COMPLEX REFRACTIVE INDEX CALCULATION FOR SUB-MICRON AEROSOL USING A SIMULATED ANNEALING APPROACH

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INTRODUCTION

A retrieval algorithm is based on a specific inversion procedure providing an estimation of atmospheric parameters from their indirect measurement. This procedure defines the numerical strategy to be followed [1]. Here we apply a metaheuristic approach for estimating the complex refractive index for both an urban and a suburban site, with an inversion based on Simulated Annealing (SA), employing both Mie and Rayleigh scattering. La Merced site is an urban zone with a wholesale food market, characterized by an intense circulation of heavy duty trucks, buses, and light duty vehicles. Tula site is a suburban and agricultural zone near to a refinery, a power plant, cement plants, and open-sky mines. The data for the first site were obtained in Nov/2004. For the second site, experimental data correspond to MILAGRO campaign in 2006.

This optimization scheme is a Monte Carlo method suited for finding the global minimum of a non-linear error function, based on the analogy with the process of gradually cooling and annealing of molten metals. [2,3]

In this work, hourly sub-micrometer refractive index retrievals are presented for both sites as well as the estimation of the scattering coefficient for three chosen days for each campaign.

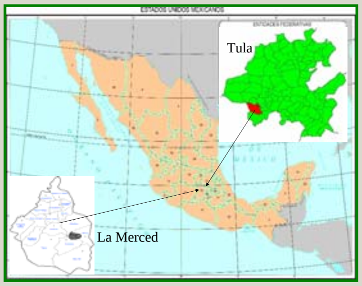

Fig. 1) Measurments sites

Fig. 2) upper: Nephelometer; lower SMPS

METHODOLOGY

Experimental data were collected from two sites in two different periods. The first data set was taken at La Merced site, a place located near the center of Mexico City, with light-duty vehicles and modern heavy-duty diesel buses [Vega, et al], from 11/26/2004 to 11/28/2004. The second experimental data set were from measurements carried out in Tula region at Hidalgo State in Mexico, during the MILAGRO campaign from 04//2006 to 11/28/200. In both sites were measured the number distribution by size, for submicron particles, using a Scanning Mobility Particle Sizer system (TSI, Inc.; model 3936 SMPS) in the range of 15–791 nm. This equipment supply particles mass and surface distribution too, assuming that these particles are spherical and they have a density of 1.2 g/cm^3. At the same sites a Model 3563 TSI Integrating Nephelometer was installed too, in order to measure the light scattering coefficients by atmospheric particles for wavelengths of 450, 550, and 700 nm.

The inversion method solves the first-kind Fredholm integral equation, $\int_0^\infty \pi r^2 Q_{sc}(\lambda, r) N(r) dr$,employing the experimental data of both Particle Size Distribution (PSD) and light scattering coefficient. Mie scattering were solved by means of the algorithm from Shen and Cai [4]. This algorithm is efficient and robust in a wide range for both, particle size and refractive index. However, since the SMPS spans for nanometric particles, Rayleigh theory was taken into account for particle size below 100 nm. In addition, because of both data sets were taken all day, here we show the hourly complex refractive index along the day for each one of the three wavelengths, for number distribution as a first approximation.

RESULTS

La Merced

$\int_0^\infty \pi r^2 Q_{sc}(\lambda, r) N(r) dr$

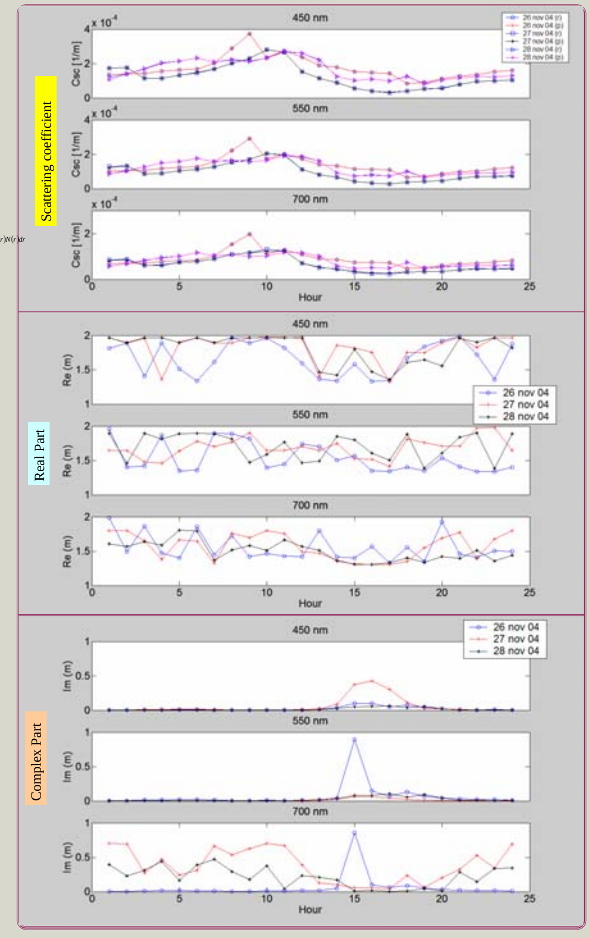

Fig. 3 , Upper) Scattering Coefficient; Middle) Real component; Lower) Complex component

Figures are organized as follows: the left ones show the results for La Merced site and those in the right, the results for Tula site. Both panels presents the results from three chosen days in each measurements campaign.

Data from both sites were chosen since in those days the data values were maximum, minimum and a combination of maximum and minimum in number for the PSD.

From the upper panels, it can be seen that the experimental **(r)** and the estimated values **(p)** show a very little difference. It means that the retrieved refractive indexes reproduced correctly the experimental light scattering coefficients. It can be noted that in both regions there are similar trends in early hours, and the increasing trends are slightly more pronounced at Tula for late hours.

The middle panels show that the real part fluctuates more at La Merced than at Tula. However, the trends for the scattering coefficients values from 11/26/04 and 03/28/06 are slightly similar at the first two wavelengths in the morning from 5 h to 10 h.

The lower panels show the behavior from the complex part of the refractive index.

Two similar trends are present at La Merced for 450 and 550 nm. The trends in the visible range show that at night the absorption decreases, which could be due to the presence of either, light organic material or sulphates [5]. In average, from mid-day to 19 hrs. the trend is well-defined, which may suggests particle growth since large particles may be dependent on the imaginary part of the refractive index [6].

Nevertheless, the results from Tula were greater than from La Merced, which could suggest that in Tula, particles have larger content of organic compounds. Also, the trends in Tula are present in early hours with a tendency to increase at night.

The aforementioned results could be representative for the period under study, since the Objective Function were always lower than the Nephelometer precision (1E-07), since even values up to 1E-30 were reached [8], as shown in Figure 5.

Tula

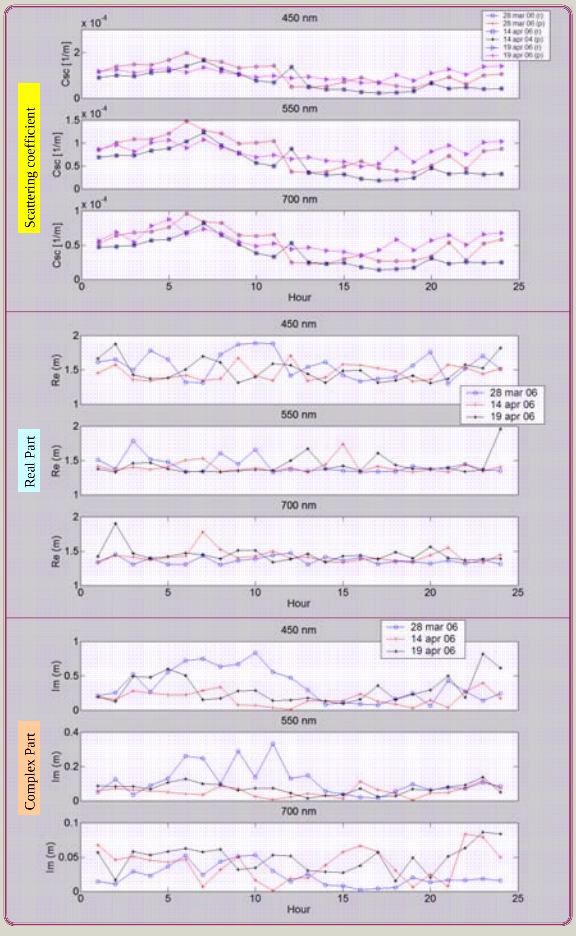

Fig. 4 , Upper) Scattering Coefficient; Middle) Real component; Lower) Complex component

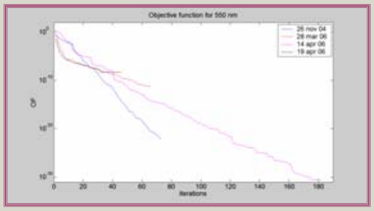

Fig. 5, Ojective Function for selected days at each site

CONCLUSIONS

1. Simulated Annealing yield representative results for both regions.
2. The hourly evolution along the entire day of the refractive index was obtained for both regions, which allows to consider its role in aerosols studies in a more detailed manner.
3. The refractive index could be related in a formal way to the chemical composition of the particles, for a specific hour of the day.
4. Since the imaginary part at Tula is bigger than in La Merced, then higher levels of organic compounds could be present in the former one.

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