Selecting a fast air quality calculator for an optimization meta-model

L. Aleluia Reis[1], D.S. Zachary[1], U. Leopold[1] & B. Peters[2]
[1]*Resource Centre for Environmental Technologies, Public Research Centre Henri Tudor, Luxembourg.*
[2]*Faculty of Science, Technology and Communication (FSTC), University of Luxembourg.*

Abstract

Air pollution models have been developed over the last few decades, ranging from large detailed models, involving complex physical-chemical phenomena, to less detailed models. Air pollution models can also be grouped according to their scale. The air quality model, AYLTP, to be presented in this paper, aims at a spatial grid specificity that falls outside of the typical air quality scales approach. This model requires a spatial domain of approximately 100 km $\times$ 100 km, a spatial grid spacing of approximately 100-500 m, a time step of 10 minutes and a temporal domain of 24 hours. Moreover AYLTP requires a fast core calculator, as it will be incorporated on the Luxembourg Energy and Air Quality meta-model (LEAQ), which is built in an optimization framework. This paper aims at selecting the most suitable code to serve as a core calculator to be incorporated in AYLTP. A set of criteria was established to carry out an analysis of different open source air quality models suitable for the LEAQ meta-model. The selection of the models was based on a space-time graph. For each model, areas of influence were determined, based on the assumption that for a fixed CPU time, the grid spacing increases with the spatial domain size. Two models, AUSTAL2000 and METRAS, fit the required criteria. The choice between these two models was based according to the model's flexibility in terms of resolution and CPU performance. In this paper we briefly review the LEAQ project and discuss the criteria used to find a suitable core calculator. AUSTAL2000 is the model that better suits the criteria due to its simpler characteristics and faster transport calculator.

Keywords : Meta-model, air quality model, Scales, model comparison

1 Introduction

Air quality is directly related to emissions, air transport and pollutants chemistry. The complexity of the phenomena influencing pollutants concentrations call for the use of modeling tools, termed air pollution models.

This paper presents the ideal attempt to improve the performance of the AYLTP prototype (TAPOM-Lite) [1], by adding the effects of terrain, turbulence and improving the influence of the meteorological factors. The goal of this paper is to find an air quality model, to serve as a core calculator which in turn would be embedded in the AsYmptotic Level Transport Pollution Model (AYLTP).

The Luxembourg Energy and Air quality meta-model (LEAQ) consists of two models, an energy model, GEOECU (Geo-Spatial Energy Optimization CalcUlator), and an Air quality model, AYLTP. The two models are coupled by an optimization routine called OBOE (Oracle Based Optimization Engine) which uses an Analytic Center Cutting point Method (ACCPM) [2]. The energy model, is by itself an energy optimization model which calculates the lowest cost energy arrangement with emission and energy constraints, e.g. demand, operational, technological and seasonal, etc.. ACCPM is used to determine an optimal solution for the meta-model. The energy model passes the total cost (objective) to ACCPM, via the procedure called the Oracle. ACCPM uses the objective as well as directional information, termed subgradients, to guide the method to an optimal solution. Subgradients are defined as the sensitivity of change of total cost per change in employed technological device [3]. External constraints, breaches of air quality over maximum allowable levels, are also used as directional information by ACCPM. For each iteration of the optimization routine, the objective and subgradients are then used to calculate new levels of maximum primary emissions levels. The entire process is repeated until a lowest cost energy solution is determined by GEOECU and no air quality breaches are found. Finally a lowest cost energy solution with air quality constraints is achieved.

By their nature, both models are distinct, therefore they have different temporal and spatial scales. GEOECU produces emission data for a 30-40 year time period with a few years time step, e.g. 5 year time steps. This emission value will be distributed over periods of 24 hours for a typical and worst day of a season. The emission distribution will be done according to land use and scheduled corresponding to each economic sector daily emissions profile. Economic sectors are defined as groups of economic activities that share a common feature in terms of the spatio-temporal distribution of their total emissions for example transportation, industry, residential, and commercial.

In the atmosphere, phenomena occur at various scales, although for practical purposes, there is a need to develop specific-scale models. A specific-scale approach allows approximations and parametrization of the different phenomena at different scales [4]. For example, urban scale models include the effects of topography and land-sea-breezes. Smaller scale phenomena such as turbulence, are naturally treated by local scale models. The AYLTP model incorporates large scale characteristics including topographic effects and small scale characteristics such as turbulence. These characteristics, added to the fact that the model must run fast, make the selection of the core calculator challenging. The analysis of the suitability of the most appropriated model is a separate project itself. Therefore this paper presents a simple procedure to guide the AYLTP project in the right direction.

2 AYLTP design

The development of AYLTP rises from the need of an air quality model with specific requirements. AYLTP is connected to an optimization routine that iterates several times until it finds the optimal solution. Potentially, AYLTP model needs to be run approximately 1000 times (30-50 iterations times the number of subgradients). Practically, the air quality model must be run, using no more then a few minutes.

2.1 AYLPT requirements

Generally, air quality models involving detailed chemical reactions are CPU expensive [5]. In order to meet this demand, AYLTP is designed to calculate only the slow ozone reactions, i.e. asymptotic ozone levels. Accordingly, the fast photochemical equations are omitted. Particularly, this will be done using the core calculator, that will calculate ozone using the tabulated asymptotic ozone level for each time step. The 24 hour air quality result is based on the average primary emissions from each five year technoeconomic period of the energy model. Approximations are therefore acceptable. As the GEOECU model predicts for such a long term the whole meta-model has inherently large uncertainties associated with long time scales. Consequently, a highly accurately, CPU costly air quality model would not be required in this application. Accordingly, emissions of the most problematic pollutants will be included, such as NO_x, VOC, SO_2, CO, CO_2, PM_{10} and $PM_{2.5}$, and photochemistry for ozone. Furthermore, AYLTP will treat transport and diffusion of pollutants, turbulence and meteorology and dry deposition.

Despite the need for a simple air quality calculator, this model will include the most significant meteorological factors. The improvement of the meteorological package is important for photochemical reactions. Hence this package will include wind direction and speed, solar irradiation, humidity and temperature.

Air pollution is intimately related with meteorology. Wind can force the movement of the pollutants and affect their mixing ratios by accelerating or slowing the chemical reactions between pollutants. Radiation influences the photochemical processes that generate ozone. Atmospheric stability, is important in the dispersion of the pollutants and influences the chemical reactions. The above relations will be addressed in the model. Turbulence, is also important in fluid flow thus, this model attempts to incorporate turbulence in a very simple way.

The model is currently being constructed for Luxembourg, but it will be applicable to any other city. Luxembourg is a country of small dimensions with irregular terrain. Terrain irregularities play an important role in air flow phenomena. In order to have a good understanding of pollutant transport over Luxembourg, a grid domain of 50 $\times$ 80 km with a 100-500 m resolution will be applied. The border regions of the neighbouring countries need to be included in the simulation.

Terrain features will be incorporated due to its importance considering 3D wind fields. The SRTM (Shuttle Radar Topographic Mission) 90m Digital Elevation Data is available on a global scale, with a average resolution of approximately 90 meters [6]. The availability of such a detailed topographic information, is one of the reasons for the choice of the target grid spacing (100-500 m). A summary of the AYLTP requirements is shown in Table 1. The list of requirements are those which would be applicable to a general city/region.

2.2 Inputs and Outputs

As inputs, the model requires emission values, terrain and meteorological information. GEOECU will output emission values for each of the pollutants considered. Land use maps will be used to distribute these emission values over space. Emission values will be distributed according to economic sectors. The emissions will be scheduled accordingly to the daily profiles of each sector. Even tough the time step strongly depends on the input data available, a 10 minute time step is targeted, because is the time required to track the slow photochemical reactions. Table 1 summarizes the AYLTP inputs.

The model outputs 3D hourly concentration maps for each pollutant for 24 hours period. As the meteorological input represents a typical meteorological day and the daily profile scheduling represents a typical emissions day, the output will represent the 'typical' air quality levels related in a certain energy scenario arrangement.

Table 1: AYLTP requirements and inputs

AYLTP Requirements	
Spatial Domain	100 km × 100 km
Horizontal resolution	100 m to 500 m
Vertical resolution	20 layers
Temporal Domain	24 hour
Temporal resolution	10 min
N^o of cells	20 000 000 cells
CPU time	few minutes, no more then 30 min
AYLTP Inputs	
Meteorology	Wind speed and direction, solar irradiation, humidity, temperature, atmospheric stability
Terrain	Terrain elevation profile
Land use	Urban, agriculture, industrial and transport
Emissions	Sectoral emissions calculated by GEOECU

Atypical days with poor air quality will also be simulated. Air quality values, averaged over a threshold 60 ppb (AOT60), will be spatially calculated and air quality breaches will be addressed. Furthermore, 3D wind fields will be plotted as well.

3 Core calculator selection

Air pollution modeling is a growing research domain, its applications have been used to support environmental management [4]. There exists a wide range of air pollution models. A review on open source air pollution models was carried out in order to choose the most appropriate code as a basis for AYLTP. The review was based on the list provided by the Model Documentation System [7] developed at the Aristotle University of Thessaloniki and on the COST 728/732 Model Inventory [8].

The model selection was based on a space-time graph. All the graphs presented in this paper were built using R [9]. First, the spatial and temporal scales as well as the resolution were evaluated. Air pollution models can be classified according to their scale focus. Figure 1 shows a comparison between the local, urban and mesoscale models and the AYLTP required scales. AUSTAL2000 was also included in Figure 1 because it was the final choice core calculator. Figure 1 shows that AYLPT does not completely match any of the scale classification models. The spatial domain of AYLTP falls in the range of urban to mesoscale models, whereas the resolution is typical of a local scale model. All these specificities called for a different selection approach of a core calculator.

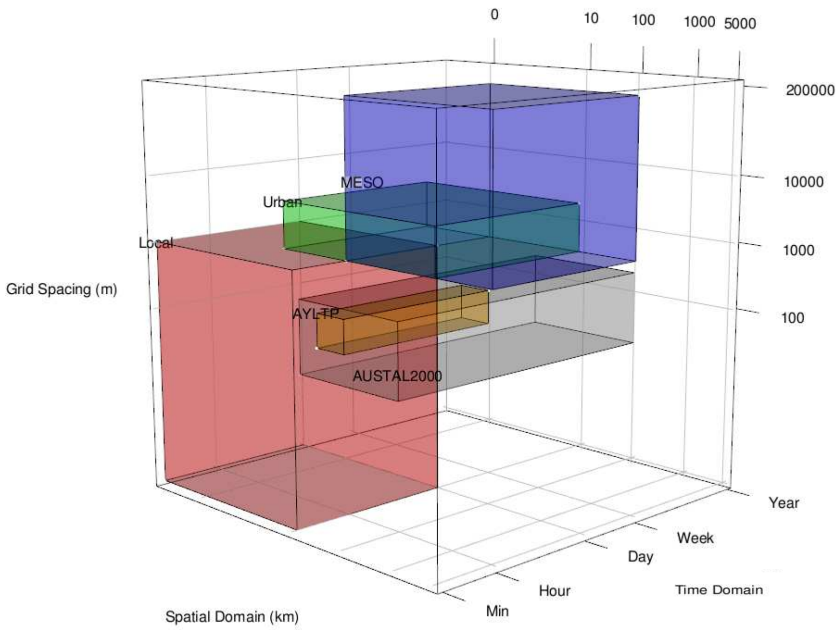

Figure 1: Schematic representation of air pollution models' scales. Red represents local scale models, green represents urban scale, blue the mesoscale. Orange stands for the AYLTP and gray describes AUSTAL2000.

The analysis of the criteria was made graphically (Figure 2). The graph was constructed using the range of spatial domain and resolution found for each model. Only the open source models were included in this selection process. The models in which the information about the spatial and temporal scale was not available are not shown. In this analysis it is assumed that the grid spacing increases linearly with the spatial domain increases when keeping the CPU time constant.

Thus instead of a range box, a triangle is used to convey this relationship. The triangles show that the smallest grid spacing available for each model is in fact not applicable for all domain sizes, if one imposes the constant CPU constraint. In practice, imposing a CPU time constraint, the combinations of grid spacing and spatial domain available lie on the shaded area above the triangle's hypotenuse.

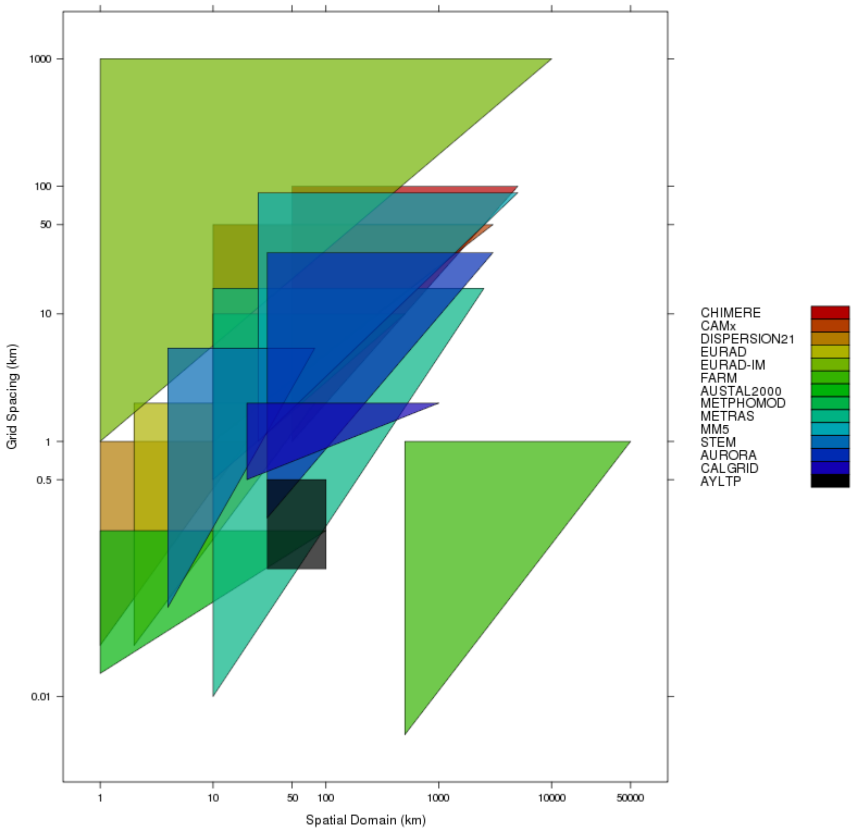

Figure 2: Compilation of models' spatial applications. The black point represents an example of how for a certain domain, the grid spacing applicable lies on the shaded area about the horizontal line.

Taking the FARM model as an example, symbolized by the black point in Figure 2. Assuming a spatial domain of 10 000 km, the grid spacing applicable, in practice, would be the range from the horizontal line that crosses the black point up to the top of the shaded area. The same type of analysis can be carried out for grid spacing, i.e. for a certain desired grid spacing, the maximum domain size that can be applied lies on the point where the horizontal line crosses the triangle hypotenuse.

4 Results and comparison

One observes that AUSTAL2000, and METRAS are the models that overlap the AYLTP box. Likewise one may observe that the model AURORA also overlaps the AYLPT range. However the CPU time found for AURORA, for a simple grid (60×60×35) for a month calculation, on a Intel Xeon 2GHz, is on the order of 70 hours [7]. As a result of the selection process, two models, AUSTAL2000 and METRAS, were found to be the best suited to serve as a core calculator (Figure 3). Both models overlap the AYLTP range, although none of them can, for a fixed CPU time, run with the largest domain and the highest resolution. Therefore, an extended analysis on these two models was carried out. A time step and time domain graph was built. Figure 3 shows the time criteria for the two models and its relation with AYLTP time requirements. Neither METRAS nor AUSTAL2000 overlap AYLTP range, though AUSTAL2000 touches the left upper limit of the AYLTP box. This means that the smallest time step allowed by AUSTAL2000 is the highest allowed by AYLTP. Thus, given a fixed CPU time AYLTP could be run with AUSTAL2000 smallest time step, but only for a time domain of one hour. Then METRAS model's time characteristics are quite different from the AYLTP requirements. The METRAS model's smallest temporal domain is equivalent to the largest of AYLTP and the time step falls under AYLTP requirements. Both models fit the spatial prerequisites, the main difference between them is their fluid motion approach. AUSTAL2000 is a Lagrangian particle model while METRAS is an Eulerian model.

The METRAS model calculates atmospheric flows, mesoscale effects, transport of pollutants and deposition of species. It contains turbulence, it can handle a complex terrain and chemistry. Eulerian models use a 3-dimensional computational grid. For each grid cell the mass balance of incoming and outgoing fluxes of the pollutants is calculated, solving the advection diffusion equation.

AUSTAL2000 is a Lagrangian particle model the official reference model of the German Regulation on air quality control [10]. It simulates the trajectories of tracer

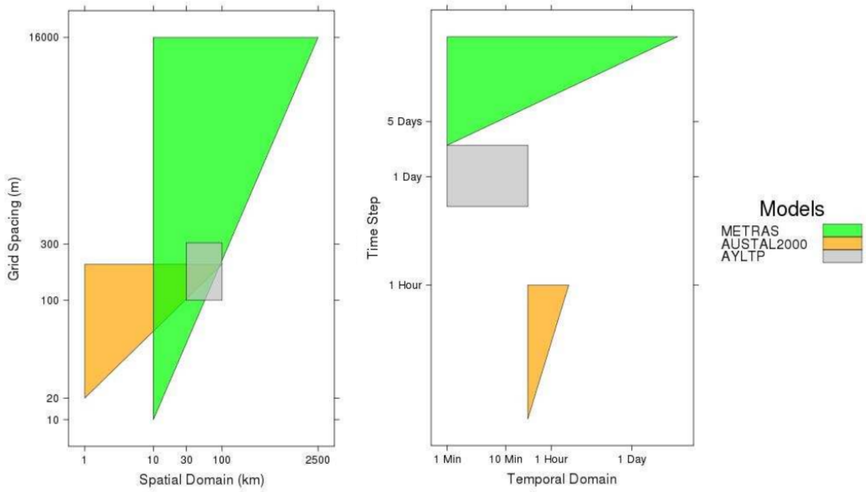

Figure 3: Spacial (left figure) and temporal (right figure) comparison of METRAS and AUSTAL2000 models with AYLTP.

particles immediately instead of investigating the fluxes. This approach offers in general more flexibility and precision in modelling the physical processes involved [11]. It simulates transport by the mean wind field, dispersion in the atmosphere, sedimentation of heavy aerosols, ground deposition and chemical conversion of NO to NO_2. The effect of turbulence on the particles is simulated by a random walk model [11].

Comparing the two models, regarding the AYLTP targeted processes, one observes that METRAS model is more complete, including all the aimed features. Thus, it uses rather complex chemical and dry deposition mechanisms. Nevertheless, ozone chemistry needs to be implemented in AUSTAL2000. The issue arising from this analysis is to decide between the simplification of the chemistry module of METRAS or the implementation of a simplified chemistry package for AUSTAL2000.

As mentioned above CPU time is a key factor for this project. Flexibility is another important issue, as the LEAQ meta-model is meant to be applicable to any city. Hence, a flexible grid spacing is desirable. This point is important when one takes into account the availability of the different quality input information for each city, and the city's dimensions and terrain particularities.

AUSTAL2000 uses a faster methodology to calculate pollutant's transport, whereas reliable numerical schemes, used in Eulerian models, are CPU expensive [12]. Concerning chemistry, AUSTAL2000 only yields a very simple NO to NO_2 conversion. Likewise, Lagrangian dispersion modeling is not based on the advection diffusion equation, but simulates the trajectories of a sample of particles. This approach is simpler and CPU inexpensive [11]. The particle approach yields more flexibility, because for a fixed grid spacing and spatial domain, it still allows the adjustment of the number of particles. This adjustment enables a compromise between statistical uncertainty and CPU time, tuning the number of particles[13].

In this sense, AUSTAL2000 better serves the purpose of this work. Its approach is faster and the model structure involves less parameters, thus is more readily adaptable. Nevertheless, it has some disadvantages, mainly because the Lagrangian particle approach is less flexible when dealing with chemistry.

4.1 A trade-off between accuracy and calculation time

This meta-modeling approach has inherently large uncertainties associated with it, which are propagated along the meta-model. Another parallel project will be carried out with the focus on uncertainty propagation through LEAQ [14]. As explained above, AYLTP is an air quality model embedded in a optimization framework. Despite the attempt to include the most important factors influencing air quality, a compromise between CPU time and accuracy had to be performed. Hence, phenomena are treated on a simple level, and more complex physical and chemical interactions are ignored. Typical meteorological scenarios are assumed as being representative of a season. The air quality model is dependent on the energy model, which calculates the energy scenarios for a five year interval. Accordingly, certain assumptions and simplifications can be done.

4.2 Core calculator adaptations to AYLTP

The AUSTAL2000 calculator has some of the requirements already implemented including: turbulence, dry deposition and the inclusion of the species SO_2, NO_x, $PM_{2.5}$ and PM_{10}. Full inclusion into the AYLPT model will require a simple chemistry module, involving the relation of NO_x and VOC in ozone formation. This will be done in a simple way, using an asymptotic level of photochemistry. The number of sources allowed is limited in AUSTAL2000, for input format reasons, thus modifications are needed to make this parameter flexible. The model also needs to incorporate the following species: VOC, O_3 and CO. The pollutant CO_2 is a output of GEOECU model, but it will not be incorporated in AYLPT, as it is its quantitative emission value that is important for decision processes. The meteorology already accounted in AUSTAL2000 includes the wind direction and speed and the atmospheric stability. Therefore, the effect of solar irradiation, temperature and humidity, will still need to be implemented.

5 Conclusions

The increasing concerns with air pollution and the strict EU legislation has triggered the development of a wide number of air quality models. A variety of models are currently available and deal with different scales and parametrization levels according to their scope of application. The LEAQ project requires an efficient air quality model. The AYLTP prototype, embedded in LEAQ, is now under development and a well suitable air quality core calculator is being selected. The spatial domain of AYLTP falls between urban and mesoscale. However, the resolution is typical of a local scale model. A set of criteria has been established to help select the core calculator. The criteria included spatial and temporal domain, resolution and CPU time. Two open source models were found to be suitable for AYLTP specificities. The choice was made based on less expensive CPU demands and spatio-temporal characteristics. The Lagrangian approach, AUSTAL2000, was chosen because it tends to have lower CPU demand and offers a larger flexibility regarding calculation time and resolution scale. The incorporation of AUSTAL2000 in AYLTP will require adaptations. The adaptations will include a fast ozone calculator module, adaptation of the time step, introduction of the species VOC, O_3 and CO, and improvement of the meteorological package. The meteorological package will include wind speed and direction, solar radiation, humidity and temperature. The selection of the most suitable model is a time demanding task, the procedure used in this paper is a simple approach to guide the project in the direction of the LEAQ requirements.

Acknowledgments

We acknowledge FNR - Fonds National de la Recherche Luxembourg for the grant founding, AFR - Aide à la Formation-Recherche, under the grant identifier PHD-08-004. We also would like to thank the LEAQ research team. We acknowledge, as well, Professor Dimitris Melas from the Aristotle University of Thessaloniki and Dr. Ulf Janicke from Janicke Consulting, for the useful comments.

References

[1] Haurie, A., Zachary, D.S. & Sivergina I., A Reduced-Order Photo-chemical Air Quality Model, 2003.

[2] Carlson, D., Haurie, A., Vial, J.P. & Zachary, D., Large-scale convex optimization method for air quality policy assessment. *Automatica*, **40(3)**, pp. 385–395, March 2004.

[3] Drouet, L., Beltran, C., Edwards, N., Haurie, A., Vial, J.P. & Zachary, D., An oracle method to couple climate and economic dynamics. *The Coupling of Climate and Economic Dynamics Essays on Integrated Assessment Series: Advances in Global Change Research Coupling Climate and Economic Dynamics*, eds. A. Haurie & L. Viguier, Kluwer, volume 34, 2005.

[4] Moussiopoulos, N., *Air Quality in Cities*. Springer, 2003.

[5] Grell, G., Duddhia, J. & Stauffer, D., Ncar mesoscale model(MM5). Technical Report NCAR/TN-398+STR, NCAR, 1994.

[6] CGIAR - Consortium for Spatial Information (CGIAR-CSI), *SRTM 90m Digital Elevation Data, VERSION 4*. http://srtm.csi.cgiar.org/, 2008.

[7] Moussiopoulos, N., MDS - Model Documentation System. http://pandora.meng.auth.gr/mds/, 2009.

[8] COST 728/732, *COST 728/732 - Model Inventory*. http://www.mi.uni-hamburg.de/Summary-Tables.510.0.html, 2007.

[9] R Development Core Team, *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2009. ISBN 3-900051-07-0.

[10] Consulting, J., TA Luft / AUSTAL2000, 2009.

[11] Janicke, L., *Lagrangian dispersion modelling*. 235, 37-41, Particulate Matter in and from Agriculture, 2002.

[12] Mathur, R., Hanna, A., Odmanm O., Coats, C., Alapaty, K., Trayanov, A., Xiu, A., Jang, C., Fine, S., Byun, D., Schere, K., Dennis, R., Novak, J., Pierce, T., Young, J. & Gipson, G., The Multiscale Air Quality Simulation Platform (MAQSIP): Model Formulation and Process Considerations. Technical report, arolina Environmental Program, University of North Carolina at Chapel Hill, 2004.

[13] L. Aleluia Reis, U.L..B.P., D.S. Zachary, Selecting a fast air quality calculator for an optimizations meta-model. *Air Pollution XVII*, ed. V.P. C.A. Brebbia, WIT Press, 2009.

[14] Zachary, D. & Leopold, U., The unLEAQ project, UNcertainty analysis for the Luxembourg Energy Air Quality project, a Luxembourg national research (FNR) proposal. Technical report, Public Research Centre Henri Tudor, 2009.