Comparison of 2D & 3D parameter-based models in urban fine dust distribution modelling

This is an early draft version. It might be cited as: Ghassoun, Y., Löwner, M.-O. (2016): Comparison of 2D & 3D parameterbased models in urban fine dust distribution modelling. In: Lecture Notes in Geoinformation and Cartography, Springer.

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Keywords: Fine dust distribution modelling, 3D City Models, Land Use Regression Modelling

Abstract: In the present study two Land Use Regression Models for the estimation of urban fine dust distribution were established and compared. The first model used 2D parameters derived from an Open Street Map project data (OSM) and the second model used 3D parameters derived from a CityGML-based 3D city model. Both models predict fine-dust concentrations by using urban morphological (2D resp. 3D) and additional semantic parameters. The models were applied to a 2 km² study area in Berlin, Germany. The 2D-LUR model explained 84 % of the variance of TNC for the full data set with root mean square error (RMSE) of 3284 cm⁻³ while the 3D-LUR explained 79 % of the variance with an RMSE of 3534 cm⁻³. Both models are capable to depict the spatial variation of TNC across the study area and showed relatively similar deviation from the measured TNC. The 3D-LUR needed less parameters than the 2D-LUR model. Furthermore, the semantic parameters (e.g. streets type) played a significant role in both models.

1. Introduction and problem statement

Many epidemiological and toxicological studies have discussed the health effects of ultrafine particles (UFP) (WHO, 2013). These studies have proved that the particulate air pollution in urban area is associated with significant impacts on human health (Heal et al., 2012; HEI, 2013, Zhang, 2015) especially, among children who are the most susceptible group in regard to particulate exposure compared to adults (Burtscher, 2012). Ultrafine particles with diameter less than 0.1 microns often are the direct product of the combustion of fossil fuels by road transport (Geiser et al., 2005).

The UFP concentration can be estimated from measurements of the particle number size distribution. At street canyon or near traffic sites, the number of UFP generally accounts for the majority of total particle number concentrations, i.e., greater than 80 % to 90 % (Morawska et al., 2008; Weber et al., 2013). The combustion source air pollution, especially from traffic has been considered as the most significant factor of premature death where numerous toxic materials produced by combustion processes are in the ultrafine size range (Jerrett, 2011; Burtscher, 2012). Therefore, detailed assessment of exposure by measurement and modelling of fine dust distribution is necessary in the field of urban planning, traffic management and city system modelling.

UFP concentrations are affected by different sources of combustion, secondary production pathways that change their number, shape, size and chemical composition (Sabaliaukas, 2015). The spatial distribution pattern of urban UFP concentrations are mostly affected by the local wind field and, therefore, by different factors of the urban complexity, i.e., the urban morphology that influences it.

Urban morphology can be analyzed concerning geometrical properties of street canyons (Vardoulakis et al., 2002), building density, alignment of streets towards the prevailing wind direction, and characteristics of crossing sections (Brand & Löwner, 2014). Especially, the buildings structure is considered in addition of the meteorological factors the main parameters for modelling air ventilation (Wong et al., 2011). However, urban morphology has to be viewed as a 3D phenomenon.

Land use regression (LUR) models have been presented as a promising approach for the prediction of long-term, local-scale variation in traffic pollution and to obtain accurate, small scale air pollutant concentrations without a detailed pollutant emission inventory (Briggs et al., 2000; Brauer et al., 2003, Zhang, 2015, Ghassoun et al. 2015A). LUR models are multiple linear regression approaches that assume independent residuals and use GIS-based explanatory variables to predict pollutant concentrations at cer-

tain locations (Hoek et al., 2008; Mercer et al., 2011). They have been widely applied in cities of North America, Europe, and Asia (e.g. Arain et al., 2007; Kashima, 2009; Chen et al, 2010; Saraswat et al, 2013; Tang et al., 2013; Rivera et al., 2012; Abernethy et al., 2013). Different studies tried to enhance the LUR models by incorporating meteorological parameters (Arain, 2007; Chen, 2010; Kim, 2011; Zhang, 2015; Li, 2015).

Few studies used 3D spatial data to enhance the representation of land use (or the urban morphology) and the dispersion field in LUR, such as using the 3D data of building, street canyons and porosity, i.e. the chance for the air to pass through a building block, in LUR modelling (Tang, 2013, Ghassoun et al., 2015B) or examining the influence of different heights from ground level on the predicted values of PM2.5 (Ho et al., 2015). 3D parameters not only exhibited an enhancement of the LUR models but also simplify the models by using less parameter than 2D model (Ghassoun et al., 2015B).

Today, 3D city models for semantically enriched virtual 3D city models are increasingly available due to the standardization processes like CityGML (Gröger et al., 2012). However, until today no comparative study has been performed to evaluate the benefit of 3D parameters in the development of LUR for fine dust distribution modelling in urban areas.

Here, two LUR models were established and compared, the first model used 2D parameters derived from an Open Street Map project data (OSM) and the second model used only 3D parameters derived from a CityGML-based 3D city model. Both models predict fine-dust concentrations by using urban morphological and semantic parameters.

2. Methods and materials

2.1. Study area and data source

The present study developed LUR models for 25 sites in an area of 1*2 km in the City of Berlin City Fig. 1. The study area is characterized by street canyons with different traffic intensities and different microenvironment. Site positions were chosen to cover the whole study area at which mobile measurements of particulate air pollutants were conducted. At each site, the average concentration of total number concentration were calculated over 1 min. the measurements were carried out during 6 campaigns in winter (January 2015) during stable weather conditions without rain and low wind speeds < 4 ms⁻¹. Total number concentrations (TNC) were measured with a hand-held particle counter device (TSI 3007). The TSI 3007 is a fully battery operated handheld sensor for the measurement of particle number concentrations. The instrument detects particles ranging in size



from 10 to about 1000 nm. The concentration range is between 0 and 100,000 particles cm-3.

Fig. 1. Research area in "Berlin Mitte" and the 25 measurement locations.

To perform the parametrization of the urban morphology different data resources have been used in our study, Open Street Map and CityGML. OpenStreetMap (OSM) has been used to extract 2D and semantically data. The latter went into both, the 2D-based and the 3D based model. OSM is one of the most well-known data of a collaborative mapping project and it receives a huge amount of contributions from across the world (Jokar et al., 2015). It provides an abundant data source for geospatial data update. Many studies have tested the quality assessment of OSM data according to its completeness, temporal accuracy, thematic accuracy and positional accuracy (Ming et al., 2013). However, OSM is a function of contributor activity. Therefore, many studies represented that the degree and nature of such activity shows significant spatial heterogeneity. A main problem of using OSM data is that we have not enough information about the people who collect these data or the patterns of data collection and the data are not complete and comprehensive (Haklay, 2009). Haklay (2009) presented the satisfactory of using OSM for many application concerning the positional accuracy and completeness in major urban area and concluded that the OSM quality is beyond good enough. OSM data became not only a source for 2D data but also have been used to generate 3D city model by integrated the OSM data into the height information (Over et al., 2010). Here,

OSM data was only used to get the information regarding the streets and land use information.

CityGML (Gröger et al. 2012) as an international standard of the Open Geospatial Consortium (OGC) has been used to extract 3D for the second LUR model. It is a common information model and encoding standard for the representation, storage, and exchange of virtual 3D city and landscape models. It provides 3D geometric representations next to concepts for the representation of their semantics and their relations. CityGML is commonly accepted in the field of 3D city models; the number of available city models and their applications has increased significantly in the last ten years (r.f. Löwner et al. 2013). Applications that rely on CityGML are e.g. the Energy Atlas of Berlin (Kaden and Kolbe 2013), noise simulation and mapping (Czerwinski et al. 2013B). Here, CityGML data was used to extract the 3D information for the establishment of a 3D based model.

Volume of buildings have been calculated using an SQL script based on the migration script from 3DCityDB 2.x to 3DCityDB 3.x and explicitly adapted for the Berlin data (where thematically surface are used). The SQL-script cannot be applied without modification to other database with mostly only one roof surface for a whole building or no Ground- Wall- or RoofSurfaces is available. However, data inconsistencies have been ignored in this study. The volume calculation achieved 98.23 % of the whole buildings and only 25 buildings out of 1412 were left out due to error in their geometry probably. Changing the tolerance value from 0.0005 given in the original 3DCityDB to 0.01 did not bring any improvement. Therefore, the remaining building's volumes were calculated out of their height and area information. In addition, the output table contains the information about the measured height, maximum and minimum height. The volume of the trees has also been extracted out of the 3D CityDB data. Therefore, Oracle SQL Developer (free software) was used to export the results for using them in developing the 3D-LUR model.

3. Model developing

3.1. Geographical parameters

In order to compare 2D and 3D parameter-based models in the field of urban fine dust distribution modelling, distinction has been made between three types of parameters. First, semantical parameters have been used to describe none geometrically properties of the urban system. In our research, semantical parameters represent the attributes of different type of streets (primary, secondary, etc.) in the study area within different radii buffer. Street types serve as a proxy for traffic intensity. Therefore, they do not stand for a geometrically property but for additionally information and are classified as semantically. Here, these parameters will be extracted out of OSM data and used in developing both, 2D-LUR and 3D-LUR (rf. Tab. 1). Hence, the two models developed just differ in terms of dimensions of the geometric parameters.

2D parameters are exclusively used for the development of the 2D based model that has been used to compare with the 3D based model. The potential 2D parameters were extracted from OSM data using different radii buffer around each measurement site to reflect their spatial influence on the air pollution concentrations around these sites. They are described in Tab. 1, also.

3D parameters are used to describe the morphology of the urban area in 3D and its impact on the fine dust distributions and urban ventilation Tab. 1. They are used for development of the 3D based model, only. 3D parameters have been extracted to build a model that really incorporates f.i. local wind field as a function of the built environment. Parameters are extracted from a CityGML-based database. To use City-GML-based database within GIS environment, Feature Manipulation Engine (FME) have been used to transfer the data into shapefiles and Oracle SQL Developer software to export their attributes and then the traditional LUR circular buffer have been used to extract the 3D parameters and they can be described as following (rf. Tab 1):

- Height of the buildings adjacent to the street (H),

- Ratio of height and width of the street canyon (H/W),

- Volumetric density which describes the ratio of built volume and air (Vb),

- Volumetric tree density which describes the ratio of tree volume and the air (Vtree),

- Porosity, which is based on the input parameters of building volume, total areas and the height of the highest building within the buffer radii. It has calculated by the following equations of Burghardt (2015):

$$P_{h-var} = (AT * h_{UCL} - V) / AT * h_{UCL}$$

- Volumetrically averaged building height and it is calculated as following:

$$\boldsymbol{H} = \sum_{i=1}^{n} \boldsymbol{V}_i * \boldsymbol{h}_i / \sum_{i=1}^{n} \boldsymbol{V}_i$$

Sub-categories	Buffer Radii	Source	Methods
	[m]		
Length of different types of	50, 100 & 200	OSM Data	Using Esri's Model Builder: gen-
streets (Primary, Secondary,			erate buffer, intersect with the
Tertiary, Residential, living)			street, and summarize according
			the type of the street.
Total area of building	100, 200	OSM Data	Using Esri's Model Builder: gen-
Total area of different land use			erate buffer, intersect with the
			buildings, and summarize accord-
			ing the type of the building.
Distance parameters			The distance to nearest primary
			roads
Plan area ratio			$\lambda_p = A_f / A_T$
The height of the buildings (H)	50, 100 & 200	CityGML	
The ratio of height and width			
(H/W)			
Volumetric density (V _b).			
Volumetric trees density (V _{tree}).			
Porosity (Ph-var)			
Volumetrically averaged build-			
ing height (H)			
	Sub-categories Length of different types of streets (Primary, Secondary, Tertiary, Residential, living) Total area of building Total area of building Total area of different land use Distance parameters Plan area ratio The height of the buildings (H) The ratio of height and width (H/W) Volumetric density (Vb). Volumetric trees density (Vtree). Porosity (Ph-var) Volumetrically averaged build- ing height (H)	Sub-categoriesBuffer Radii[m]Length of different types of streets (Primary, Secondary, Tertiary, Residential, living)50, 100 & 200Total area of building Total area of building100, 200Total area of different land use100, 200Distance parameters100, 200Plan area ratio50, 100 & 200The height of the buildings (H) (H/W)50, 100 & 200The ratio of height and width (H/W)50, 100 & 200Volumetric density (Vb).Volumetric trees density (Vtree).Porosity (Ph-var) Volumetrically averaged build- ing height (H)100, 200	Sub-categoriesBuffer RadiiSource[m][m]Length of different types of streets (Primary, Secondary, Tertiary, Residential, living)50, 100 & 200OSM DataTotal area of building Total area of different land use100, 200OSM DataDistance parametersImage: Comparison of the buildings (H) The ratio of height and width (H/W)50, 100 & 200CityGMLThe height of the buildings (W) Volumetric density (Vb). Volumetric density (Vb).50, 100 & 200CityGMLPorosity (Ph-var) Volumetric ally averaged build- ing height (H)Image: Comparison of the building the set of the buildingImage: Comparison of the set of the

Tab. 1. List of used spatial parameters and their source next to their extraction method in Esri's ArcGIS 10.0.

3.2. LUR model using 2D parameters

A total of 22 2D parameters and 5 semantical parameters were included into the process of land use regression model and these parameters were grouped depending on the process impact on pollutant concentrations into three categories of emission, dilution and deposition. In our study, a model building algorithm described by Henderson et al. (2007) was used to build the LUR model for the fine dust concentrations according to the following procedures:

- 1. All variables were ranked by the absolute strength of their correlation with the measured pollutant.
- 2. The highest-ranking variable in each sub-category was identified.
- 3. Afterwards the variables in each sub-category that are correlated (i.e. Pearson's $r \ge 0.6$) with the most highly ranked variables were eliminated to avoid autocorrelation and collinearity.
- 4. All remaining variables were implemented into robust linear regression models.
- 5. Hence, variables that were not significant at a 90 % confidence level or that had a coefficient with a counter intuitive sign were rejected.
- 6. Finally, the last two steps were repeated to convergence.

Before applying the aforementioned procedures, buffers of different radii were generated for each measured site using ESRI's ArcGIS 10.2. All the available data (streets, buildings and recreational area) were extracted and stored in order to use them in the process of LUR model. Buffer radii of 50 m, 100 m, and 200 m were used to derive the length of streets, whereas buffers radii of 100 m, 200 m, and 300 m were used to derive the building area. Buffer radii of 500 m were used to derive the area of recreational area. Specify the buffer radii reflects the scale of environmental processes appropriate for each variable. For example, effects of emission from road traffic are typically localized, so the buffer radii should be small. The effect of land use are often more extensive and more complex, therefore, larger buffer radii might be used.

The most significant parameters were selected and used in the multi regression model in order to build the models for fine dust concentrations. The LUR model was evaluated using leave-one-out cross validation (in which one observation is left out in each iteration and the model was rerun and then used to predict the excluded observation) to confirm the model fit.

3.3. LUR model using 3D parameters

For the development of the 3D based model, the 3D parameters derived form CityGML-based database were extracted and transferred into ArcGIS. The 3D parameters, i.e. the height of the buildings (H), the ratio of height and width (H/W), volumetric density (V_b), volumetric trees density (V_{tree}), porosity (P_{h-var}), and volumetrically averaged building height (H)) were extracted within buffers of radii 50 m, 100 m and 200 m for each measured site. Volumetric density was calculated as a ratio of built volume and air. Air volume was calculated as a cylinder. The top surface of this cylinder is generated as a TIN surface represents the height of the buildings lying within a buffer around the site (V_b). Porosity is one of the roughness parameters and it is a measure of how penetrable the area is for the airflow (Gàl et al., 2009). It represents the correlation between the penetrable and impenetrable parts of an air layer over a certain area. It could be calculated as the ratio of the volume of the open air and the volume of urban canopy layer regardless the orientation. The volumetrically averaged building height can be calculated after determining the volumes and the heights of each building in each buffer. Trees are considered as passive controls in reduction of pedestrian exposure (Abhijith et al., 2015). Therefore, volumetric trees density was calculated as ratio of trees volume and the air volume was calculated same in volumetric density.

In addition semantical information as a proxy for traffic intensities have been extracted from OSM data. This is the sum of length of different type of streets within LUR buffers was used. Then, all the 3D parameters were entered into multiple linear regression and same aforementioned LUR procedures were used to select the most significant variables and implemented them in building 3D model for fine dust concentrations.

4. Results

4.1. Measurements

The descriptive statistics of the measured and modeled TNC for the study area are presented in (Tab. 2). Mobile measurements at 25 spots were conducted to analyze the spatial variation of TNC across the study area.

Mean of measured TNC concentration was 23569 cm⁻³ in ranging from 14332 cm⁻³ at sampling spot 13 to 40972 cm⁻³ at sampling spot 9.

Generally, it is evident that the minimum concentrations were at the measurement spots close to park place while the area close to the major roads with high traffic intensity were characterized by highest concentrations.

	Meas.	2D-LUR	3D-LUR	
Mean (cm ⁻³)	23569	23569	23292	
SD (cm ⁻³)	7148	6558	6262	
Max (cm ⁻³)	40972(9)	38016(9)	34579(9)	
Min(cm ⁻³)	14332(13)	14586(13)	14731(16)	

Tab. 2. Descriptive statistics of measured TNC concentrations and TNC output from 2D-LUR and 3D-LUR models. Values in brackets represent corresponding sampling points.

4.2. Comparison of 2D & 3D models

27 parameters were extracted from the data available and the final 2D-LUR model included parameters that incorporated site position, length of primary and residential streets, width of the streets and commercial and residential land use. Each parameter took the expected sign and matches the predefined direction of effect. Width of the streets and the length of primary streets (semantic parameters that represents high traffic intensity) within 100 m buffer resulted with higher TNC concentration, whereas commercial land use within 500 m buffer resulted in lower TNC concentrations. Fig. 2 depicts the standardized regression coefficients and the influence explanatory parameters on the dependent parameter. The standardized coefficients of each parameter used in the final 2D-LUR and their errors are presented in Tab. 3.



Fig. 2. Corresponding standardized regression coefficients for 2D-LUR model.

Standardized coefficients:					
Source	Value	Standard error	t	Pr > t	
Υ	1.142	0.414	2.761	0.013	
Primary100	1.480	0.578	2.560	0.020	
Resid50	1.057	0.219	4.827	0.000	
Comercial500	0.442	0.309	1.433	0.169	
Width	-2.045	0.596	-3.429	0.003	
Residential500	-0.718	0.191	-3.752	0.001	
R ²	0.84				

Tab. 3. Model coefficients for 2D-LUR model.

The 2D-LUR model expressed 84 % of the variance of the measured fine dust concentrations with root mean square errors (RMSE) of 3284 cm⁻³. Fig. 3a shows the plot of measured TNC concentrations against predicted one and the model gives the evidence for a linear trend with no outliers.



Fig. 3. Plot of residuals between measured and predicted TNC a) 2D-LUR model, b) 3D-LUR model

In contrast, 35 parameters were extracted from the 3D data and 5 semantical parameters available and the final 3D-LUR model included only the most significant parameters that incorporated length of secondary and tertiary streets, the ratio of height and width of the street canyon and volumetric trees density. Also, the parameters reflect the direction of their influence of the TNC. The secondary streets within 100 m buffer and the ratio of width and height of the streets resulted with higher TNC concentration, whereas tertiary streets and volumetric trees density within 50 m buffer resulted in lower TNC concentrations.

Fig. 4 shows the standardized regression coefficients and the influence explanatory parameters on the dependent parameter. The standardized coefficients of each parameter used in the final 3D-LUR and their errors are presented in Tab. 4.



TNC / Standardized coefficients

Fig. 4. Corresponding standardized regression coefficients for 3D-LUR model.

|--|

Standardized coefficie	ents:			
Source	Value	Standard	t	Pr > t
		error		
W_H200	0.410	0.117	3.495	0.002
Tertiary50	0.313	0.105	2.973	0.008
V.tree ratio50	0.299	0.115	2.600	0.018
Secondary100	0.675	0.117	5.789	< 0.0001
R ²	0.79			

The 3D explanatory parameters show a high auto-correlation therefore, many parameters could not show there influence in predicting TNC concentrations and they have been deleted during the LUR processing.

The 3D-LUR model explained 79 % of the variance of the measured fine dust concentrations with root square error (RMSE) of 3534 cm⁻³. Fig. 3b shows the plot of measured TNC concentrations against predicted one and the 3D-LUR model gives the evidence for a linear trend with no outliers too. The 2D-LUR model showed slightly better performance in predicting the fine dust concentration in comparison of the 3D-LUR model. In both model, the semantical explanatory parameters show significant impact on the final 2D and 3D models.

Standardized deviation for 2D-LUR accounts to 14 % and it was calculated by the ratio of the RMSE to the average measured TNC concentration across the study area. The visual errors were illustrated in Fig. 5a and it shows that 2D-LUR model predicts the TNC concentration very well in most of the sites and the large errors between measured and predicted TNC account on the site spots 11and 3, where the blue area represent the pixels that have the maximum error between the measured and predicted TNC values.

The standardized deviation for 3D-LUR accounts to 15 %. 3D-LUR shows a very slight deviation in most of the measured sites comparing to 2D-LUR and Fig. 5b shows a large error of predicting TNC on the spots 1 and 14.



Fig. 5. The visual RMSE in each site station between the measured and predicted TNC concentration for a) 2D-LUR model and b) 3D-LUR model.



Fig. 6. IDW interpolation illustrates map of TNC concentration resulted from a) 3D-LUR and b) 2D-LUR models in comparison with c) the measured TNC.

Mean absolute deviations between measured and modelled TNC concentrations were calculated for the 2D-LUR and 3D-LUR. Generally, 2D-LUR shows smaller deviation than 3D-LUR and is characterized by a deviation of 22 % while the mean absolute deviation for 3D-LUR turns out with 23 %. Leave-one-out cross validation was applied to validate both 2D-LUR and 3D-LUR models estimation. The deviation for 2D-LUR model accounts 17 % and it is relatively close to original model, while the deviation for the 3D-LUR model accounts to 18 %.

Inverse distance weighted interpolation was carried out for the TNC data and the results indicate that both models generally show a similar spatial distribution of modeled TNC Fig. 6. The Highest TNC concentrations are distributed on the main road intersections where traffic lights and high traffic intensities.

5. Conclusion

To predict the TNC concentrations and their variation across the study area in Berlin, Germany three kinds of parameters were used in order to build an LUR models (the semantical parameters, 2D parameters and 3D parameters). Both models show approximately similar results and are able to depict the variance of TNC concentrations and the residuals for both models appear to behave randomly, it suggests that the model fits the data well. However, the 3D-LUR needs less parameters than the 2D-LUR and the parameters show similar significant values where the 2D-LUR parameters show big variance of influence on getting the best model. The high autocorrelation among the 3D parameters has a negative role on presenting the strength of some parameters in predicting TNC.

In this study the 3D parameters have been used as static parameters without taking into account the interaction between these parameters and the meteorological parameters such as the wind direction and its correlation with the porosity and that lead us to consider it as a dynamic parameters. We believe that the use of this approach can result an enhancement of the traditional LUR model or the LUR model that use 3D parameters. The LUR is temporally static and trained by urban morphology parameters.

As further work, we believe that LUR can be used with meteorological data or with spatial parameters that interacts with the meteorological data in order to make it dynamic. Also, the combination of traditional LUR and the urban ventilation are our promising approach for enhancing the model.

Acknowledgment

We acknowledge the support of Stephan Weber from the institute of geoecology of the Technische Universität Braunschweig for the supply of the measurement device that was used to perform this study.

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