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Aerosols in the Atmosphere

A Matlab user interface for optical properties of aerosols in internal and external mixture

Una interfaz en Matlab de las propiedades ópticas de aerosoles en mezcla interna y externa

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ABSTRACT:

The purpose of the interface is to provide a simple platform to compute aerosol optical properties when its constitutive components are in external or internal mixture. External mixture means that there is no physical or chemical interaction between the particles of different components. Internal mixture consists of a component that is coated by a concentric shell of another material. The most common case is a light-absorbing carbon (soot) coated with a weakly absorbing material (sulphate). The user can select to combine the six basic components (soot, nitrate, sulphate, sea salt, dust and organic carbon) either in external mixture, internal mixture or a combination of both. The interface will output the absorption, extinction and scattering coefficients, as well as the single scattering albedo and the asymmetry parameter. The platform includes some predefined values for the key parameters describing the basic components: the refractive index, and the parameters of the lognormal size distribution. For those cases when there is not a general agreement in the Scientific Community, such as the refractive index of soot, the user can input its own parameters. The scattering is described with the Mie scattering theory. The main drawback of this approach is that aerosols are considered spherical. We plan to extend the platform for spheroid-like particles.

Keywords: Aerosols, Optical Properties, Internal Mixture, External Mixture, Mie Scattering.

RESUMEN:

El propósito de la interfaz es proporcionar una plataforma sencilla para que el usuario pueda calcular las propiedades ópticas de aerosoles que tengan sus componentes constitutivos en mezcla externa o interna. La mezcla externa supone que no existe interacción física o química entre los distintos componentes. La mezcla interna consiste en que un componente se encuentra recubierto por una capa concéntrica de otro material. El caso más común es carbono que absorbe luz (hollín) recubierto de un material débilmente absorbente (sulfato). El usuario puede combinar los seis componentes básicos (hollín, nitrato, sulfato, sal marina, polvo y carbono orgánico) tanto en mezcla externa como en mezcla interna, así como en una combinación de ambas. La interfaz proporciona como salida los coeficientes de absorción, extinción y dispersión, así como el albedo de dispersión simple y el factor de asimetría. La interfaz incluye algunos valores predefinidos de los parámetros que describen los componentes básicos: índice de refracción, y los parámetros de la distribución lognormal de tamaños. En aquellos casos en los que no exista acuerdo en la Comunidad Científica, como en el índice de refracción del hollín, el usuario puede introducir sus propios parámetros. La dispersión se describe con la teoría de Mie. El inconveniente del enfoque presentado es la consideración de aerosoles esféricos. Planeamos extender la plataforma a partículas esferoides.

Palabras clave: Aerosoles, Propiedades Ópticas, Mezcla Interna, Mezcla Externa, Dispersión de Mie.

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1. Introduction

Atmospheric aerosols are a microscopic liquid or solid particles suspended in Earth's atmosphere. Aerosols can harm human health as well as influence climate by absorbing and reflecting solar radiation and modifying cloud formation acting as cloud condensation nuclei (CCN) [1]. Aerosol optical properties are essential for Remote Sensing, in two ways: they provide information about the aerosols, and also they help to unravel hidden information, i.e. the atmospheric correction of data. To make such optical properties available and easy to handle we present a simple platform for constitutive aerosol components in external or internal mixture.

The aerosol chemical composition and size distribution are the main factors for determining the aerosol optical properties. The aerosol chemical composition is complex and includes carbonaceous matter, primary wind driven components such as sea salt and mineral dust, as well as secondary components such as sulphate and nitrate. Black carbon (BC) is a primary emitted species whereas organic carbon (OC) can be emitted directly to the atmosphere, or result from secondary formation. OC consists of a variety of chemical constituents and the processes leading to the formation of all constituents are still not well resolved. In recent years there have been considerable advances in the extent and quality of aerosol observations. Aircraft, shipboard, and ground-station measurements during field campaigns as well as long term measurements at ground stations give direct information on chemical composition, but they often have limited spatial coverage. The network of sunphotometers within AERONET is essential for validation of satellite data and global aerosol models, in particular for aerosol optical depth (AOD). The near global coverage of AOD through satellites has given much insight into the aerosol distribution.

On the other hand, the radiative forcing (RF) is a measure of the influence that a factor has in altering the balance of incoming and outgoing energy in the Earth-atmosphere system and is an index of the importance of the factor as a potential climate change mechanism. Positive forcing tends to warm the surface while negative forcing tends to cool it. To better quantify the direct aerosol effect and to quantify its uncertainty there is a need to improve the aerosol models and to investigate those parts of the RF calculation due to the direct aerosol effect.

The properties of aerosol particles are highly variable, both in time and space. This applies to the number density, i.e. the amount of particles per volume, for the microphysical properties like size distribution, refractive index and shape, and for the height distribution. Moreover, in most cases the actual properties are not known. For this reason, it is impossible to model aerosols in detail. It is necessary to reduce the variability of naturally occurring aerosols to typical cases, but without neglecting possible fluctuations. For this we include a dataset of typical aerosol components, which can be combined both or internal external mixture to describe a wide range of tropospheric aerosols. The distinction between internal or external determines which chemical reactions take place on mineral surfaces and how the original particles change during atmospheric transport [2].

2. Aerosol components

The oxidation of sulphur-bearing gases (natural and anthropogenic) in the atmosphere ends as a stable form: sulphate. Sulphate particles are one of the main cooling aerosols. Nevertheless, in the remote oceanic atmosphere sulphate can be aggregated with soot decreasing the cooling effect of sulphate [2]. Soot is a by-product of inefficient combustion, is not soluble in water and therefore the particles are assumed not to grow with increasing relative humidity. Although soot is a small fraction of the aerosol mass, it is the dominant aerosol absorber of solar radiation in the atmosphere and is an important component of the anthropogenic climate forcing. Natural dust is produced in arid regions. It contains a mixture of quartz and clay minerals. Anthropogenic mineral dust is difficult to estimate, with values from 20 to 50% of the total, according to the source. Cooling or heating depends on size distribution, chemical composition and shape, vertical distribution and surface albedo. The global mean short-wave radiative forcing is usually negative and the global mean long-wave forcing will be positive. Nitrate is an end product of a wide variety of reactions in the atmosphere involving trace gases. The trace gases produced either naturally of anthropogenically are: nitrogen oxides, volatile nitrogen-bearing acids and gaseous nitrates. Currently most global aerosol models still exclude ammonium-nitrate when the direct aerosol radiative forcing is studied. However, nitrate aerosols are expected to become more important in the future atmosphere due to the expected increase in nitrate precursor emissions and the decline of ammonium sulphate aerosols in wide regions of this planet. There are two types of organic carbon: primary carbon, which is emitted directly to the atmosphere; and secondary carbon, which is produced via photo-oxidation of hydrocarbon precursors. The organic carbon has a negative climate forcing. Sea salt is formed predominantly by the bursting of entrained air bubbles during whitecap formation. Sea salt particles are important light scatterers and contributors to cloud condensation nuclei.

3. Scattering theory

Different particle types (mineral dust, sulphates, nitrates, sea salt, organic carbon and soot) can occur in the same air mass. An important question is whether the particles are internally or externally mixed. External mixture means that there is no physical or chemical interaction between particles of different components. Internal mixture consists of a component that is coated by a concentric shell of another material. Changes from predominantly external to internal mixtures can occur when particles grow by coagulation with different species, a process that is especially common during entrainment into clouds [2]. The differences between internal and external mixtures can significantly affect the optical properties and radiative efficiency of the aerosol and its ability to act as CCN. Next, we are going to briefly describe the scattering approach of external and internal mixture of aerosol components

3.a. External mixture

Optical properties of aerosols are determined by the size distribution and the refractive index. For those aerosols that are able to take up water, the mode radius, as well as the limiting radii, are increased with increasing relative humidity. Six values of relative humidity have been applied for the calculations: 0%, 50%, 70%, 80%, 90%, and 99%. Regarding to the refractive index, the platform includes values for sulphate [3], soot [4], nitrate, dust, sea salt [3], and organic carbon [5]. The user can also include other values for the refractive index. The refractive index of hygroscopic aerosols changes with the additional amount of water that is absorbed in response to changing relative humidity. This change in refractive index has also been included

[3]. The aerosol optical properties are calculated with Mie theory [6]. The interface outputs the absorption, extinction and scattering coefficients, the single scattering albedo and the asymmetry parameter. It is also possible to compute the aerosol optical thickness once the mixing layer is defined by the user with the parameters of an exponential aerosol decrease. The interface also includes the possibility of including a lidar retrieved aerosol extinction profile.

3.b. Internal mixture: core-shell particles

Only a few aerosol components absorb light, with the most powerful actors being strongly absorbing carbon particles or soot. Modelled absorption depends on whether the strongly absorbing substance is assumed to be externally mixed— that is, located in particles that are physically separated from other, weakly absorbing material—or internally mixed— that is, contained in the same particle as weakly absorbing material. In the approach we will follow [4], we will consider that soot is perfectly mixed with other material at the molecular level, and that the soot particle remains solid but it is covered with other material or encapsulated. We will use concentric sphere geometry [7] since it is more plausible. It could be caused by organic or ionic species condensing on insoluble soot. It has been predicted [7] that most absorbing particles would be mixed with non absorbing species within a few days after emission. The aerosol optical properties of the spherical core-shell particles are calculated with Mie theory [6].

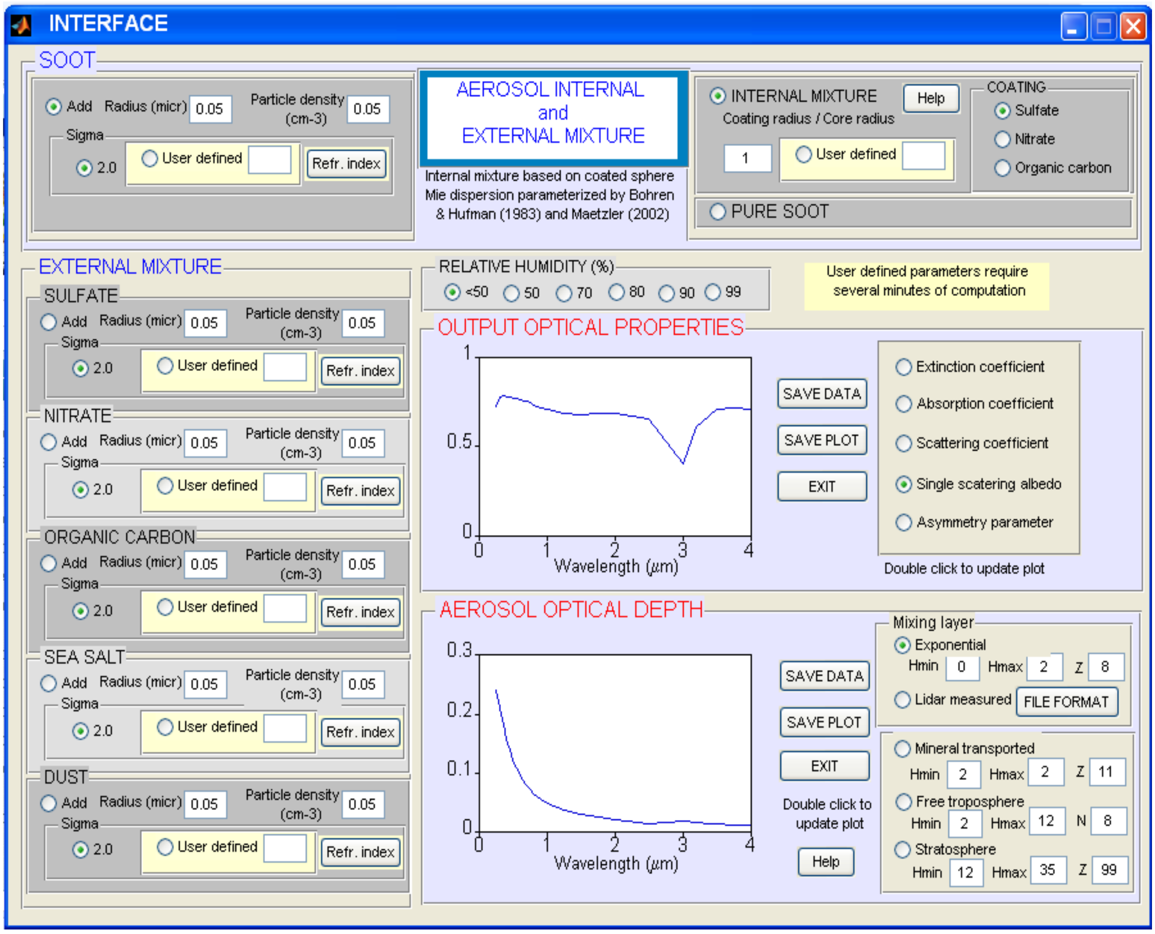

Fig.1. Screen capture of the user interface.

4. The interface

The interface has been designed in Matlab. A general view of the interface can be seen in Fig. 1, showing five main parts: (i) internal mixture of soot area; (ii) control of external mixture area; (iii) relative humidity selection; (iv) output optical properties; (v) aerosol optical depth calculation. The internal mixture of soot area allows the selection between pure soot or soot coated with one of the following components: sulphate, nitrate and organic carbon. The user must select the particle density as well as the parameters of the lognormal size distribution for soot (radius and width of the distribution σ).

Another possibility is to use the predefined values. For the core-shell model, the user can select the ratio of coating radius to core radius. The properties of the coating particle are selected in the external mixture area. The external mixture area controls the aerosol components included. For the selected aerosols, the user must introduce the particle densities, radius and σ of the lognormal distribution or to use the predefined values. The relative humidity selection determines the refractive index and the radius of the hygroscopic components (nitrate, sulphate and sea salt). In the output optical properties area the user can access the optical properties of the combination of the selected aerosol components. It is possible to plot the wavelength dependency of the selected aerosol property as well as save the data. Finally the aerosol optical depth area is designed to compute that aerosol parameter. For this, the user has to input the aerosol height profile in the mixing layer. There are two possibilities: (1) the user provides the minimum and maximum height of the mixing layer, and the slope parameter Z (in meters) of an exponential profile; (2) the user enters a lidar measured aerosol extinction coefficient.

5. Conclusions

The interface is intended to serve as a tool to users who need to describe the optical properties of aerosols for climate-modelling purposes. It therefore consists of a platform to calculate optical properties with easy-to-use software from input data or a set of predefined values, both for external and internal mixtures. Various user-defined combinations are possible and a set of typical mixtures is also provided. Combinations of different individual radiative calculations have the advantage of convenient use and also easy improvements. This can be done by changing the properties of single components. Particularly, we intend to include properties of non spherical aerosols particles instead of the results of Mie calculations for dust.

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