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Software Package for Aerosol Size Distribution

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Abstract: *The "Software Package for Aerosol Size Distribution" is a novel graphical user interface application software used for the study of atmospheric aerosol size distribution from various aerosol models (Continental clean, Continental average, Continental polluted, Urban, Desert, Maritime clean, Maritime polluted, Maritime tropical, Arctic, Antarctic) and/or with different aerosol components (insoluble, water soluble, soot, sea salt (accumulation mode), sea salt (coarse mode), mineral (nucleation mode), mineral (accumulation mode), mineral (coarse mode), mineral (transported), sulfate), as a function of radius. This article discussed about the atmospheric aerosol, aerosol size distribution and the software description. Application case studies to generate the aerosol size distribution for an urban aerosol model and with different components have also been presented in this note.*

Keywords—Aerosol, Size distribution, Lognormal, aerosol models, aerosol components, number concentration

1. Introduction to Atmospheric aerosols

Atmospheric aerosols are tiny solid and/or liquid particles suspended in the atmosphere. Aerosols vary considerably in shape, size, concentration and composition depending on (i) the strength and nature of sources, (ii) production mechanisms, (iii) the mixing characteristics, (iv) the dilution capacity of the air, (v) scavenging processes and (vi) background burden of particles. Aerosols of different sizes, magnitude and composition play a vital role in many atmospheric processes such as visibility, radiation balance, air pollution, atmospheric electricity, cloud formation etc. These are produced by natural or anthropogenic sources and can be transported to different regions depending upon the meteorological conditions. The sizes (radius 'r') of atmospheric aerosols extend over five orders of magnitude from 0.001 µm to 100 µm. Based on their sizes and production mechanisms, the atmospheric aerosol can be divided into (Figure 1)

- Nucleation mode (0.001 µm < r < 0.1 µm)
- Accumulation mode (0.1 µm < r < 1.0 µm)
- Coarse mode (r > 1.0 µm)

Size of aerosol is one of the most important parameters that determines its interaction with the solar and terrestrial radiation, and also affects the physical and chemical properties and their lifetime.

Atmospheric aerosols are produced by various processes of terrestrial and extra terrestrial origin. Depending on their source aerosols are classified as natural and anthropogenic (manmade). Windblown dust, pollen grains, sea salt particles, black carbon from combustion of fossil fuel or biomass burning emissions are directly injected into the atmosphere and hence they are known as primary aerosols. Several inorganic species in the atmosphere such as sulfates, nitrates etc. produced from precursor gases released into the atmosphere get converted into particles and these are known as secondary aerosols. Aerosols in the nucleation mode are formed mostly through gas-to-particle conversion processes. Usually nucleation mode particles are the most predominant in terms of number, however, due to their smaller size, these aerosols constitute only a few percent of the total mass concentration of aerosols in the atmosphere. Aerosols in the accumulation mode size range are produced either by coagulation of smaller particles or by heterogeneous condensation of gas vapor onto existing smaller nucleation mode particles. Coarse mode aerosols such as windblown dust and sea salt (produced by breaking of sea waves and bursting of bubbles) are generated by mechanical processes. Chemical nature of aerosols is mainly decided by their production source while the size distribution of aerosols depends on their production mechanism (Figure 2).

Depending on the size, the aerosols are removed from the atmosphere by coagulation, dry deposition, or wet deposition. Residence time of aerosols indicates the mean lifetime of particles in the atmosphere and depends on their size and altitude at which they are present. The residence time is of the order of few days within the atmospheric boundary layer, few weeks in free troposphere and few years in the stratosphere. Nucleation mode aerosols have higher rate of condensation growth and coagulation processes, resulting in their transformation into accumulation mode aerosols. The residence times for coarse (r > 10 µm) and small (r < 0.01 µm) particles are rather short compared to that of the particles in 0.1 µm to 1.0 µm range.

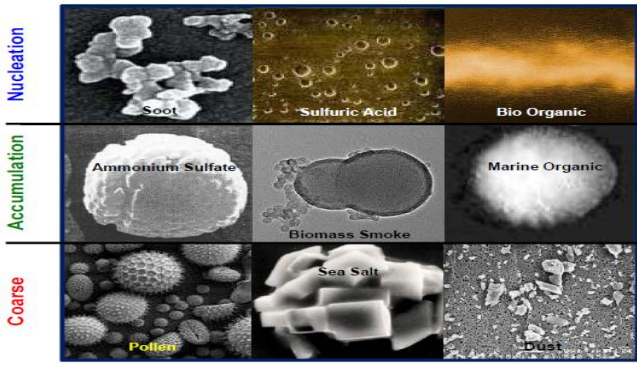

Figure 1: Different aerosol types in the nucleation, accumulation and coarse modes [1]

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2. Aerosol size distribution

The spread in the sizes of aerosols result from intricate processes by which the particles are produced, the interactions among themselves and removal processes. The spread of the atmospheric aerosols population over the vast size range is described by a size distribution function. It describes the number of particles per specified interval of radius. The various size distributions used for characterising the atmospheric aerosols are (i) Junge power law size distribution (ii) Lognormal size distribution (iii) Modified Gamma distribution (iv) Zold distribution. In the present work, the commonly used Junge power law and lognormal size distribution will be discussed and are used in the software package for aerosol size distribution.

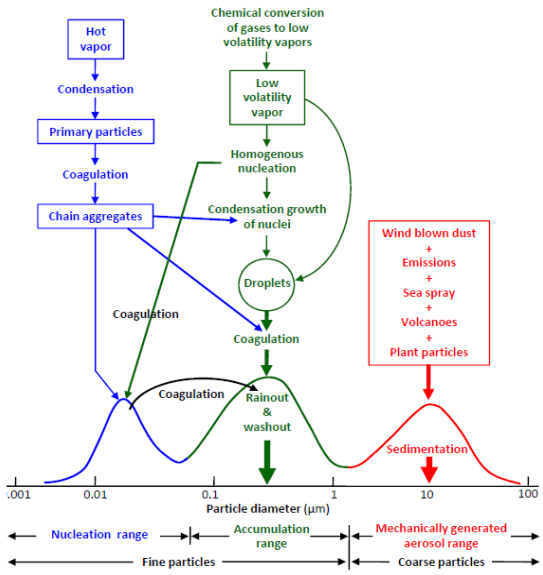

Figure 2: Schematic of an atmospheric aerosol size distribution as a function of particle diameter. Figure shows the three modes of aerosol distribution, major production and removal mechanisms [6].

Junge power law size distribution

Junge based on experimental observations, proposed a power law size distribution function of the form

$$\frac{dN(r)}{dLog(r)} = C\, r^{-\gamma}$$

where dN represents the number of particles with radii between r and r+dr, C and γ are constants. As γ value decreases the number of larger particles increases compared to the number of smaller particles and viceversa. The Junge power law size distribution assumes the aerosol number concentration decreases monotonically with increasing particle size. The power law is rigorously valid for all the wavelengths only if the particle size distribution is mono-modal. However, the Junge power law distribution is accurate only over a limited size range, and extrapolation to smaller or larger sizes may introduce significant errors of the ambient aerosol size distribution which is generally multimodal. Therefore, the Junge power law distribution is not appropriate for all environments and locations as well as in extended wavelength bands. The advantage of Junge power law size distribution is that the aerosol size distribution can be described from the knowledge of γ alone [5].

Lognormal size distribution

Atmospheric aerosol size distributions show modal structure and can be represented best by a lognormal size distribution function [3]. The lognormal distributions to describe the aerosol population can be given in terms of the number concentration, area, volume distribution or mass distribution. The aerosol lognormal number size distribution can be represented as

$$\frac{dN(r)}{dLog(r)} = \sum \left[\frac{N_i}{\sqrt{2\pi}\,\log\sigma_i}\right] Exp\left[\frac{-[\log(r) - \log(r)_{mi}]^2}{2\,log\sigma_i^2}\right]$$

where r_{mi} and σ_i are the mode radius and the standard deviation respectively of the i^{th} mode and N_i its total number density. For a mixture of particles originating from multiple independent sources, the resulting size distribution is a combination of all individual sources. Each component has its specific mode radius, standard deviation (σ) and total number density. The above equation, if summed for i = 1 to 3, represents trimodal distribution, which will have, three values of N_i, r_{mi} and σ_i. When i varies from 1 to 2, the resulting distribution will be bi-modal and when i = 1, it will be a monomodal size distribution. The log normal distributions to describe the aerosol population can be given in terms of the number concentration, surface distribution or volume distribution. Number distributions are for instance of interest when the ability of the aerosol to act as cloud condensation or ice nucleus are studied. Surface distributions are relevant when the radiative properties of the aerosols are of interest as the surface area of the aerosol determines the amount of solar radiation that it scatters. Volume or mass distributions are used to obtain information about the total mass of the aerosol in the atmosphere or the mass that is deposited. The surface area S(r) and volume V(r) size distributions are represented as

- $S(r) = 4\pi r^2 \left[\frac{dN(r)}{dLog(r)}\right]$
- $V(r) = \frac{4}{3}\pi r^3 \left[\frac{dN(r)}{dLog(r)}\right]$

The log normal distributions are best suited to characterise the aerosol components, the aerosol types and their spatial and temporal variability and hence it is widely used for tropospheric aerosol studies [5].

3. Software description

The "Software package for aerosol size distribution" was designed and developed in Microsoft Visual Basic 6.0, which is an event-driven object-oriented programming language and enables the rapid application development of graphical user interface (GUI) applications [2]. The present application uses DynaPlot ActiveX chart control component (DynaPlot v.3.7.4 from wilhelm-kurz-software) for real-time chart control. It features dynamic scaling of chart elements with control size, linear and logarithmic scaling, cursors and markers, scroll, pan, stacked zoom, auto scale, and original scale functions.

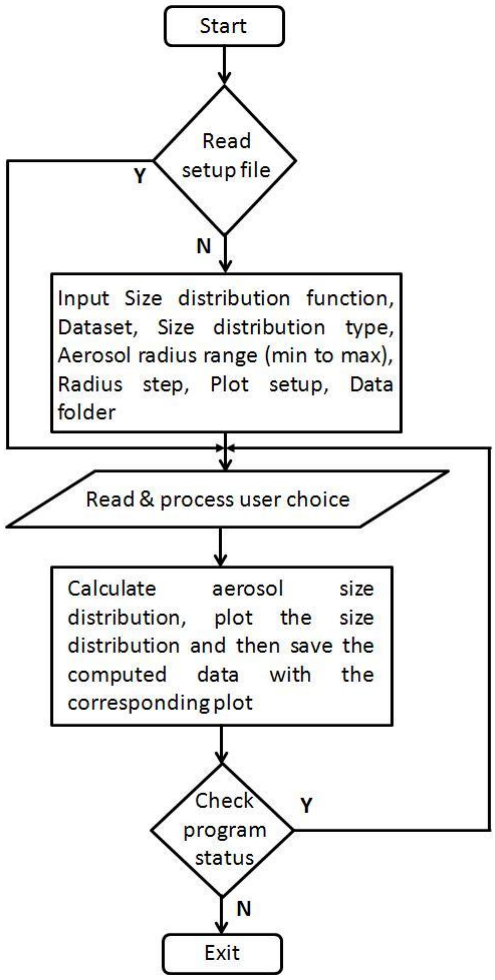

Figure 3: Flowchart for the software package for aerosol size distribution

The flowchart for the present work is shown in Figure 3. The GUI application software has five menus tab (1) Setup (2) Aerosol size distribution (3) Refresh (4) About (5) Exit, as illustrated in Figure 4. In order to run the application software, it requires a setup file "Setup.dat" which is configured by a user as per the objective and requirement (Figure 5). The various software configurable setup parameters are (1) Size distribution function: User can select either Lognormal or Junge power law distribution (2) Dataset: This is non editable combo box and is set to default as Hess et al. 1998 dataset (3) Size distribution: The user can choose Number, Surface or Volume size distribution (4) Aerosol radius range: The aerosol minimum and maximum radius (μm) are configured for the size distribution computations (5) Radius step: Aerosol radius increment step (μm) is used for aerosol size distribution calculation from minimum to maximum radius range with uniform radius step increment (6) Save plot: The online generated plot can be saved at the configured data folder (7) Plot X-axis range: The x-axis minimum and maximum scale can be set for the plots (dN/dLog(r) plot and dSordV/dLog(r) plot) (8) Plot Y-axis range: The y-axis minimum and maximum scale can be set for the plots (dN/dLog(r) plot and dSordV/dLog(r) plot) (9) Plot total mode: User can choose to plot only the total mode (10) Plot number SD: The user can configure the GUI to plot only number size distribution although surface or volume size distribution are computed (11) Select data folder: The default program and data folder path is "C:\ASD".

International Journal of Scientific Engineering and Technology (ISSN : 2277-1581)
Volume 2 Issue 4, PP : 249-255 1 April 2013

Figure 4: GUI application software default screen

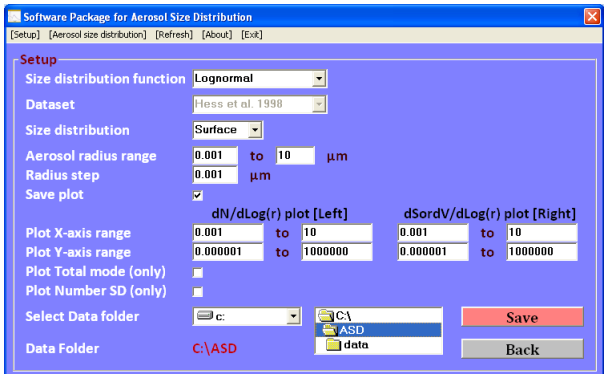

Figure 5: GUI Setup frame with Lognormal size distribution function

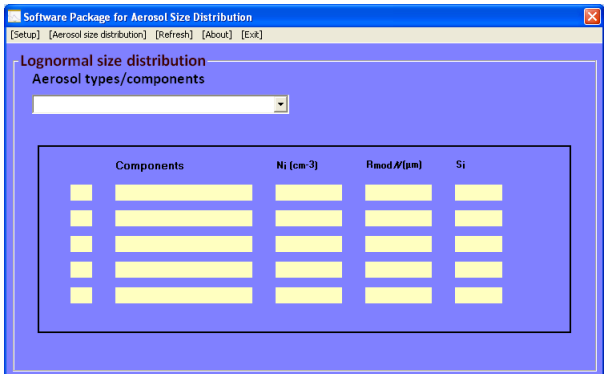

Figure 6: Lognormal size distribution frame with user selectable Aerosol types/components

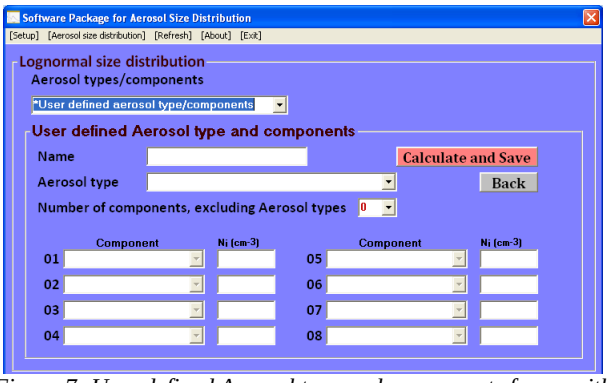

Figure 7: User defined Aerosol type and components frame with input fields

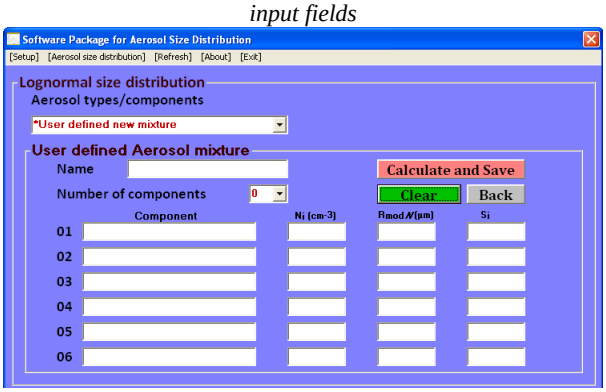

Figure 8: User defined Aerosol mixture frame with various input fields

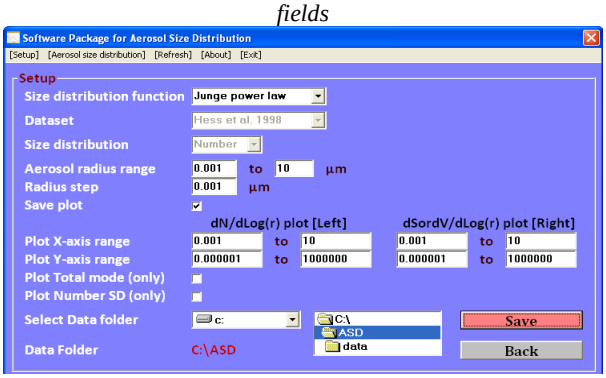

Figure 9: Setup frame with Junge power law size distribution function

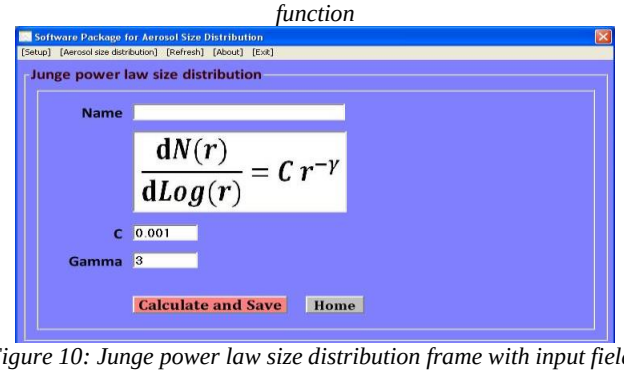

Figure 10: Junge power law size distribution frame with input fields

The Aerosol size distribution menu is the main thread of this application software. As per the user configuration it can compute aerosol size distribution based on Lognormal or Junge power law size distribution function. When configured for lognormal size distribution, user can select the Aerosol types/components from the dropdown combo box (Figure 6). The various aerosol types/components are (1) Continental clean (2) Continental average (3) Continental polluted (4) Urban (5) Desert (6) Maritime clean (7) Maritime polluted (8) Maritime tropical (9) Arctic (10) Antarctic (11) User defined aerosol type/components (12) User defined new mixture. When aerosol types/components 1 to 10 are selected, the application software computes the aerosol size distribution and displays the various aerosol components along with number concentration, mode radius and sigma. It also plots the aerosol size distribution on the screen.

When "User defined aerosol type/components" is clicked, the GUI displays a new frame titled "User defined Aerosol type and components" in order to configure the aerosol type and components (Figure 7). The user can choose the aerosol models as (1) Continental clean (2) Continental average (3) Continental polluted (4) Urban (5) Desert (6) Maritime clean (7) Maritime polluted (8) Maritime tropical (9) Arctic (10) Antarctic and the aerosol component as (1) insoluble (2) water soluble (3) soot (4) sea salt (accumulation mode) (5) sea salt (coarse mode) (6) mineral (nucleation mode) (7) mineral (accumulation mode) (8) mineral (coarse mode) (9) mineral (transported) or (10) sulfate along with its number concentration (cm^{-3}). When "Calculate and Save" command is executed it computes the aerosol size distribution, displays the plots in the graph section and saves the data in ASCII format.

When "User defined new mixture" is selected, the application software displays a new frame entitled "User defined Aerosol mixture" in order to configure the aerosol components (Figure 8). The user can create its own aerosol mixture comprises of various aerosol components. The aerosol size distribution can be calculated by clicking the "Calculate and Save" command button and after successful computation it displays the plots and saves the data in a file. When the software is configured to compute aerosol size distribution using Junge power law size distribution function (Figure 9), it enables "Junge power law size distribution" frame where user can enter the C and gamma values in order to calculate the aerosol size distribution (Figure 10). The GUI application software menu tab "Refresh" is used to reinitialize the program variables and reload the programs and the "Exit" menu is used to terminate the application software.

4. Application example and results

Atmospheric aerosols result from different sources and processes. At any place in the atmosphere there exists a mixture of particles of different origin. To describe the wide range of possible compositions, the aerosol particles are modeled as mixture of components [4]. We can study the various aerosol types (Continental clean, Continental average, Continental polluted, Urban, Desert, Maritime clean, Maritime polluted, Maritime tropical, Arctic, Antarctic) and its components (insoluble, Water soluble, soot, sea salt (accumulation mode), sea salt (coarse mode), mineral (nucleation mode), mineral (accumulation mode), mineral (coarse mode), mineral (transported), sulfate) using the "Software package for aerosol size distribution". As an application case study, we will run this software package to generate the Urban aerosol model components using Hess et al, 1998 aerosol dataset [4]. The size distribution of an urban aerosol model is made up of water soluble, insoluble and soot components. Table 1 illustrates the lognormal size distributions parameters for an urban aerosol model.

In the setup frame, configure the size distribution function as "Lognormal" and when the "Urban" aerosol types/components is selected in the "Aerosol size distribution" menu, the software display the various aerosol components along with the lognormal size distribution parameters (N_i is the total particle number density, R_{modN} is the mode radius and S_i measures the width of the distribution) used in an urban aerosol model (Figure 11). Figure 12 shows the lognormal size number distribution along with surface distribution for an urban aerosol model.

The main advantage of the present software is to study the aerosol size distribution from different sources (e.g., the dust, sea salt particles effect on the total aerosol size distribution over an urban location comprising of water soluble, insoluble and soot particles). In order to study the dust effect on an urban aerosol model, select the "User defined aerosol type/components" component in the "Aerosol size distribution" menu as illustrated in Figure 14. With the basic aerosol model type defined as "Urban" choose a dust component mineral (accumulation mode) with particle number density (124 cm^{-3}), the software computes the lognormal size distribution, logs the calculated size distribution data and display the aerosol size distribution plot (Figure 13).

Finally, in order to calculate the aerosol size distribution for various aerosol components, select the "User defined new mixture" option in the "Aerosol size distribution" menu (Figure 14). In the user defined aerosol mixture frame, define the number of aerosol components, total particle number density, component mode radius and width of the distribution. Figure 14 shows a new aerosol mixture defined as "Urban_user" with three components, soot, insoluble (IS) and water soluble (WS). In order to validate the newly defined aerosol mixture, the aerosol components and lognormal size distribution parameters were kept same as an urban aerosol model, software computes the aerosol size distribution for this newly defined aerosol mixture which is identical to an urban aerosol model size distribution. Figure 14 illustrates the user defined aerosol mixture and the size distribution plot which is identical to the urban aerosol size distribution in Figure 11.

Table 1: Lognormal size distributions parameters of an urban aerosol model [4].

Aerosol types	Components	$N_i(cm^{-3})$	r_{modN} (µm)	σ
Urban	Water Soluble	28000	0.0212	2.24
	Insoluble	1.5	0.4710	2.51
	Soot	130000	0.0118	2.00

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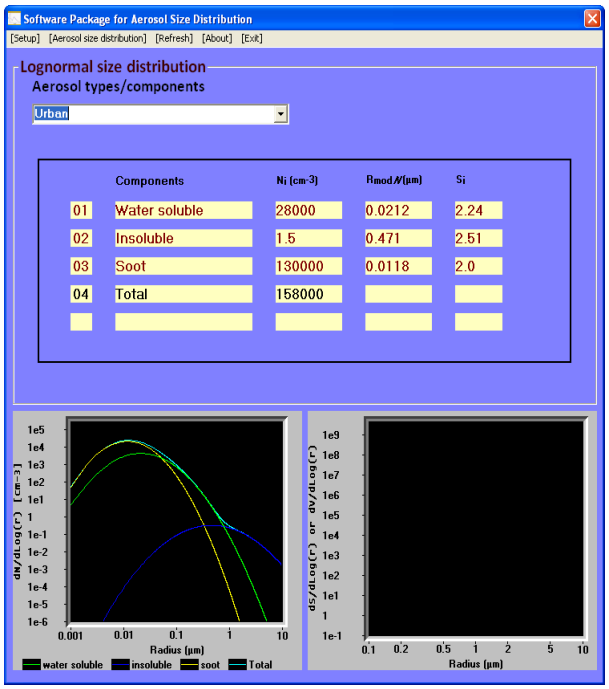

Figure 11: Lognormal size distribution data and plot for an urban aerosol model.

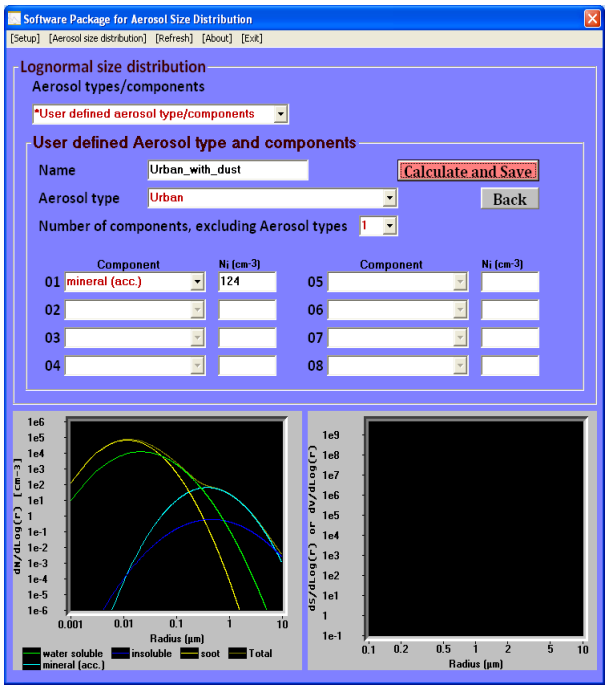

Figure 13: Lognormal size distribution for an urban aerosol model with dust component.

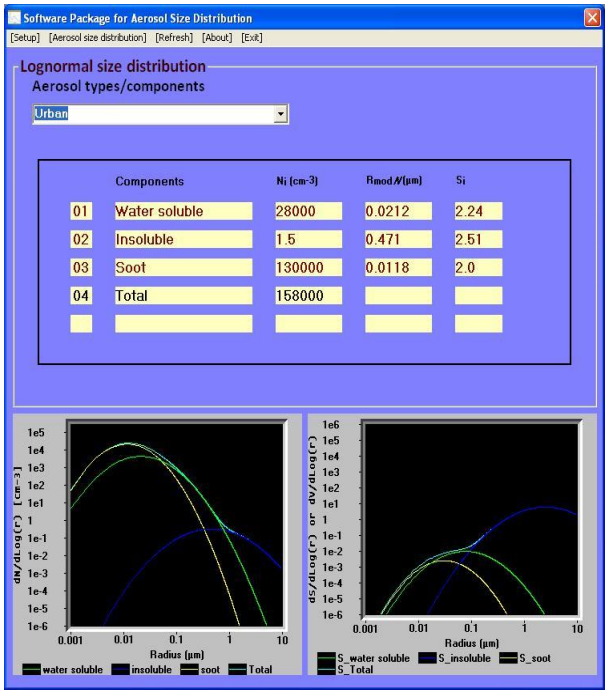

Figure 12: Lognormal size number and surface distribution for an urban aerosol model.

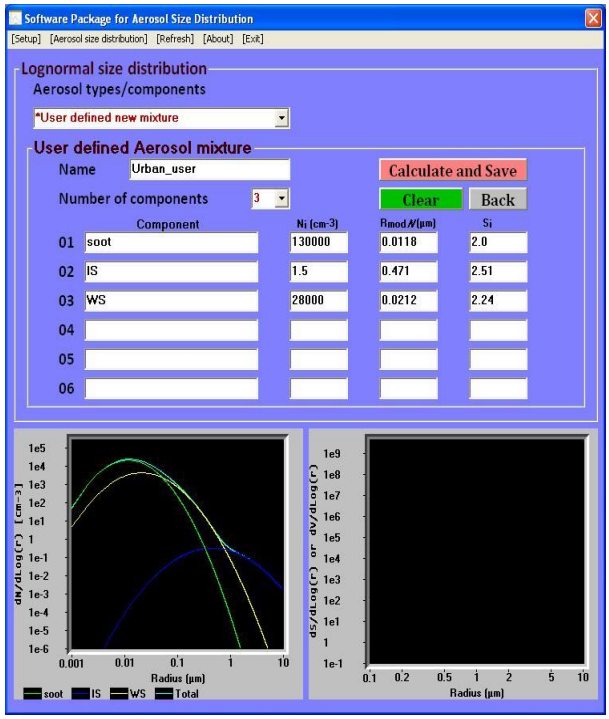

Figure 14: Lognormal size distribution for an urban aerosol model with dust component.

5. Summary

The aerosol size distribution is the basic aerosol parameter used in determining various properties of aerosols (for the known composition and physical state of aerosols). The software package for Aerosol Size Distribution can be used to study the atmospheric aerosol size distribution for various aerosol models (Continental clean, Continental average, Continental polluted, Urban, Desert, Maritime clean, Maritime polluted, Maritime tropical, Arctic, Antarctic) and/or with different aerosol components (insoluble, water soluble, soot, sea salt (accumulation mode), sea salt (coarse mode), mineral (nucleation mode), mineral (accumulation mode), mineral (coarse mode), mineral (transported), sulfate), as a function of radius. In addition to aerosol number size distribution the application software can also be configured to compute and generate aerosol surface or volume size distribution. The present software package uses Hess et al 1998 aerosol dataset for the computation of aerosol size distribution. However, it can also be configured to calculate the size distribution with user defined aerosol mixture with user defined aerosol components, total particle number density, component mode radius and width of the distribution. The software compute, plot and logs the aerosol size distribution data as a function of aerosol size (radius). It also can be configured to save the online computed aerosol size distribution plot along with the data in ASCII format. The GUI application software in the distribution package can be made available to any user on request. The present software uses Junge power law and lognormal size distribution functions, however, it can be upgraded in future for handling other size distribution functions like modified Gamma distribution, Zold distribution etc.

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6. Acknowledgements

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7. References

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