher numbers of tracers is not possible with this concept.

In ATHAM two main assumptions are applied to circumvent the problem of dealing with a very large equation system (Oberhuber et al., 98):

- dynamic equilibrium
  instantaneous exchange of momentum between particles and gas
  large particles move with their terminal fall velocity

- thermal equilibrium
  tracers can act as a source of heat
  the system to exchange heat instantaneously
  particles and gas have the same in situ temperature

-> diagnose gas particle interaction
-> neglect dynamic interaction between particles

These assumptions require that all particles are small compared to the time scales needed to reach both equilibria.

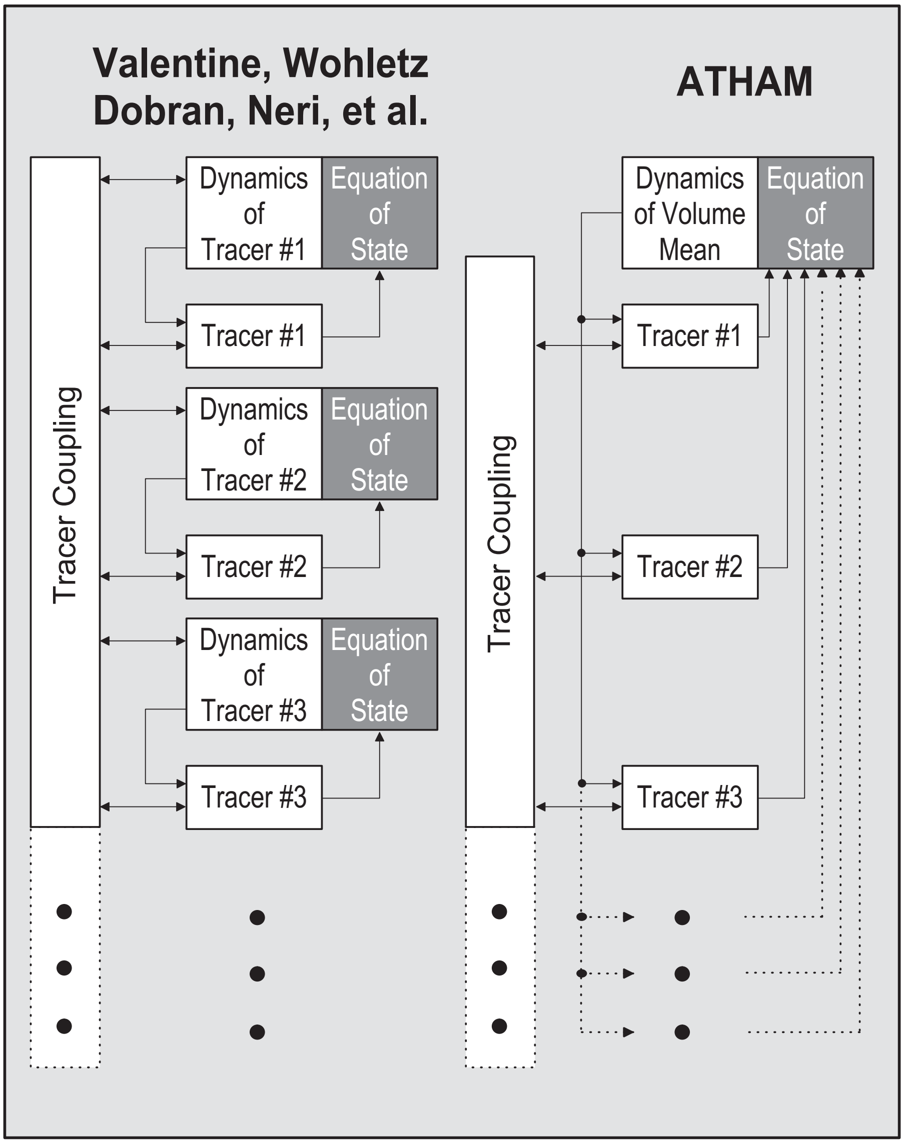
Restriction: time resolution of the model must be large compared to the time needed
to achieve both equilibria.
Advantage: strong reduction in the number of prognostic equations

Equations for the dynamics

Five equations for three momentum components
heat
pressure
-> for the mixture.

One additional transport equation
-> for each tracer concerning its specific fall velocity.

Coupling of active tracers and dynamical variables is done by the bulk density and the heat capacity of the mixture in the equation of state. Further diagnostic equations describe the interactions between the tracers and close the equation system. (Herzog, 98 and Oberhuber et al., 98)



Summary of model equations for the dynamics

Based on the assumption of thermal and dynamic equilibrium, the dynamics of the gas-particle-mixture is shortly decribed by the equations given in this section. For detailed descriptions of the model equations see [?] and [?].

The system consists of four prognostic basic equations:

- the Navier-Stokes-equations for the momentum of the volume mean:

$$
\begin{aligned}
\frac{\partial}{\partial t}\rho u_i &= -\frac{\partial}{\partial x_j}\rho u_i u_j && \text{advection} \\
&+ \frac{\partial}{\partial x_j}\left(\rho K_j \frac{\partial}{\partial x_j} u_i\right) && \text{turbulent diffusion} \\
&- \frac{\partial}{\partial x_i} P && \text{pressure gradient force} \\
&- \rho\, g\, \delta_{i3} && \text{gravitation} \\
&+ 2\, \rho\, \epsilon_{ijk}\, \omega_j\, (u_k - u_k^*) && \text{Coriolis force} \\
&+ \rho\, Q_i && \text{source term}
\end{aligned}
$$

  for i = 1,2,3

- the equation of pressure for the whole system:

$$
\begin{aligned}
\frac{\partial}{\partial t} P = \frac{c_{p,g}}{c_{v,g}} P \Big[& -\frac{1}{\rho q_g}\frac{\partial}{\partial x_i}(q_g\, \rho u_i) && \text{divergenz} \\
& -\frac{1}{\rho q_g}\frac{\partial}{\partial z}(q_g\, \rho\, \Delta u_{3,g}) && \text{correction for velocity} \\
& -\frac{\rho_g}{\rho q_g}\frac{\partial}{\partial t}\frac{\rho q_g}{\rho_g} && \text{correction for volume} \\
& +\frac{1}{\Theta_g}\frac{\partial \Theta_g}{\partial t} \Big] && \text{correction for temperature}
\end{aligned}
$$

- the tracer equation for active tracers:

$$
\begin{aligned}
\frac{\partial}{\partial t}\rho q &= -\frac{\partial}{\partial x_i}\rho q\, u_{i,q} && \text{advection} \\
&+ \frac{\partial}{\partial x_j}\left(K_{j,q} \frac{\partial}{\partial x_j}\rho q\right) && \text{turbulent diffusion} \\
&+ \rho\, Q_q && \text{external sources and sinks}
\end{aligned}
$$

- the temperature equation for the potential temperature of the mixture:

$$\begin{aligned}\frac{\partial}{\partial t}\Theta &= -u_{i,\theta}\frac{\partial}{\partial x_i}\Theta && \text{advection}\\ &\quad +\frac{1}{\rho\, c_p}\,\frac{\partial}{\partial x_j}\left(\rho\, c_p\, K_{j,\theta}\frac{\partial}{\partial x_j}\Theta\right) && \text{turbulent diffusion}\\ &\quad +Q_\theta && \text{external sources and sinks}\end{aligned}$$

The equations for the tracer and the temperature equation are coupled by the equations for momentum and pressure via the equations of state given below.

$$\frac{1}{\rho} = \sum_{i=1}^{N}\frac{q_i}{\rho_i}$$

$$P_g = R_g\,\rho_g\,T_g \quad \text{mit } R_g = c_{p,g} - c_{v,g},$$

The turbulence closure scheme for the determination of turbulent exchange coefficients contributes three additional prognostic equations.

Numerical Solution

Spatial discretisation

finite difference scheme
Arakawa C grid (Arakawa and Mesinger 1976)

Transport

Transport of tracers	centered differences + diffusion term (similar to Smolarkiewicz, 1984)
Transport of heat	semi-Lagrange (similar to Crowley, 1968)

Temporal descretisation

Implicit time step scheme, Cranck-Nicholson (25% forward, 75% backward)

Parallel iteration of dynamic quantities to account for the temporal coupling of the equations with updated density (6 iterations).

Conservation of mass and momentum explicitly guaranteed
Flux form for the equations of motion and continuity of the tracers

Solution of the matrix equations

Efficient realisation of the ADLSOR scheme: Alternating-Direction-Successive-OverRelaxation method (O'Brien, 1986; Lautenschlager, 1986; Oberhuber 1990, 1993)

Model time step

adaptive time step with CFL $\overset{=}{<}$ 0.8

Boundary conditions

lower boundary	fixed bottom, deposition of tracers
upper boundary	damping of pressure and temperature anomalies
lateral boundaries	open boundaries Neumann boundary condition (fixed derivatives, open for sound waves)

Initialisation

- Vertical profiles for horizontal wind, temperature, relative humidity and gaseous species
- Orography, geometry of the volcano
- Volcanic forcing: vertical velocities, temperature and composition of the emissions
- Fire forcing: fluxes of heat, moisture, gases and particles, no vertical velocity.

The simulation of volcanoes begins just after the decompression phase within the crater, fire emissions are distributed within the lowest atmospheric grid cells. Hence, small scale processes in the vicinity of the source in the hot temperature regime are not resolved in the concept of ATHAM.

Turbulent Exchange Processes

Entrainment of ambient air into the plume is important for:

- plume dynamics
- microphysics
- plume chemistry

⇒ Turbulence is a highly important process

Turbulent exchange coefficient based on an extended Kolmogorov - Prandtl formulation:

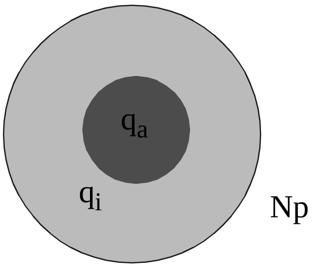
$$\mathrm{K_{hor}} = \mathrm{const}\,\Lambda\,\sqrt{3/2\,\mathrm{B_{hor}}} \qquad \mathrm{B_{hor}} = \overline{\mathrm{u'u'}} + \overline{\mathrm{v'v'}}$$

$$\mathrm{K_{ver}} = \mathrm{const}\,\Lambda\,\sqrt{3\,\mathrm{B_{ver}}} \qquad \mathrm{B_{ver}} = \overline{\mathrm{w'w'}}$$

$\mathrm{K_{hor}}$, $\mathrm{K_{ver}}$:	hor./vert. exchange coefficient
$\mathrm{B_{hor}}$, $\mathrm{B_{ver}}$:	hor./vert. turbulent energy
Λ:	turbulent length scale
$\overline{\mathrm{u'u'}}$, $\overline{\mathrm{v'v'}}$, $\overline{\mathrm{w'w'}}$:	turbulent correlations

$\mathrm{B_{hor}}$, $\mathrm{B_{ver}}$, Λ prognostically treated
through a set of 3 coupled linear differential equations
1.5 order scheme

Cloud Microphysics and Ash aggregation in the twomoment scheme



Prognostic Quantities
mass mixing ratio of ash q_a and hydrometeors q_i
number concentration Np of particles

Categories

Hydrometeors [kg/kg $_{tot}$] [mass mixing ratio]			Ash [kg/kg $_{tot}$] [mass mixing ratio]		Number [#/kg $_{tot}$] [number content]	
small warm	Hydrometeor	(cloud water)	small warm	ash	small warm	particles
large warm	Hydrometeor	(rain)	large warm	ash	large warm	particles
small cold	Hydrometeor	(cloud ice)	small cold	ash	small cold	particles
large cold	Hydrometeor	(graupel)	large cold	ash	large cold	particles

Assumptions

Ash is always active as cloud or ice condensation nuclei.
Ash can be treated like a pure hydrometeor as soon as it is covered by water or ice.

Advantage

No additional Parameterization for the ash microphysics necessary!
The ash-water relation in the particle influences:

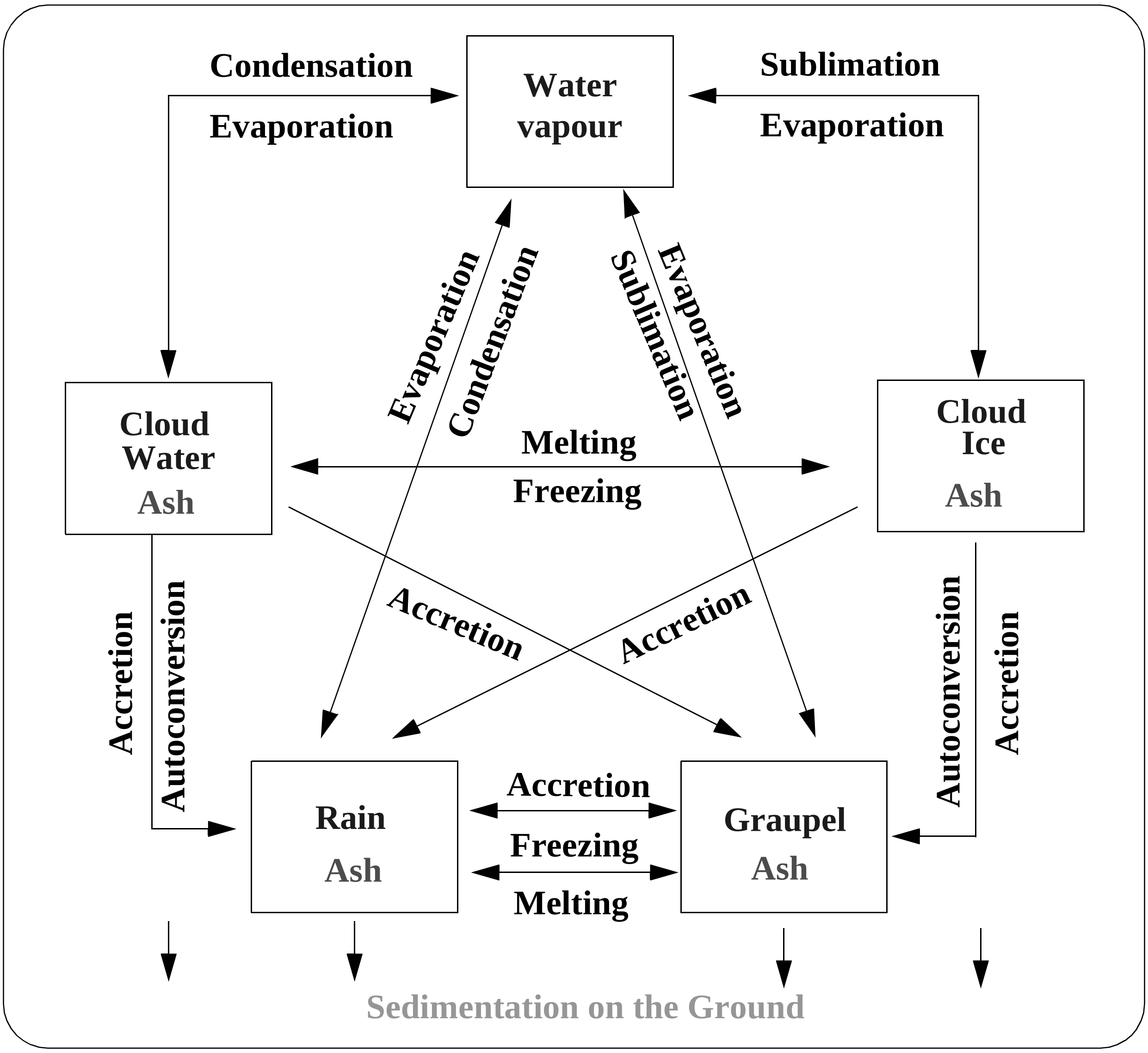
- collision-coalescence efficiency
- skewness parameter of the size distribution function
- particle density

Disadvantage

- It is not possible to tell which part of the ash at a certain grid point is not covered by water or ice.
- It is not possible to tell which part of a hydrometeor at a certain grid point is not covered by water or ice.

-> Dry ash and pure hydrometeors never exist at the same time at one grid point.
-> Instead, aggregates are formed.

Schematic representation of the microphysics



- **Kessler-type microphysics (One-moment scheme)**
  Very simple representation of cloud microphysics, does not include particle aggregation, but is suitable for the investigation of latent heat effect.

- **Two-moment scheme**
  The size distributions are described by normalized gamma functions following the concept of Walko et al. (1995) and Meyer et al. (1997).
  The interaction between aerosol particles and hydrometeors is taken into account.

All classes of hydrometeors and particles are assumed to be spherical.

Microphysics: Two-moment scheme

Normalised gamma functions as size distributions:

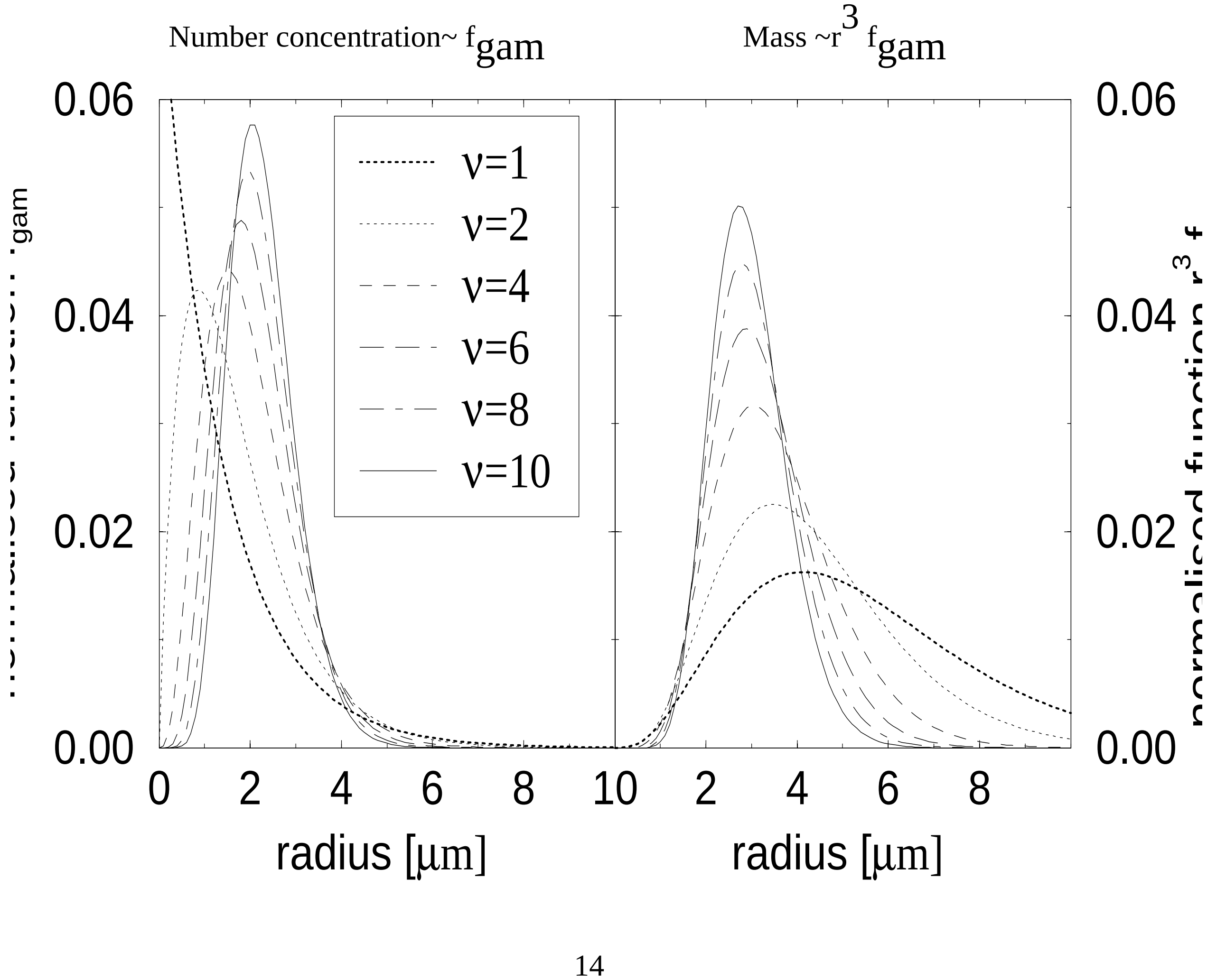
$$N(r) = N_t f_{gam}(r)$$

with
$$f_{gam}(r) = \frac{1}{\Gamma(\nu)}\left(\frac{r}{r_n}\right)^{\nu-1}\frac{1}{r_n}\exp\left(\frac{r}{r_n}\right)$$

and $r_n = f(\bar{r}, \nu)$ with $\bar{r}$ =f (mass, number),ν=const

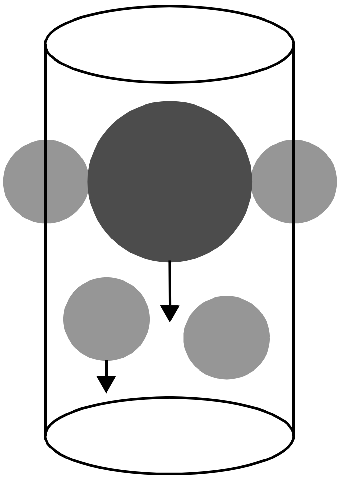
The skewness of the size distribution is determined by mass, number and ν.

Normalised gamma function for $\bar{r}$=2.5 µm



Parameterization of particle aggregation in the twomoment-scheme

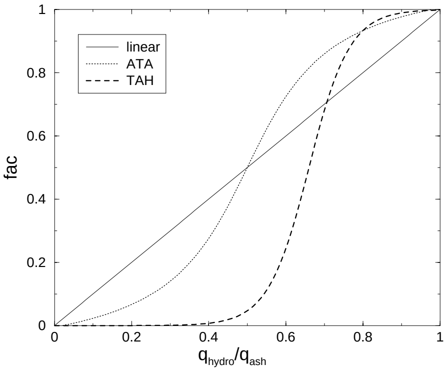
Volume swept by large particles colliding with smaller ones



- Difference in fall velocity leads to collision.
- Coalescence if particles are hydrometeors or ash particles coated with water or ice.
- Dry ash can be allowed to aggregate to reflect the effect of electrostatic forces or mechanical interlocking.

- Wet or icy ash behaves like pure water or ice
- Use of Parameterization for cloud microphysics
- Aggregation coefficient E_{agg} dependent on the fraction of water or ice and ash can be varied with precompiler flags (mo_twomoment.F):

no flag	linear approach
ATA	arcus tangens function
TAH	tangens hyperbolicus function
ELEC	aggregation of dry ash due to electrostatic forces E=0.2



E_{agg}=fac*E_{hyd}, 0<=fac<=1

linear	fac=q_{hyd}/q_{ash}
ATA	fac=0.5*atan(2π*(q_{hyd}/q_{ash}-0.5))*.8+0.5
TAH	fac=0.5*tanh(3π*(q_{hyd}/q_{ash}-0.66))+.5

(The functions are chosen by educated guess!)

Fall velocities

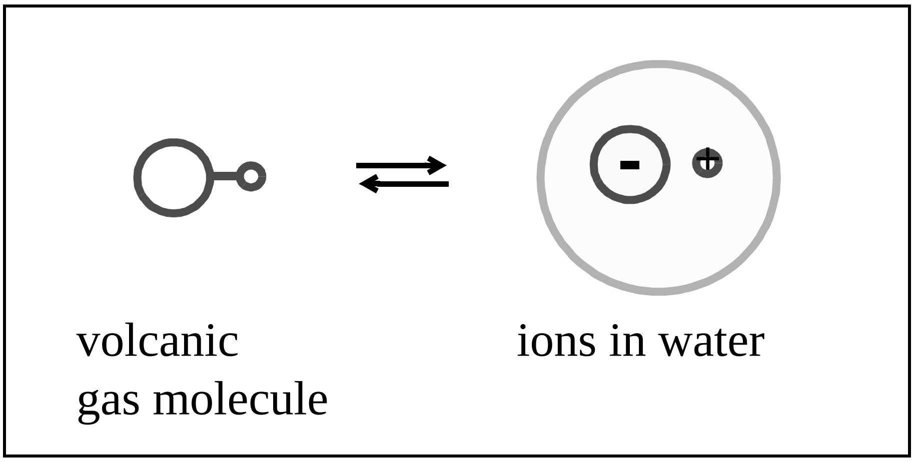
small particles (<35 µm)	$w \sim \overline{r}^{2}$	Stokes friction
large particles (>500 µm)	$w \sim \overline{r}^{1/2}$	Newtonian motion
intermediate particles (50-500µm)	$w \sim \overline{r}$	

The effect of decreasing density in the atmosphere is included.

Scavenging of gases through water drops

Kinetics of the phase transfer

Dissociation of acidic gases in water

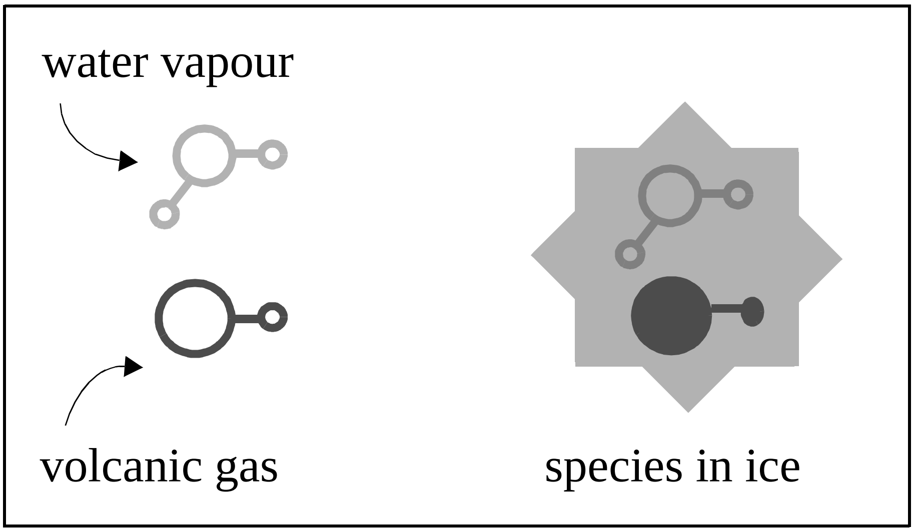


$$\frac{\Delta c_{aq,\,i}}{\Delta t} = k_t L (c_{g,\,i} - c_{g,\,i,\,eq})$$

$c_{aq,i}$	concentration of species i in water
$c_{g,i}$	concentration of species i in the gas phase
$c_{g,i,eq}$	equilibrium concentration of species i in the gas phase
k_t	phase transfer constant $k_t = f\,(r_{aq})$
L	liquid water content

Scavenging of gases through ice particles

Deposition and sublimation of volcanic gases proportional to the transfer of water vapour



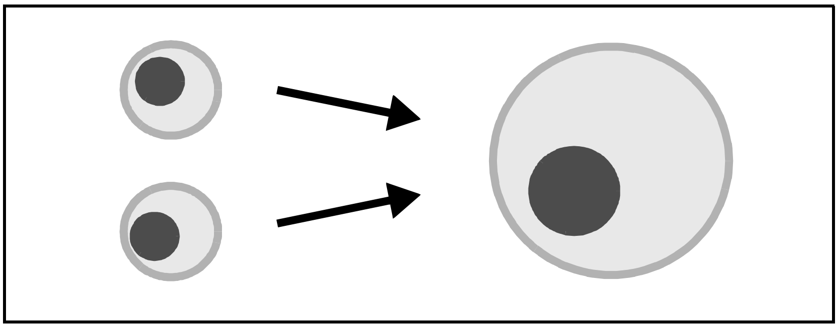
Concentration of gases in ice is determined by the kinetics condensation.

$$\frac{\Delta c_i}{\Delta t}\frac{1}{c_i}\alpha_i\bar{v}_i = \frac{\Delta q_v}{\Delta t}\frac{1}{q_v}\alpha_v\bar{v}_v$$

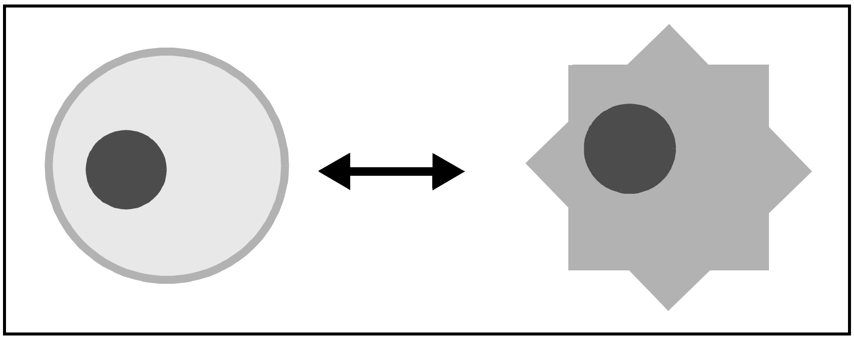
c_i	Concentration of species i in the gas phase [mol/kg $_{\text{tot. mass}}$]
q_{wet}	Specific concentration of water vapour [kg/kg $_{\text{tot. mass}}$]
Δt	time step
α	Sticking coefficient

Transfer of scavenged gases and particles

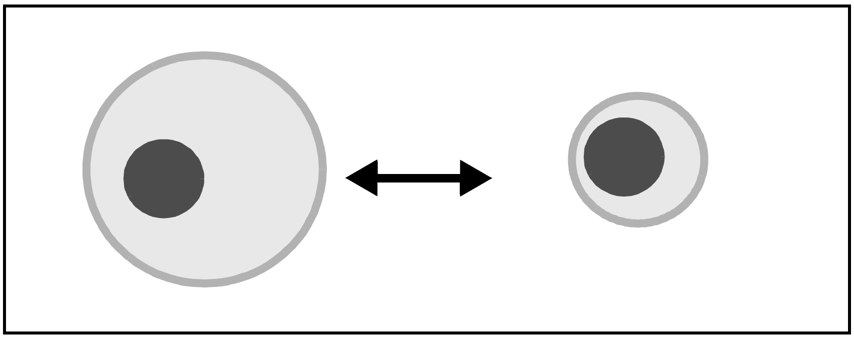
Coagulation of hydrometeors by accretion processes:
Mixture of contained species.



Melting and freezing of solutions:
Retention of contained species.



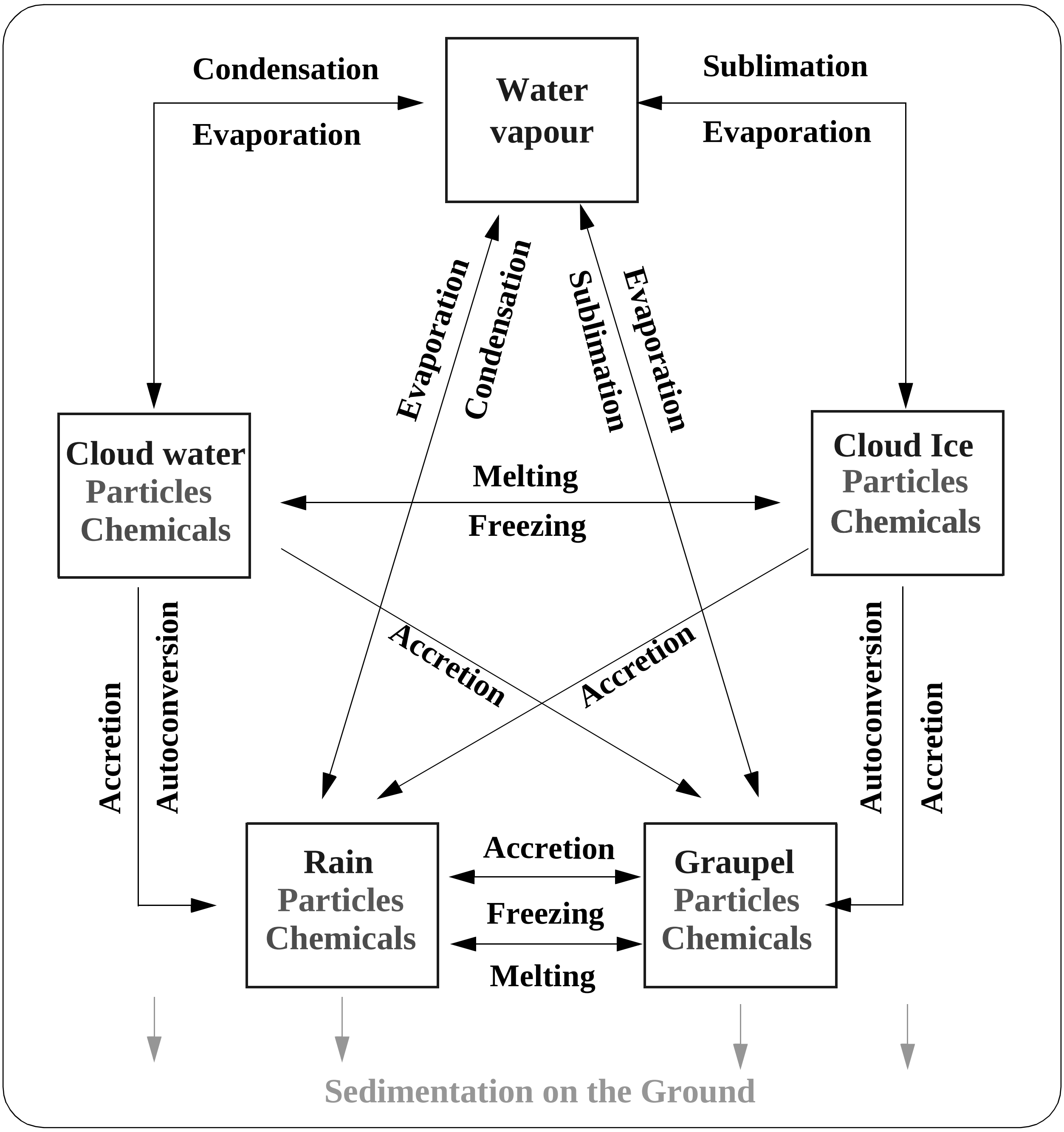
Evaporation and condensation of liquid droplets:
increasing - decreasing concentration in the solution.



water drop: ○ ice crystal: ✶ scavenged material: ●

Parameterization of the gas scavenging in ATHAM

Two-moment scheme of microphysical processes considering
the interaction between hydrometeors and volcanic particles



Hydrometeors:	cloud water cloud ice rain graupel	**Particles**: **Chemicals**:	4 classes like hydrometeor classes 3 species

Program structure of ATHAM

main program in file atham.F

```
program atham

  initialize parallel ATHAM                                        call mpiinit
  initialize dynamical variables                                   call initial
  initialize twomoment microphysics                                call twoinit
  initialize volcano/fire                                          call volcinit/fireinit
  initialize accuracies for transport                              call accur
  initialize gas scavenging                                        call scainit
  initialize model geometry, background etc.                       call atminit
  initialize grads                                                 call gradsinit
  inititialize deposition                                          call depinit
  calculate equation of state                                      call makeall
  determine tropopause height                                      call tropopause
  calculate terminal fall velocities                               call fallvel
  calculate sun zenit angle                                        call szwini
  initialization of grid for the photolysis frequency calculations call atmos_rad
  initialization of photolysis module                              call ini_photo



-> start time stepping loop
        set fluxes to zero for next time step
        add volcanic/fire forcing                                  call volcforc/fireforc
        calculate equation of state                                call makeall
        calculate equation of microphysics                         call microphys
          and transfer of scavenged gases                              call cheflux
        diagnose effective vertical velocity w.r.t. mixture        call diawind
        calculate turbulence                                       call atmturb
        calculate transport                                        call atmstep
        calculate terminal fall velocities                         call fallvel
        calculate gas scavenging                                   call gasscav
        calculate deposition                                       call deposition
        compute the photolysis frequencies                         call calc_photo
        compute the gas chemistry                                  call chemistry
        update time control and time step                          call timestep
-> go to start of time loop

  write output for GrADS                                           call gradsmov
  do final operations                                              call atmstop

end
```

The program structure of ATHAM

main program

atham.F	program control, time loop

Subroutines

name	Flag	purpose
dynamic.F		Calculation of the dynamics (transport, therm. energy, pressure equation, turbulence)
initial.F		initial conditions and constants for dynamics
mpiinit.F	MPI	initialisation of processor communication for parallel code
background.F		construction of the background profiles for temperature, humidity and wind from MARPTS and KINETIK
	SCA	initialise vertical profiles for other tracers
	DIA	determination of k value for tropopause height
microphys.F		environment for microphysics, internal time step for microphysics
kessler.F	KES	Kessler microphysics
twomoment.F	TWO	twomoment microphysics
correct.F	TWO	correct numerical inaccuracies for transport of mass and number
reclass.F	TWO	reclassification of dry ash according to the temperature for the twomoment scheme
fallvel_kes.F	KES	calculation of the fall velocity for Kessler microphysics
fallvel_two.F	TWO	calculation of the fall velocity for twomoment scheme
scav.F	SCA	gas scavenging
cheflux.F	SCA	transfer of dissolved gases proportional to transferred hydrometeors
atham_chem.F	CHEM	gas phase chemistry
jval.F	CHEM	calculation of photolysis frequencies
diagnose.F	DIA	vertical- and horizontal profiles, total mass, plume shape *
grads.F		creates output files for GrADS
gradsscav.F	SCA	creates output files for GrADS for gaseous tracers
volc.F	VOLC	initialisation of the volcanic parameters, shape and forcing
fire.F	FIRE	initialisation of the fire parameters

Modules

name	Flag	purpose
mo_params.F		definition of basic universal constants, explanation of variables
mo_dyn.F		definition of variables for the dynamics, run time control, grid geometry, material constants, convergence parameters, turbulence, file names, and names for alternative use
mo_grads.F		definition of variables for the grads files
mo_kessler.F	KES	definition of variables for the Kessler microphysics
mo_mpi.F	MPI	definition of variables for the twomoment scheme
mo_scav.F	SCA	definition of variables for gas scavenging
mo_twomoment.F	TWO	definition of variables for twomoment microphysics
mo_volc.F	VOLC	definition of variables for the volcano
mo_fire.F	FIRE	definition of variables for the fire
mo_rad.F	CHEM	definition of variables for the photolysis and chemistry

Input files

MARPTS	DATA for vertical background profiles of temperature, relative humidity and horizontal wind.
KINETIK	DATA for vertical background profiles of kinetic viscosity, mean free path.

for chemistry:

atham_chem.h	declaration of variables for chemistry
atham_chem_s.h	declaration of variables for chemistry, Jacobean matrix
CHEM_BACK	background profiles of chemicals
jval.com	declaration of common blocks for photolysis rates
lookt.dat	look-up table for photolysis rate calculation
aer.dat	aerosol optical data
constant.dat	universal constants for photolysis rates

Explanation of tracer indices

Units:
Generally, SI units are used in ATHAM.
The tracer units are in relation to the total mass in kg at a grid point.

active incompressible tracers
tracnew(nx,ny,nz,ntrac)

	kg/kg	t=1	cloud water
	kg/kg	t=2	precipitable water
	kg/kg	t=3	cloud ice
	kg/kg	t=4	graupel
not TWO	kg/kg	t=5	ash particle
	kg/kg	t=6	lapilli
TWO	kg/kg	t=5	warm small ash
	kg/kg	t=6	warm large ash
	kg/kg	t=7	cold small ash
	kg/kg	t=8	cold large ash

active compressible tracers
tgasnew(nx,ny,nz,ntgas)

	kg/kg	g=1	water vapor	
SCA	kg/kg	g=2	ghcl	hcl in the gas phase
	kgl/kg	g=3	gso2	so2 in the gas phase
	kg/kg	g=4	gh2s	h2s in the gas phase

passive tracers
tpasnew(nx,ny,nz,ntpas)

	kg/kg	p=1		inert gas
TWO	#/kg	p=2		number of cloud water/ash/aggregates
	#/kg	p=3		number of cloud ice /ash/aggregates
	#/kg	p=4		number of graupel /ash/aggregates
	#/kg	p=5		number of hail /ash/aggregates
SCA	mol/kg	p=6	chcl	hcl in cloud water
	mol/kg	p=7	phcl	hcl in rain
	mol/kg	p=8	ehcl	hcl in cloud ice
	mol/kg	p=9	hhcl	hcl in graupel
	mol/kg	p=10	cso2	
	mol/kg	p=11	pso2	
	mol/kg	p=12	eso2	
	mol/kg	p=13	hso2	
	mol/kg	p=14	ch2s	
	mol/kg	p=15	ph2s	
	mol/kg	p=16	eh2s	
	mol/kg	p=17	hh2s	
ENT	kg/kg	p=ntpas-nchem		entrained tracer
CHEM	mol/kg	p=ntpas-nchem+1 -> ntpas, with nchem=number of chemicals		

Implementation of additional tracers

How to introduce an incompressible active tracer tracnew

-> change number of incompressible tracers ntrac

-> be sure to set

tracmin(ntrac)	in initial
actrac(ntrac)	in initial
cptrac(ntrac)	in initial
cvtrac(ntrac)	in initial
rhotrac(ntrac)	in initial
radtrac(ntrac)	in initial
voltrac(ntrac)	in volcinit
wtrac(ntrac)	in fallvel

How to introduce a compressible active tracer tgasnew

-> change number of compressible tracers ntgas

->be sure to set

tgasmin(ntgas)	in initial
actgas(ntgas)	in initial
cptgas(ntgas)	in initial
cvtgas(ntgas)	in initial
voltgas(ntgas)	in volcinit

How to introduce a passive tracer tpasnew

-> change number of passive tracers ntpas

-> be sure to set

tpasmin(ntgas)	in initial
actpas(ntgas)	in initial
voltpas(ntgas)	in volcinit
wtpas(ntpas)	in fallvel

-> Check nnum, nash, nhyd and nsca in mo_params.F.

-> if necessary, add equivalences in mo_dyn.F

Explanation of model versions controlled by precompiler flags

flagname	code	meaning
VOLC	mo_volc. volc.F	volcanic eruption
FIRE	mo_fire.F fire.F	vegetation fire
MPI	mpiinit.F	message passing interface: parallel version - for cartesian coordinates only -
PAS		passive tracers
SUN		sun architecture
KES	mo_kessler.F kessler.F fallvel_kes.F	kessler microphysics
TWO	mo_twomoment.F twomoment.F fallvel_two.F reclass.F correct.F	twomoment scheme (needs PAS)
MUD		twomoment scheme including particle aggregation (needs TWO, PAS)
ATA		atan function for aggregation coefficient (needs TWO, PAS)
TAH		tah function for aggregation coefficient (needs TWO, PAS)
ELEC		aggregation of dry ash (needs TWO, PAS)
SCA	mo_scav.F scav.F cheflux.F gradsscav.F	scavenging of gases (needs TWO)
DIA	diagnosis.F	output of diagnosis files
NOIN		no incorporation of gases into growing ice
FREEZE		freezing point/vapour pressure depression
DITCH		topography of volcano, see volc.F
MtHelen		topography of volcano, see volc.F
PULSE		pulsating eruption

flagname	code	meaning
SHORT		do a short test run, e.g. nrep=1,periodt=1.
NOM		no microphysics, but you must choose KES or TWO, for the calculation of the fall-velocities
CHEM	atham_chem.F	gas phase chemistry
	atham_chem.h	declaration of variables for chemistry
	atham_chem_s.h	declaration of variables for chemistry, Jacobean matrix
	CHEM_BACK	background profiles of chemicals
	jval.F	calculation of photolysis frequencies
	jval.com	declaration of common blocks for photolysis rates
	mo_rad.F	definition of variables for the photolysis and chemistry
	lookt.dat	look-up table for photolysis rate calculation
	aer.dat	aerosol optical data
	constant.dat	universal constants for photolysis rates
DEP	deposition.F	calculate deposition of particles

The modules must be compiled before the routines, which use them!

Some options are always necessary:
You must decide for either VOLC or FIRE. For the calculation of the
particle terminal fall velocity you must choose either KES or TWO,
even if the microphysics is not calculated (NOM).

The gas phase chemistry module is built by the KPP© - The Kinetic PreProcessor:

“KPP analyses the chemical mechanism and builds the derivative function and the Jacobian describing the chemical transformations. Kpp offers transparent support for treating sparsity, checks chemical equations for balance, and provides links to different numerical integrators; the output is C or Fortran code (ready to run).“

http://www.cs.mtu.edu/~asandu/Software/software.html

V. Damian-Iordache. KPP -- chemistry simulation development environment. Master's thesis, University of Iowa, 1996.

Examples for Pre-Compiler flags

-DVOLC -DKES -DNOM

mo_dyn.F
mo_volc.F
mo_params.F
mo_grads.F
mo_kessler.F
dynamic.F
atham.F
grads.F
initial.F
volc.F
background.F
fallvel_kes.F

-DVOLC -DKES

mo_dyn.F
mo_volc.F
mo_params.F
mo_grads.F
mo_kessler.F
dynamic.F
atham.F
grads.F
initial.F
volc.F
background.F
fallvel_kes.F
microphys.F
kessler.F

-DVOLC -DTWO -DPAS -DMUD

mo_dyn.F
mo_volc.F
mo_params.F
mo_grads.F
mo_twomoment.F
dynamic.F
atham.F
grads.F
initial.F
volc.F
background.F
fallvel_two.F
correct.F
twomoment.F
microphys.F
reclass.F

-DVOLC -DTWO -DDIA -DPAS -DMUD -DSCA

dynamic.F

```
atham.F
mo_dyn.F
mo_volc.F
mo_params.F
mo_grads.F
mo_scav.F
mo_twomoment.F
grads.F
initial.F
volc.F
background.F
fallvel_two.F
correct.F
twomoment.F
microphys.F
diagnose.F
reclass.F
cheflux.F
scav.F
gradsscav.F
```

-DFIRE -DKES

```
mo_params.F
mo_dyn.F
mo_fire.F
mo_grads.F
mo_kessler.F
grads.F
dynamic.F
initial.F
atham.F
fire.F
background.F
fallvel_kes.F
```

-DFIRE -DTWO -DDIA -DPAS -DMUD -DCHEM

```
mo_params.F
mo_dyn.F
mo_fire.F
mo_grads.F
mo_twomoment.F
mo_rad.F
dynamic.F
atham.F
grads.F
initial.F
fire.F
background.F
fallvel_two.F
correct.F
twomoment.F
microphys.F
diagnose.F
reclass.F
jval.F
atham_chem.F
```

atham_chem.h
atham_chem_s.h
CHEM_BACK
jval.F
jval.com
mo_rad.F
lookt.dat
aer.dat
constant.dat

output files

volcano	shape of volcano
horipro	horizontal profile of tracers, integrated over a vertical column
horisum	cumulative horizontal profile
vertpro	vertical profile of tracers, integrated over a horizontal plane
vertsum	cumulative vertical profile
total	total mass of tracer in the model domain as a function of time
plume	specific characteristics of the plume (max, mean height) as a function of time
spsum	total mass of tracer above the as a function of time
grads_pic.des	descriptor file for grads picture file
grads_pic.dat	data of grads picture file, written to at time 'nrep'*'periodt'
grads_mov.des	descriptor file for grads movie file
grads_mov.dat	data of grads movie file, written to 'nrep' times periodt
mask.des	descriptor file for mask
mask.dat	data of grads file for mask: topography
liste	data of grid structure and background profiles
README_xxx	source code used for run xxx

Makefile or Unix-script?
For test runs use Makefiles, output is created in the same directory.
For longer simulations use Unix-script to create restart files and output files with consecutive numbers.

Compiler

FORTRAN90 or FORTRAN95

options	for nag f90 compiler
fixed format	-fixed
preprocessor	-fpp
double precision for chemistry	-r8
optimization	-O3

How to get started

set simulation time in initial.F

total simulated time:	nrep*periodt
periodt	after this period write to the movie file
nrep	number of periodt, number of pictures in a movie file

change forcing in volc.F/ fire.F

change topography in volc.F

change background profiles in MARPTS, be careful with data formats in background.F!

change size of model domain in mo_params.F

change grid resolution in mo_params.F

change 2dim to 3dim in mo_params.F

switch from cartesian to cylindrical coordinates in initial.F

change variables written to grads-output in grads.F

Try ATHAM!

Run model with Makefile (make run)

Look at output with qview

Goto workshop/work/gradsout and look at grads output, play around with qview

Change simulation time from 1 sec to 6 sec with 3 pictures in grads movie files

Create a restart file after 3.5 sec

Run ATHAM with twomoment scheme instead of Kessler microphysics

Switch on gas scavenging

Switch from cylindrical to cartesian coordinates

Introduce a passive tracer

Introduce an active tracer

References

Graf, H.-F., M. Herzog, J.M. Oberhuber, and Textor, C.: The effect of environmental conditions on volcanic plume rise, J. Geophys. Res., 104, 24309-24320,1999.

Herzog, M.: Simulation der Dynamik eines Multikomponentensystems am Beispiel vulkanischer Eruptionswolken, phd thesis, University of Hamburg, 1999.

Herzog, M., H.-F. Graf, C. Textor, and J.M. Oberhuber, The effect of phase changes of water on the development of volcanic plumes, J. Volcanol. Geotherm. Res., 87, 55-74, 1998.

Landgraf, J., and P. J. Crutzen, An efficient method for online calculations of photolysis and heating rates, J. Atmos. Sci., 55, 863-878, 1998.

Oberhuber, J.M., M. Herzog, H.-F. Graf, and K. Schwanke, Volcanic plume simulations on large scales, J. Volcanol. Geotherm. Res., 87, 29-53, 1998.

Textor, C., Graf, H.-F., Herzog, M. Oberhuber, J.M.O.: Scavenging of Volcanic Gases in the Eruption Column, to be submitted to journal of Geophysical Research, 2002.

Textor, C: Numerical Simulation of Scavenging Processes in Explosive Volcanic Eruption Clouds, phd thesis, University of Hamburg, 1999.

Textor, C., Graf, H.-F., Herzog, M. Oberhuber, J.M.O., Rose W. I., Ernst G. G. J.: Volcanic Particle Aggregation in Explosive Eruption Columns Part I: Parameterisation of the Microphysics of Hydrometeors and Ash, accepted at Journal of Volcanology and Geothermal Research, 2002.

Textor, C., Graf, H.-F., Herzog, M. Oberhuber, J.M.O., Rose W. I., Ernst G. G. J.: Volcanic Particle Aggregation in Explosive Eruption Columns Part II: Numerical Experiments, accepted at Journal of Volcanology and Geothermal Research, 2002.

Trentmann, J., M. O. Andreae, H.-F. Graf, P. V. Hobbs, R. D. Ottmar, T. Trautmann, Simulation of a biomass-burning plume: Comparison of model results with observations, J. Geophys. Res., 107, 10.1029/2001JD000410, 2002

Trentmann, J., M.O. Andreae, H.F. Graf, M. Herzog, P.V: Hobbs, J.M. Oberhuber, R.D. Ottmar, T. Trautmann, C. Textor, Atmospheric Processes in a Biomass Burning Plume, Poster presented at the IGAC Conference, Bologna, 1999.

Volcanic eruptions:	http://www.mpimet.mpg.de/Depts/Klima/adac/atham/ (to be updated!)
Biomass Burning:	http://www.mpch-mainz.mpg.de/~jtrent