Cloud parameterisation for Brown Dwarfs and exoplanets: Cloud2Con discussion session report

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Below we define the cloud structure (i.e. the density of the cloud) and the opacity.

1 Cloud structure

There are two types of cloud structures in the Brewster parameterisation: a deck cloud and a slab cloud. On top of that we recognise that for the transiting planets the cloud deck might not provide the best representation for low pressures, so we propose an alternative which we call the Layer cloud.

1.1 Brewster parameterisation

1.1.1 Cloud deck

The cloud deck is a cloud that extends to high enough pressures that we cannot see through the cloud. For simplicity we therefore model it as infinite towards high pressures.

The cloud deck is parameterised using the prescription from Brewster (see e.g. Burningham et al. 2021). What is set is 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 $\kappa = f_{\mathrm{cloud}}\kappa_{\mathrm{cloud}}$, where f_{cloud} is the mass fraction of the local atmosphere in cloud particles ($f_{\mathrm{cloud}} = \rho_{\mathrm{cloud}}/\rho_{gas}$). Working this all out we find that

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

Where the scaling constant is determined by where the optical depth reaches a value of one at the reference wavelength. Note 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.

The value for C is determined such that the optical depth reaches unity at the pressure $P = P_\tau$. To find the value for C we need to integrate $\partial\tau$ from $P = 0$ to $P = P_\tau$ which gives,

$$1 = C \int_0^{P_\tau} \exp\left((P - P_\tau)/\Phi\right) dP = C\,\Phi\left[1 - \exp\left(-P_\tau/\Phi\right)\right] \tag{4}$$

So we end up with

$$C = \frac{1}{\Phi\left[1 - \exp\left(-P_\tau/\Phi\right)\right]} \tag{5}$$

Filling this all in we have the cloud parameterised by using the mass fraction

$$f_{\mathrm{cloud}} = \frac{g}{\kappa_{\mathrm{cloud}}} \frac{\exp\left((P - P_\tau)/\Phi\right)}{\Phi\left[1 - \exp\left(-P_\tau/\Phi\right)\right]}. \tag{6}$$

In this equation κ_{cloud} can vary with pressure. As long as f_{cloud} is computed at all pressures using Eq. 6 this is all still consistent with the initial parameterisation of $\partial\tau/\partial P$.

1.1.2 Cloud slab

A cloud slab is significantly more simple. We take here that

$$\frac{\partial \tau}{\partial P} = C\,P. \tag{7}$$

in the range where the cloud exists, which is in the range $P_{\rm top} < P < P_{\rm bottom}$. Using again Eq. 2 we get

$$f_{\rm cloud} = \frac{g}{\kappa_{\rm cloud}} C\, P. \tag{8}$$

The constant C is now computed assuming a total optical depth $\tau_{\rm cloud}$ at the reference wavelength between $P_{\rm top}$ and $P_{\rm bottom}$. Integrating again Eq. 7 we get that

$$\tau_{\rm cloud} = C \int_{P_{\rm top}}^{P_{\rm bottom}} P\, dP = \frac{C}{2}(P_{\rm bottom}^2 - P_{\rm top}^2), \tag{9}$$

from which we get that

$$C = \frac{2\tau_{\rm cloud}}{P_{\rm bottom}^2 - P_{\rm top}^2}. \tag{10}$$

So we arrive at the final equation for the mass fraction of cloud material for pressures with $P_{\rm top} < P < P_{\rm bottom}$.

$$f_{\rm cloud} = \frac{2\, g\, P\, \tau_{\rm cloud}}{\kappa_{\rm cloud}(P_{\rm bottom}^2 - P_{\rm top}^2)} \tag{11}$$

1.2 Cloud Layer

The cloud layer is parameterised over the range $P_{\rm bottom} < P < P_{\rm top}$ (although it can also be extended throughout the entire atmosphere) and parameterised using the pressure where the cloud reaches a given optical depth at the reference wavelength. However, to ensure that the cloud density drops to zero at low pressures we parameterise the gradient of optical depth as

$$\frac{\partial \tau}{\partial P} = C\, P^{(\xi - 1)}, \tag{12}$$

The value of ξ determines how fast the cloud decreases towards high altitudes compared to the pressure scale height,

$$\xi = \left(\frac{H_{\rm gas}}{H_\tau}\right)^2, \tag{13}$$

with $H_{\rm gas}$ the gas scale height and H_τ the opacity scale height. This means we have $\xi > 0$. For a cloud with constant opacity per unit mass (i.e. homogeneous particles throughout the cloud), the opacity scale height is the density scale height of the cloud. We might argue that for a condensation cloud it is expected that $\xi > 1$ while for a haze layer $\xi \leq 1$.

Using the same formalism as above we arrive at

$$f_{\mathrm{cloud}} = \frac{g\,\xi\,\tau_{\mathrm{cloud}}\,P^{(\xi-1)}}{\kappa_{\mathrm{cloud}}\left(P_\tau^\xi - P_{\mathrm{top}}^\xi\right)}, \tag{14}$$

where P_τ is now the pressure at which the optical depth of the cloud reaches the value τ_{cloud} and P_{top} is the top of the cloud layer. We generalise the concept by setting $f_{\mathrm{cloud}} = 0$ for $P > P_{\mathrm{bottom}}$.

We could in general simplify to make a simple cloud extending to the entire atmosphere if we take $P_{\mathrm{top}} = 0$, $\tau_{\mathrm{cloud}} = 1$ and $P_{\mathrm{bottom}} = \infty$

$$f_{\mathrm{cloud}} = \frac{g\,\xi\,P^{(\xi-1)}}{\kappa_{\mathrm{cloud}} P_\tau^\xi}. \tag{15}$$

For this setup it is best to take $\xi > 1$ to make sure that the cloud specific density decreases with decreasing pressure.

Note that the Cloud Slab is a special case of the Cloud Layer by setting: $\xi = 2$ and $P_\tau = P_{\mathrm{bottom}}$ (see Eqs. 11 and 14).

1.3 Gaussian cloud layer

The Gaussian cloud layer is parameterised over the entire atmosphere. It has a central pressure and a width. We parameterise the optical depth as:

$$\frac{\partial \tau}{\partial P} = \frac{C}{P} \exp\left(-\frac{1}{2\sigma_P^2}\left[\log\frac{P}{P_0}\right]^2\right), \tag{16}$$

The value of σ_P determines how fast the cloud decreases towards lower and higher altitudes.

Using the same formalism as above we arrive at

$$f_{\mathrm{cloud}} = \frac{g\,\tau_{\mathrm{cloud}}}{\kappa_{\mathrm{cloud}}\,P\,\sigma_P\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma_P^2}\left[\log\frac{P}{P_0}\right]^2\right). \tag{17}$$

2 Opacities

For the cloud opacities we have three levels of complexity. The choice taken is based on the availability of observations.

2.1 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

$$\kappa_{\rm ext} = \frac{\kappa_0}{1+\left(\frac{\lambda}{\lambda_0}\right)^p} \tag{18}$$

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.

2.2 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.

$$n(r)dr \propto r^{\frac{1-3v_{\rm eff}}{v_{\rm eff}}} \exp\left(-\frac{r}{r_{\rm eff}v_{\rm eff}}\right) \tag{19}$$

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

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

$$r_{\rm eff} = r_{\rm nuc} + (r_{\rm eff,0} - r_{\rm nuc})\left(\frac{P}{P_0}\right)^\gamma \tag{20}$$

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: $v_{\rm eff}, r_{\rm eff,0}$ and γ.

2.2.1 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 $m = n + ik$.

2.2.2 Real materials measured in the lab

The final model complexity is obtained by using wavelength dependent refractive indices measured in the lab. There are tables available from various sources. In a single cloud the particles of different composition are expected to be mixed together. The effective refractive index of a mixture of materials can be approximated using effective medium theory. In effective medium theory it is assumed that the mixing of materials takes place on the smallest possible scales, such that at any resolution one only observes an effective refractive index, m_{eff}. In this way the computational methods for single material particles can again be applied.

Consider an infinite medium with complex refractive index m_m which we will call the matrix material. The polarizability of a small spherical inhomogeneity with complex refractive index m_i in that medium is given by,

$$\alpha_i = 3V \frac{(m_i/m_m)^2 - 1}{(m_i/m_m)^2 + 2}. \tag{21}$$

Now the two most commonly used effective medium theories state that the polarizability of the effective medium inside this matrix material is the average of the polarizabilities of the materials that make up the medium,

$$\frac{(m_{\text{eff}}/m_m)^2 - 1}{(m_{\text{eff}}/m_m)^2 + 2} = \sum_i w_i \frac{(m_i/m_m)^2 - 1}{(m_i/m_m)^2 + 2}, \tag{22}$$

where w_i is the volume fraction of material i. To solve for m_{eff}, the quantity which we want to derive, we have to define what the matrix material, m_m, is. In the Garnett mixing rule one choses the dominant material in the mixture, so $m_m = m_j$. This makes it possible to write down a closed form solution of Eq. 22, and is a good approximation if one wants to look at the effects of small abundance polutions in a material. In the Bruggeman mixing rule one makes the logical choice that $m_m = m_{\text{eff}}$ (so the left hand side of Eq. 22

becomes zero). This makes physically more sense, but also makes it more difficult to solve for m_{eff}. In practice however, a simple iterative scheme usually converges relatively fast.

3 Retrieval complexity

The above setup allows for various combinations of complexity in the cloud setup. One can in principle have multiple layers of different composition. The setup with the least numbers of parameters (infinetly extended cloud deck or layer combined with a parameterised opacity or a single lab material cloud) requires only 4 parameters in total. Note that the parameter κ_0 is in fact meaningless since the cloud density is scaled to reach a given optical depth. This means that the opacity of the cloud in the end does not depend on the choice of κ_0, and it can be fixed to an arbitrary value in a retrieval setup. A more complex generalised cloud layer containing parameterised refractive index particles requires up to 9 parameters. Different combination can be chosen depending on the information content of the observations. Tables 1 and 2 give the parameters for different setups and suggested reasonable ranges that might be expected.

Table 1: Retrieved parameters for the cloud structure with some suggested reasonable ranges for these parameters

Cloud deck (Eq. 6)	
P_τ	10^{-3} – 10^{3} bar
Φ	10^{-3} – 10^{3} bar
Cloud slab (Eq. 11)	
P_{top}	10^{-3} – 10^{3} bar
P_{bottom}	10^{-3} – 10^{3} bar
τ_{cloud}	10^{-6} – 10^{2}
Cloud layer, finite extend (Eq. 14)	
P_{top}	10^{-3} – 10^{3} bar
$P_{\mathrm{bottom}} = P_\tau$	10^{-3} – 10^{3} bar
τ_{cloud}	10^{-6} – 10^{2}
ξ	0.1 – 10
Cloud layer, infinite total τ, extended to top (Eq. 17)	
P_τ	10^{-3} – 10^{3} bar
ξ	1 – 10

Table 2: Retrieved parameters for the opacity with some suggested reasonable ranges for these parameters

Parameterised opacity (Eq. 18)	
λ_0	$10^{-2} - 10^{2}\,\mu$m
p	$0 - 4$
ω	$0 - 1$
Parameterised refractive index	
$r_{\mathrm{eff},0}$	$10^{-2} - 10^{1}\,\mu$m
v_{eff}	$10^{-2} - 0.5$
γ	$0 - 2$
n	$0.1 - 3$
k	$10^{-6} - 1$
Real materials measured in the lab	
$r_{\mathrm{eff},0}$	$10^{-2} - 10^{1}\,\mu$m
v_{eff}	$10^{-2} - 0.5$
γ	$0 - 2$
Composition	mixing ratios of various materials