Cloud setup in ARCiS

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February 19, 2025

1   Introduction

In this document the new cloud setup options are described. These option are a complete replacement of the older setup used in ARCiS. The old setup was getting very convoluted with too many option that had to be set in too many different places. Management of the code and the input files was therefor too sensitive to errors.

We have now a few different basic types of clouds. Different cloud layers can be set by using the keyword

cloud followed by a number (the number of the layer) and a ":".

After that the keywords described above follow. Example is `cloud1:Kzz=1d9` sets the K_{zz} value of cloud layer 1 to 10^9. In the remainder of this document I will always use as an example for the keywords cloud number 1.

2   Self consistent cloud formation

2.1   Condensation cloud new scheme (recommended)

This setup follows the method from Huang et al. (submitted). The clouds are formed using diffusion and sedimentation following detailed condensation physics using the Gibbs free energies.

type Has to be set to "CONDENSATION" to form this type of cloud

SigmaDot The nucleation rate in g/cm^2

globalKzz Set to .false. to use a value for K_{zz} different from the profile set globally in the atmosphere (default is .true.)

Kzz Value for K_{zz} to use. Only used when globalKzz=.false.

P The pressure of maximum nucleation rate in bar (default is 10^{-4})

dP Width of the nucleation rate profile (default is a factor of 10)

coagulation When switched on computes the coagulation of cloud particles (default is .true.)

rainout When switched on materials that are (partly) thermally stable at the lower boundary of the atmospheric setup are (partly) removed from the mixture (default is .false.)

Srainout Determines the saturation ratio at the bottom above which cloud material is rained out (default is 1)

haze Compute the cloud nuclii. In the original paper the mass and opacity of the cloud nuclii is ignored. (default is .false.)

hazetype Determines the composition of the haze particles (only when haze=.true.). Can be any of the build-in material types.

fmax Sets the maximum value used in the DHS computation (default is 0.8)

freeflow_con Sets the lower boundary condition for the condensate species to be a free-flow boundary condition in stead of fully evaporated (default is .true.)

freeflow_nuc Sets the lower boundary condition for the cloud nuclii to be a free-flow boundary condition in stead of $x_n = 0$ (default is .true.)

The list of condensates currently included is:

Silicates: SiO2, MgSiO3, Mg2SiO4, SiO

Oxides: MgO, FeO, Fe2O3, Al2O3, TiO2

Sulfides: FeS, Na2S, ZnS, MnS

Salts: NaCl, KCl, NH4Cl

Metals: Fe, Zn, Mn, Cr

Ices: H2O, NH3

By default the cloud refractive index is found in the ARCiS data directorty (($HOME)/ARCiS/Data/refind/). This might require an update of the data directory.

As an example if you want to setup a cloud layer that is computed and follows the global K_{zz} profile all you have to do is:

```
cloud1:type="CONDENSATION"
cloud1:SigmaDot=1d-12
cloud1:condensate01="SiO2"
cloud1:condensate02="MgSiO3"
cloud1:condensate03="Mg2SiO4"
```

Note that for these self-consistent cloud layers the opacities are by default computed using DHS and effective medium theory. Note that in principle any number of condensates can be defined (at the cost of increased computing time).

2.2 Condensation cloud (old scheme, not recommended)

This setup follows the method from [2]. The clouds are formed using diffusion and sedimentation. The cloud species are condensed one by one following a prescribed condensation sequence. This has the disadvantage over the method above that multiple materials might be constrained by the same atoms in the gas phase.

type Has to be set to "DIFFUSE" to form this type of cloud

SigmaDot The nucleation rate in g/cm^2

globalKzz Set to .false. to use a value for K_{zz} different from the profile set globally in the atmosphere (default is .true.)

Kzz Value for K_{zz} to use. Only used when globalKzz=.false.

coagulation When switched on computes the coagulation of cloud particles (default is .true.)

rainout When wsitched on materials that are (partly) thermally stable at the lower boundary of the atmospheric setup are (partly) removed from the mixture (default is .false.)

haze Compute the cloud nuclii. In the original paper the mass and opacity of the cloud nuclii is ignored. (default is .false.)

condensates Compute the cloud condensation species. Can be switched off to have a pure haze cloud (default is .true.)

hazetype Determiones the composition of the hze particles (only when haze=.true.). Can be any of the buildin material types.

computecryst When switched on tries to compute the crystallinity of the cloud silicates. (default is .false.)

cryst Sets the crystallinity of the cloud silicates in case computecryst=.false. (default is 1)

fmax Sets the maximum value used in the DHS computation (default is 0.8)

As an example if you want to setup a cloud layer that is computed and follows the global K_{zz} profile all you have to do is:

```
cloud1:type="DIFFUSE"
cloud1:SigmaDot=1d-12
```

Note that for these self-consistent cloud layers the opacities are always computed using DHS and effective medium theory.

3   Reading from a file

This is the most straightforward one. You have a file with a setup of the cloud from another code. All parameters should be given in the file.

type Has to be set to "FILEDRIFT" or "FILE" to form this type of cloud

file Gives the filename to read.

fmax Sets the maximum value used in the DHS computation (default is 0.8)

The structure of the possible file formats will be described in a separate document.

4   Parameterised clouds

For the parameterised cloud distribution setup we have four options: "LAYER", "SLAB", "DECK", "HOMOGENEOUS". There are a few general parameters, mostly for the particle setup, and some specific for the two types. We start with the specific ones and afterwards discuss the general ones for giving the particle size distribution and optical properties.

For details on the underlying equations, please read the document on cloud parameterisation.

4.1 Cloud layer

This is a slab with constant mass fraction of the cloud material between two pressure points. To get this you have to specify:

```
cloud1:type="LAYER"
```

You have only a few parameters specifying the cloud

type Has to be set to "LAYER" to form this type of cloud

Ptop The top pressure of the cloud (default $P_{\text{top}} = 0$)

Pbottom The bottom pressure of the cloud (default $P_{\text{bottom}} = 10^9$)

Ptau The pressure where the optical depth of τ_{cloud} is reached at the reference wavelength

tau Optical depth of the cloud at reference wavelength (default $\tau_{\text{cloud}} = 1$)

xi The powerlaw of the opacity change with pressure (default $\xi = 2$)

lam_ref Reference wavelength (in micron, default $1\,\mu$m)

4.2 Gaussian cloud layer

This is a layer with a Gaussian profile at a given pressure level with a given width and optical depth. To get this you have to specify:

```
cloud1:type="GAUSS"
```

You have only a few parameters specifying the cloud

type Has to be set to "GAUSS" to form this type of cloud

P The central pressure of the cloud (default $P = 10^{-4}$)

dP The width of the cloud (default $\sigma_P = 10$)

tau Optical depth of the cloud at reference wavelength (default $\tau_{\text{cloud}} = 1$)

xi The powerlaw of the opacity change with pressure (default $\xi = 2$)

lam_ref Reference wavelength (in micron, default $1\,\mu$m)

4.3 Homogeneous cloud

This is actually not really a cloud. It is actually a homogeneous component in the atmosphere. There is only a top pressure but no bottom pressure, the entire atmosphere is filled with the same mass fraction of cloud particles.

```
cloud1:type="HOMOGENEOUS"
```

You have only a few parameters specifying the cloud distribution

type Has to be set to "HOMOGENEOUS" to form this type of cloud

mixrat Mass mixing ratio of the cloud particles

Ptop The top pressure of the cloud (default $P_{top} = 0$)

4.4 Cloud slab

This is a slab with a mass fraction of the cloud material between two pressure points varying linearly with pressure. To get this you have to specify:

```
cloud1:type="SLAB"
```

You have only a few parameters specifying the cloud

type Has to be set to "SLAB" to form this type of cloud

Ptop The top pressure of the cloud (default $P_{top} = 0$)

Pbottom The bottom pressure of the cloud (default $P_{bottom} = 10^9$)

tau Optical depth of the cloud at reference wavelength

lam_ref Reference wavelength (in micron, default $1\,\mu$m)

4.5 Cloud deck

This is a deck with an infinite extend. The pressure at which an optical depth of 1 is reached is given as well as how the cloud mass fraction increases with pressure. To get this you have to specify:

```
cloud1:type="DECK"
```

The cloud is parameterised using the prescription from the gradient in the optical depth,

$$\frac{\partial \tau}{\partial P} = C \exp\left((P - P_\tau)/\Phi\right). \tag{1}$$

For an atmosphere in hydrostatic equilibrium we have that

$$\frac{\partial \tau}{\partial P} = \frac{\kappa}{g}, \tag{2}$$

where κ is the mass absorption coefficient of the atmosphere and g is the gravitational acceleration. Here we consider only the optical depth caused by the cloud which means that we have $\kappa = f_{\text{cloud}} \kappa_{\text{cloud}}$. Working this all out we find that (assuming gradients in f_{cloud} and κ_{cloud} can be ignored)

$$f_{\text{cloud}} = \frac{g}{\kappa_{\text{cloud}}} C \exp\left((P - P_{\text{top}})/\Phi\right). \tag{3}$$

Where the scaling constant is determined by where the optical depth reaches a value of one at the reference wavelength. Not that for very low pressures f_{cloud} reaches a constant value so the cloud reaches up with constant value to the top of the atmosphere.

You have only a few parameters specifying the cloud

type Has to be set to "DECK" to form this type of cloud

Ptop The pressure at which an optical depth op 1 is reached at the reference wavelength

dlogP The pressure range over which the cloud optical depth falls off (i.e. Φ)

lam_ref Reference wavelength (in micron, default $1\,\mu$m)

4.6 Opacities

There are two different options for the opacities in the cloud: parameterised or computed from real material optical properties. For the parameterised one can parameterise the opacity itself or parameterise the refractive index.

The opacity type of the cloud can be set by using the keyword

opacitytype which can be "PARAMETERISED", "REFIND", "MATERIAL"

4.6.1 Parameterised opacity

The simplest opacity is the parameterised opacity one. This should only be used in the case that there is no observational data on the composition of the particle available (e.g. no mid-infrared spectral resonances). In this case we simply parameterise the opacity as

$$\kappa_{\text{ext}} = \frac{\kappa_0}{1 + \left(\frac{\lambda}{\lambda_0}\right)^p} \tag{4}$$

where λ_0 is the wavelength where the opacity turns from grey into a Rayleigh slope. In principle this is an indication for the particle size as this usually happens around $\lambda \sim 2\pi r$. For Rayleigh scattering p is expected to be 4 while for Rayleigh absorption it is expected to be around 2.

When computing emission spectra it is important to know the albedo of the particles, which gives us another parameter ω, the single scattering albedo. We take this to be wavelength independent.

The parameters to set are:

opacitytype Has to be set to "PARAMETERISED" to use this opacity type

kappa The value of κ_0 in cm^2/g.

lam_kappa Reference wavelength (in micron, default $\lambda_0 = 1\,\mu$m)

pow_kappa The value of the powerlaw p (default is $p = 4$)

albedo The single scattering albedo ω

4.6.2 Computed from refractive index

When computing the particle opacity from the refractive index we have to define the size and the shape of the particle. For the shape we take either Mie theory (homogeneous spheres), DHS (simulating irregularly shaped particles, see Min et al. 2005), or aggregates.

We parameterise the size distribution of the particles using a Hansen size distribution.

$$n(r)dr \propto r^{\frac{1-3v_{\text{eff}}}{v_{\text{eff}}}} \exp\left(-\frac{r}{r_{\text{eff}}v_{\text{eff}}}\right) \tag{5}$$

for radii $r > r_{\text{nuc}}$. The smallest possible radius (the radius of a nucleus) can be set to a low value of around $r_{\text{nuc}} = 0.01\,\mu$m. In this distribution r_{eff} is the effictive radius of the size distribution and v_{eff} is the dimensionless width.

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We take a varying radius with height in the cloud parameterised as,

$$r_{\text{eff}} = r_{\text{nuc}} + r_{\text{eff},0} \left(\frac{P}{P_0} \right)^{\gamma} \tag{6}$$

For convenience we pick $P_0 = 1$ bar. Typically the larger particles will be at the bottom of the cloud (so at high pressures) so $\gamma > 0$.

So this parameterisation has 3 parameters in total: $v_{\text{eff}}, r_{\text{eff},0}$ and γ. They can be set by:

reff Value of $r_{\text{eff},0}$ in μm.

veff Value of v_{eff} (default is $v_{\text{eff}} = 0$, which uses a single size in each pressure layer)

pow_rad Value of the power of the powerlaw γ (default is $\gamma = 0$)

Pref Value of the reference pressure P_0 (default is $P_0 = 1$)

fmax Irregularity parameter for the DHS computations. When set to 0 homogeneous spheres are used (default $f_{\text{max}} = 0.8$)

rnuc Value of r_{nuc} in μm (default is $r_{\text{nuc}} = 0.01 \, \mu$m).

Parameterised refractive index

A simple thing we could do is fit the refractive index of the material. This works best if the wavelength coverage is rather narrow so the refractive index is not expected to vary too much. In that case we simply have two parameters: the real and imaginary parts of the refractive index, n and k respectively such that $m = n + ik$.

opacitytype Has to be set to "REFIND" to use this opacity type

n Real part of the refractive index

k Imaginary part of the refractive index

Real materials measured in the lab

For this a library of measured optical properties is needed. Some materials come compiled into ARCiS. You can setup a mixture of materials. Each material gets a number and you can mix materials from files and precompiled materials.

opacitytype Has to be set to "MATERIAL" to use this opacity type

lnkfile Optionally followed by a number. This keyword points to an lnk-file with three columns: wavelength [micron], real part, imaginary part of the refractive index.

lnkfilex,lnkfiley,lnkfilez Optionally followed by a number. This keyword points to an lnk-file with three columns: wavelength [micron], real part, imaginary part of the refractive index for different crystallographic axes. If one of them is set, they have to be set all. If none of them is set, the particle is supposed to have an isotropic refractive index set by the keyword **lnkfile**.

material Optionally followed by a number. This keyword points to a material compiled into ARCiS. For a list of materials see the table below.

abun Followed by a number. Sets the abundance of material with the matching lnk-file.

An example of pure forsterite cloud, using the files "forsterite_x.lnk","forsterite_y.lnk", "forsterite_z.lnk" for the refractive index.

```
cloud1:opacitytype="MATERIAL"
cloud1:lnkfilex="forsterite_x.lnk"
cloud1:lnkfiley="forsterite_y.lnk"
cloud1:lnkfilez="forsterite_z.lnk"
```

An example of mixed astrosil/forsterite cloud, using the files "astrosil.lnk" and "forsterite_x.lnk","forsterite_y.lnk", "forsterite_z.lnk" for the refractive index.

```
cloud1:opacitytype="MATERIAL"
cloud1:lnkfile01="astrosil.lnk"
cloud1:lnkfilex02="forsterite_x.lnk"
cloud1:lnkfiley02="forsterite_y.lnk"
```

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```
cloud1:lnkfilez02="forsterite_z.lnk"
cloud1:abun01=0.7
cloud1:abun02=0.3
```

An example of mixed astrosil/forsterite cloud, using the compiled material "EN-STATITE" and the files "forsterite_x.lnk","forsterite_y.lnk", "forsterite_z.lnk" for the refractive index.

```
cloud1:opacitytype="MATERIAL"
cloud1:material01="ENSTATITE"
cloud1:lnkfilex02="forsterite_x.lnk"
cloud1:lnkfiley02="forsterite_y.lnk"
cloud1:lnkfilez02="forsterite_z.lnk"
cloud1:abun01=0.4
cloud1:abun02=0.6
```

5 Examples

5.1 Cloud formation

A full setup for cloud formation similar to what was done in [1] but compute the crystallinity

```
cloud1:type="DIFFUSE"
cloud1:globalKzz=.false.
cloud1:SigmaDot=1d-12
cloud1:Kzz=1d8
cloud1:computecryst=.true.
```

5.2 A fully parameterised cloud layer

A cloud layer with parameterised structure and opacity extending to very high optical depths and reaching optical depth one at 1 bar.

```
cloud1:type="LAYER"
```

```
cloud1:Ptop=1d-3
cloud1:Ptau=1d0
cloud1:xi=4
cloud1:opacitytype="PARAMETERISED"
cloud1:kappa=100
cloud1:opacity_pow=2
cloud1:albedo=0.1
```

References

[1] Michiel Min, Chris W. Ormel, Katy Chubb, Christiane Helling, and Yui Kawashima. The ARCiS framework for exoplanet atmospheres. Modelling philosophy and retrieval. *A&A*, 642:A28, October 2020.

[2] Chris W. Ormel and Michiel Min. ARCiS framework for exoplanet atmospheres. The cloud transport model. *A&A*, 622:A121, February 2019.