# REFLECTANCE SPECTROSCOPY IN THE 400-2400 nm TO ASSESS SETTLED DUST IN DIFFERENT URBAN ENVIRONMENTS

E. Ben-Dor and A. Chudnovsky

Department of Geography and Human Environment, Tel-Aviv University,
Ramat Aviv, P.O.B. 39040, 69978, Israel
e-mail: chudnovs@post.tau.ac.il

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## ABSTRACT:

The aim of this study was to apply a spectral reflectance approach to account for small amounts of sediment dust in occupied homes. We examined the method's ability to predict the gravimetric weight of sediment dust particles solely from the reflectance data (400-2400 nm). Multivariate data analysis based on Partial Least Squares (PLS) regression was run to predict the dust loads solely from reflectance data. For both experiments use of difference index (when the dust trap background spectra was subtracted from the total measured reflectance) in the PLS analyses was found to demonstrate the best pre-treatment in PLS modeling. Maps of dust distribution, based both, on the reference gravimetric and spectrally predicted weight values was generated. Reasonable explanation was provided to the calculated distribution that can be further used by decision makers to improve the indoor life quality. We conclude that this methodology (simple and rapid in-situ spectral measurements with appropriate analyses), can be employed to assess dust in both indoor and outdoor environments (in small and high dust content). This information can be used for initial decision making, improving indoor conditions, and tracking dust contamination following environmental change.

## 1 Introduction

Today, the basic academic training related to indoor and outdoor air quality is within a single discipline and a new multidisciplinary paradigm is needed [1**].** The synergy of reflectance spectroscopy and multivariate statistical methods to quantitatively measure dust loadings could eventually become the preferred method for accurate, comprehensive, and almost real-time assessment of indoor-environment dust information.

Reflectance spectroscopy of solid particles in the Visible-, Near Infrared-, and Short Wave Infrared (VIS-NIR-SWIR) region is a well-known technique by which the chemical composition of many materials can be rapidly and quantitatively assessed [2, 3]. This method is known for its simplicity, accuracy, and ability to analyze many constituent components simultaneously. The constraints inhibiting the adoption of this method are 1) the relatively low sediment dust load that mask out the dust signals; and 2) the strong spectral responses of the target's background, that may be beyond the detection limit.

The total mass of dust particles settling in an indoor environment is an important parameter for estimating people's exposure to dust in both their residences and workplaces. Previously, we have developed a new and sensitive method aimed to assess the small amounts of artificial dust under laboratory conditions, using reflectance spectroscopy [4,5]. In this study we wish to (1) examine the potential of our method over an actual indoor dwelling environment; and (2) map the results of the gravimetrically measured and spectrally predicted samples in order to generate a pattern of settled dust distribution encompassing the study area.

## 2 Study Area

Two field experiments of one month length were conducted, one during the spring season (April 2005) and the second during the summer season (August 2005). Similar locations were used for the dust traps during the spring and the summer seasons, but, the summer experiment was expanded to a higher sample set. Forty-five dwellings from the northern and central parts of Tel Aviv city were sampled during April 2005, and one-hundred thirty five dwellings were sampled during August 2005. The traps (2-4 in each dwelling) were placed on flat surfaces (tables, shelves, and boxes) at a height of 1.3 m above the floor and positioned on surfaces where the column of air above the sampling surface was not obstructed, at least 0.5 m away from large electrical appliances (Edwards et al. 1998). Additionally, several traps were placed outdoors to identify the differences between the indoor and outdoor amounts of dust settled during both seasons.

## 3 Method

### 3.1 Dust Traps

We have found that the optimal configuration of a dust trap for spectral analysis is a glass disk (2 mm thick), with a black carbon background placed underneath. Measuring the reflectance of the dusty glass trap maximizes any meaningful spectral response of the dust mixture. Each glass trap was measured spectrally before and after exposing it to the dust in the indoor environment to enable precise identification of the spectral changes.

### 3.1 Gravimetric Weight Measurements

The traps were cleaned, numbered, and gravimetrically measured before and after they were exposed to the dust during the field study experiment, using a sensitive gravimetric weight with a precision of ±0.01 mg, and a maximal weighing capability of 60 g. The difference between the dusted and cleaned glass traps was calculated and used as reference values for the PLS modeling (Y-variable).

### 3.2 Spectral Measurements

Dust samples were scanned by the Analytical Spectral Devices FieldSpec Pro (ASD 2001) spectrometer with a total of 2100 spectral bands (350-2500 nm) by attaching the contact probe (‘potato’) device to the dust sample. The ‘potato’ was set on a stable tripod base and maintained in a constant position at a nadir-looking angle. BaSO4 was used as a white reference to calibrate the measurement data to reflectance values at the same angle. Additionally, each dust trap was measured gravimetrically using a sensitive analytical scale model Mettler AE163, with a precision of 0.01 mg, to enable us to compare the total amounts of dust that settled during each season.

Similarly to the reference gravimetric measurements, each dust trap was spectrally measured before and after the exposure to the dust.

### 3.3 Multivariate Modeling

The multivariate calibration models were calculated by Partial Least Squares (PLS) regression, with total dust loadings and NIR-SWIR spectra correlated. All data management, calculations and PLS analyses were performed using the Unscrambler software, Version 9.1 [33].

The difference between the predicted and measured gravimetric weights was expressed as a root mean square error of prediction. Root Mean Square Error of Prediction (RMSEP), and Root Mean Square Error of Calibration (RMSEC) are direct estimates of the prediction and modeling errors**,** expressed in original units. RMSEP is defined as the square root of the average of the squared differences between predicted and measured values of the validation objects:

$$RMSEP = \left[ \frac{\Sigma (X_m - X_P)^2}{n_v} \right]^{1/2} \tag{1}$$

where $X_m$ is the gravimetrically measured weight of a sample, $X_p$ is the predicted value of the sample on the basis of spectral analysis, and $n_v$ is the number of samples in the calibration stage [6].

The predictive capability of all models was compared in terms of the relative standard error for both calibration and validation sets (denoted as RMSEC (%) and RMSEP (%), respectively; see Table 3):

$$\%RMSE = \left[ \frac{\Sigma (X_m - X_P)^2}{\Sigma X^2{}_m} \right]^{1/2} \times 100 \tag{2}$$

The results of all spectral measurements were divided into three subsets: 1) A calibration set (training set) to establish the model; 2) a validation (test) set, to validate the model; and 3) the external test set (the second validation set), to examine the model’s predictive ability. A calibration set contained of 55 and 85 samples during spring and summer experiments consequently, validation sets comprised of 18 and 25 samples, and finally test sets comprised of 17 and 25 samples. In this way we were able to assess the predictive capability of the final model, and the ability of spectroscopy to quantify the small amounts of settled particulate matter.

In real world environments, reflectance spectra of dust particles may contain materials displaying various particle size distributions and mixtures of materials that may cause baseline shifts due to their reflectance properties. Different pretreatments are used to simplify the spectral signals in order to ensure stable calibration and improve the predictive ability of the final model. To eliminate undesirable variation in the spectral data, two types of pretreatments are commonly reported: differentiation and signal correction. Various orders of spectra derivatives are used to correct baseline variations. In the present case, first and second derivatives were used as pretreatments.

To minimize the effect of the glass background we calculated spectral ratio (RI) ($B_{ratio(\lambda)}$, Eq. 3) and spectral difference (DI) ($B_{\ dif(\lambda)}$, Eq. 4) indexes by calculating the apparent ratio or difference values for each waveband, taking the single-beam spectrum against that of the glass background, as follows:

$$\mathrm{RI} = B_{\ ratio(\lambda)} = B_{rad(\lambda)} \ / \ B_{\ background(\lambda)} \tag{3}$$
$$\mathrm{DI} = B_{\ dif(\lambda)} = B_{rad(\lambda)} - B_{\ background(\lambda)} \tag{4}$$

where:

$B_{\ rad(\lambda)}$ - reflectance of the mixture on the glass trap
$B_{\ background(\lambda)}$ - reflectance of the glass trap

The same pre-treatments that were applied on the raw spectra were tested also on the DI and RI indexes [6].

## 4 Results

During the spring, the gravimetric weight (90 samples) ranged from 0.01 to 3.5 mg, with an average of 1.7 mg. During the summer, the gravimetric weight (135 samples) was lower and ranged from 0.01 mg 2.5 mg, with an average of 1.1 mg. This difference may be explained by the large difference in the outdoor dust concentrations resulting from the spring dust storm events that are also partially expressed in the indoor environment. This suggests that outdoor dust has a significant effect on the indoor dust environment. An additional factor influencing the dust deposition loads is the influence of anthropogenic activity as well as the effect of crowding. Owing to the incomparable environmental conditions between the dwellings (open and closed windows, different indoor activities, etc.), it is impossible to make an unequivocal conclusion regarding the quantitative differences between settled dust among dwellings in similar locations.

### 4.1 Prediction of Gravimetric Weight for Field Survey

For both experiments the best-fit model for the calibration set is achieved when the difference manipulation is used. Applying this model to the external test set gave favorable predicted values, with a RMSEP of 7.2%, confirming the model’s relatively good predictive ability (Table 1):

| Model | Prediction on external test set | |
|---|---|---|
| **Spring** | RMSEP (%) | $r^2$ |
| DI | 7.2 | 0.93 |
| (DI)' | 10.3 | 0.90 |
| DI on 50 wavelengths | 10.8 | 0.90 |
| **Summer** | | |
| DI | 7.5 | 0.94 |
| (DI)' | 8.3 | 0.93 |

Table 1: Best results obtained for external test set prediction statistics resulted from different PLS models

The high predictive ability of the external test set, at the validation test set level, enabled us to conclude that the constructed PLS models can be used to precisely predict the gravimetric weight of loaded dust. Generally, the best model was obtained when DI was calculated and PLS calibration models were run on the full spectral range. Applying this model to the external test set gave favorable prediction values, with a RMSEP of 7.2% for spring and 7.5% for summer, confirming the model's confidence with only four PLS components (data not shown). The first four components in the PLS DI model explained 99% of the X variance (spectra), and 94% of the Y variance (weight). The score plot of the samples from the PLS modeling (figure not shown) was perfectly arranged along its axis according to their gravimetric weights, with a positive increasing. This indicates that most of the spectral variation is related to the settled dust that was modeled by PLS.

Figures 2-3 show the predicted versus the measured gravimetric values of the indoor dust for spring and summer consequently:

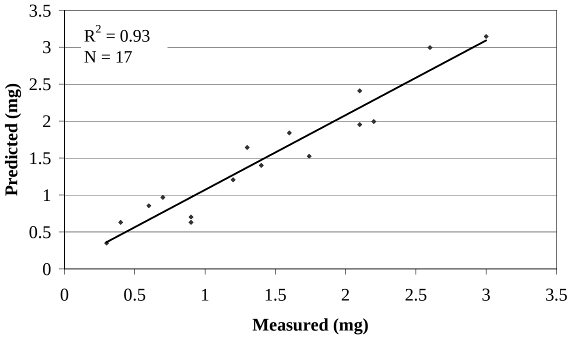


Fig. 2 Measured versus predicted gravimetric weights (run on the external 17 samples test set) accepted for spring.

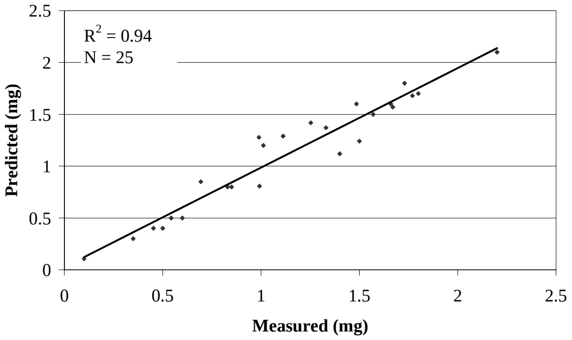


Fig. 3 Measured versus predicted gravimetric weights (run on the external 25 samples test set) accepted for summer.

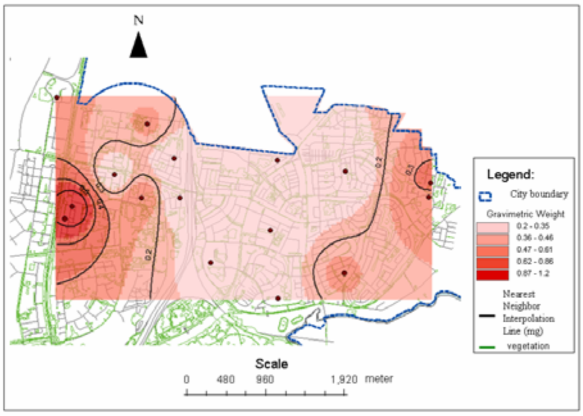
The results indicate that gravimetric weight can be predicted with a high confidence level solely on the basis of spectral measurements. Hence, many samples can be measured along large scale and in a very short time domain. RMSEP values for both experiments are quite impressive when taking into account the relatively small amount of settled dust with a narrow gravimetric weight of ±0.01 mg (min and max values are 0.12-3.5 mg for spring and 0.11-2.5 mg for summer).

## 4.2 Spatial Mapping of the Indoor Settled Dust Distribution

The maps were generated in order to demonstrate the powerful application of the multivariate spectral data modeling, facilitating the interpretation of the spectral measurements results. We used the IDW (Inverse Distant Weighted) Interpolation method within the Geographic Information System (GIS) (ArcGIS Geostatistical Analyses), the technique that calculates a grid value with the nearest real value, then produces specific, stepped contours [7].

For both experiments, Iso-Dust maps demonstrated that physical and anthropogenic factors plays an important role in total amounts of settled dust. Physical factors are the outside climate conditions, micro topography, wind regime and the distance from the Mediterranean Sea. Anthropogenic factors are the orientation of a building, the floor height, the inner structure of a dwelling unit, the density of the of the sampling location area, the "opening" of the dwelling to the oudoor environment, indoor antropogenic activity, and the existance of local sources of pollutants such as traffic and industry.

Figure 4 presents the settled dust distribution map, the *"iso-dust"* maps for Northern and Central Tel-Aviv Area during spring season:



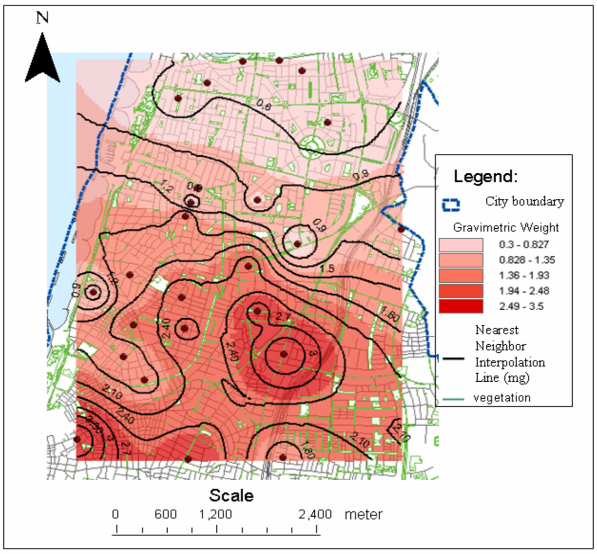


Figure 4: General spatial pattern of settled dust distribution based on the indoor environment measurements as obtained in Experiment 1: Northern (upper) and Central parts of Tel-Aviv (lower). Gravimetric weight of dust samples as a GIS layer was calculated based on the Nearest Neighbor Interpolation.

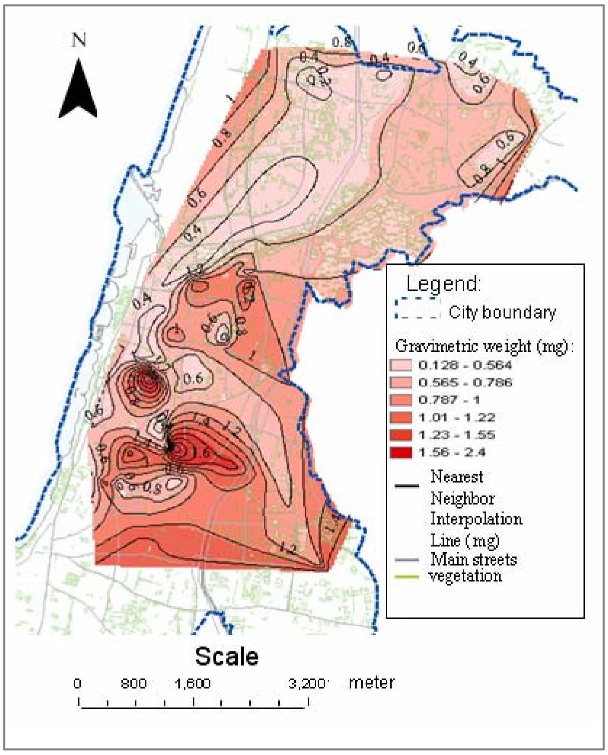


Fig. 5 Spatial Distribution of Indoor Settled Dust in Tel-Aviv during summer

As can be seen from Fig. 4, the map shows the existence of dusty areas in the urban environment. A careful examination of the iso-dust pattern reveals the following findings:

1) High amounts of dust were measured in high densely populated area, orientated to the road where at least half of a window was constantly opened allowing the fresh and polluted air penetrate the dwelling. On the contrary, sampling locations where the vegetation areas are prevealed, houses oriented to the vegetated inner side of a building characterized by low amounts of dust (under the same indoor conditions).

2) There is dinstinct quantitative difference between northern vegetated and central dense populated parts of the city. Higher amounts of dust were measured in central Tel-Aviv whereas northern part was characterized by lower amounts of dust.

3) Orientation of a dwelling has an inflence on the total amounts of settled dust. Among the dust samples from the central part Tel-Aviv area, sampls that were located at areas oriented to vegetatation or to inner side of a building (yard of a building) were characterized by lower amounts of dust (under the same indoor conditions, open, closed windows) than those oriented to the roads.

During summer experiment (Figure 5) different spacial pattern is readly observed:

1) It is clearly seen that higher amounts of dust are settled in the inner part of the city than in the vicinity of the sea shore. We may suppose that wind breeze that have mostly western direction transports dust in the urban area. In the central part of the city the wind is weaken by the densely populated buildings. Future study should explore the spatial pattern of the indoor settled dust distribution as a function of wind regime in the city.

During both experiments anthropogenic factors were found to be important. The most significant in our study area are the “opening” of the dwelling to the oudoor environment (open- closed windows), and the existance of local sources of pollutants such as traffic.

Several applicative conclusions may be proposed on the basis of the results of our study. For example: positive vegetative climate effects can be achieved by combining vegetation on walls, and around the buildings, better management of the indoor ventilation can improve the life quality.

## 5 Conclusion

It can be concluded that reflectance spectroscopy is sufficiently sensitive to detect very small amounts of dust in the real indoor environment. Since a low dust load is a much more interesting phenomenon than a high dust load (which is visible using many methods), we concluded that the presented method has high scientific merit as well as industrial applications. The method we have proposed can be utilized in a simple and low-cost mode and work under high power. Thus it can be made available to individuals, commercial organizations or governmental authorities to monitor different indoor environments. The extracted information can be used for initial decision making, improving indoor conditions, and tracking dust contamination following environmental change. We believe that the possibility of building a model or models (perhaps different for different seasons) that will give an immediate qualitative and quantitative answer regarding indoor dust conditions opens up new opportunities for more professional indoor environmental monitoring. With minor modifications, the method can be adapted for outdoor use, such as assessment of dust contamination in large areas during a short sampling time period.

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