Cloud setup in ARCiS

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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 two 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

This setup follows the method from Ormel & Min (2019). The clouds are formed using diffusion and sedimentation.

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: "soot", "tholin", "optEC", "SiC", "carbon", "corrundum", "iron", "SiO", "TiO2", "enstatite", "MIX"

fHaze followed by any of: SiO, SiO2, tholin, TiO2 corrundum, iron, enstatite or forsterite. Sets the abundance ratios of these species in case the haze type is set to "MIX"

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 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.

3.1 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 $P_{top} = 0$)

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

Pdeck 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 $\tau_{cloud} = 1$)

xi The powerlaw of the opacity change with pressure (default $\xi = 1$)

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

3.2 Homogeneous cloud

This is actually not really a cloud. It is actually a homogeneous component in the atmosphere. There is no top pressure or 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

3.3   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 $P_{\text{top}} = 0$)

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

tau Optical depth of the cloud at reference wavelength

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

3.4   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,

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

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)

3.5 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"

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

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

albedo The single scattering albedo ω

3.5.2 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.

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

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

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

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

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_{eff}, $r_{\mathrm{eff},0}$ and γ. They can be set by:

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

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

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

P0 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 $f_{max} = 0.8$)

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

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.

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

An example of pure forsterite cloud, using the file "forsterite.lnk" for the refractive index.

```
cloud1:opacitytype="MATERIAL"
cloud1:lnkfile="forsterite.lnk"
```

An example of mixed forsterite/enstatite cloud, using the files "forsterite.lnk" and "enstatite.lnk" for the refractive index.

```
cloud1:opacitytype="MATERIAL"
cloud1:lnkfile01="forsterite.lnk"
cloud1:lnkfile02="enstatite.lnk"
cloud1:abun01=0.7
cloud1:abun02=0.3
```

4 Examples

4.1 Cloud formation

A full setup for cloud formation similar to what was done in Min et al. 2020 but compute the crystallinity

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

4.2 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:Pdeck=1d0
cloud1:xi=4
cloud1:opacitytype="PARAMETERISED"
cloud1:kappa=100
cloud1:opacity_pow=2
cloud1:albedo=0.1
```

References

Ormel C. W., Min M., 2019, A&A, 622, A121. doi:10.1051/0004-6361/201833678