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# A fast air quality model using Look-up tables to address integrated environmental assessment model requirements.

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**Abstract:** The use of integrated assessment models (IAM), which combine models from different fields, raises the need for developing specific modelling concepts in order to provide results to support policy decisions within a reasonable time frame. Air quality policy support systems have been evolving towards the use of integrated assessment models that relate technologies (emitting sources) with air quality levels. Existing photochemical air quality models are not directly suitable for integrated assessment as they are time intensive in terms of input preparation and simulation speed. The objective is to present a methodology to reduce the computational burden of photochemical models, using pre-tabulated values of first order reaction rates. This approach was designed for the Luxembourg Energy and Air Quality (LEAQ) assessment model. It combines the air quality model with a technoeconomic model which computes ozone precursors emissions coming from energy consumption (e.g. traffic). The models are coupled via an optimization approach, which minimizes the total energy cost for a given ozone level. We have used an adapted version of AUSTAL2000, as a transport calculator and coupled it with a fast photochemical module, the AsYmptotic Level Transport Pollution (AYLTP). AYLTP consists of a Look-Up Table (LUT) of linear reaction coefficients. The LUT has been built using a box model by simulating a large set of possible combinations of meteorological variables and precursor concentrations. The ozone concentration variations are then obtained using the rate coefficient that is utilized to affect the mass carried by the Lagrangian particles. The loss of accuracy inherent to this approach is acceptable given the reduction of CPU time. The development of such methodologies is important when considering IAM. The use of linear reaction rates obtained with the help of the LUT represents an innovative step towards the use of simplified air quality models that involve complex chemistry.

***Keywords:*** Integrated assessment models; Fast air quality models; Photochemistry; Look-up tables; LEAQ

## 1 INTRODUCTION

Air quality (AQ) is, nowadays, a subject of major concern. Moreover the European Environment Agency reports for important damages on human health, climate and ecosystems due to air pollution, e.g. eutrophication, acidification and vegetation degradation.

The more and more rigorous air quality standards and regulations require structured answers from the policy makers. The current legislation in force in Europe still poses a problem for the members states, which report every year still a large number of exceedances. The EU states in the European Environmental Agency [2011] that: “European policies and measures increasingly seek to maximise co-benefits, managing air pollutant and greenhouse gas emissions at the least cost to society”. Integrated assessment models (IAMs) have been developed to answer these needs, connecting the economy with different fields of environment, to study the efficiency of environmental policies. Decision makers have become more exigent in demanding more integrated technical support, and air pollution is emphasize as one of the environmental factors to be accounted in urban planning. Consequentially, integrated assessment models that use air quality models, have emerged and became more common.

An IAM combines the knowledge coming from different scientific fields in order to provide knowledge that cannot be provided by a single disciplinary approach. IAMs have both of the following characteristics: (i) provide added value compared to single disciplinary models; and (ii) supply technical information for decision makers Rotmans and Asselt [1996]. Likewise, IAMs using air quality models, aim at solving problems related to air pollution and an emitter element. The IAM links human and natural aspects related to atmospheric pollution, though a common component: emissions.

Despite the influence of meteorology, air pollution is highly dependent on emissions. On the other hand, emissions depend on the implementation of technologies over many years such as power plants, industry facilities and cars. Therefore the implementation of air quality policies must be designed for long time-horizons. Pollutant concentration reductions are undertaken via emission reductions, however for some pollutants the relation between emissions and concentrations is not direct. That is the case of ozone, a secondary pollutant which is formed by its precursors - $NO_x$ and VOC - in the presence of sunlight. Ozone concentrations must be controlled via the abatement of the emissions of its precursors, even tough this relation is non-linear. That is the reduction of $NO_x$ emission does not always lead to a decrease in ozone levels. Ozone concentrations will increase or decrease with the reduction of $NO_x$ depending on the VOC/$NO_x$ ratio.

Air quality-IAMs can be used in *simulation* or *optimisation* mode. In a *simulation* mode, the sub-models of the IAM are run subsequently to assess the air quality impacts of a socio-economic scenario. Accordingly IAMs which run in *simulation* mode are useful to assess the response of air quality to policy scenarios. This mode allows the use of complex air quality models yielding a detailed view of the future. This mode is the most used, however it is not able to assess the best policy for a given air quality threshold, Carnevale et al. [2011]. On the other hand the *optimisation* mode determines the best policy amongst a set of possible policies. The “optimal” policy is found by solving an optimisation mathematical problem, such that a given set of constraints are met.

## 2 LEAQ - The Luxembourg Energy Air Quality model

The Luxembourg Energy-Air Quality model (LEAQ, `http://crteweb.tudor.lu/leaq/`), developed by the Centre de Recherche Public Henri Tudor, is an air quality integrated assessment model designed for the Grand Duchy of Luxembourg, Zachary et al. [2009, 2011].

Carlson et al. [2004] applied an air quality integrated assessment model in optimization mode to the Geneva canton. The LEAQ model is based on the same integrated assessment architecture and operating mode. The goal of LEAQ is to built an integrated assessment policy support tool for Luxembourg that is able to run both in simulation and optimization mode. The model permits users to explore possible long term policy measures for Luxembourg. On the assumption that LEAQ is run in simulation mode the outcome is the quantitative evaluation of a policy measure in terms of air quality and cost. Whereas in case it operates in optimization mode, the outcome will be the most cost-effective policy measure that satisfies the air quality standards, Zachary et al. [2011]. Therefore allowing to assess efficient policy strategies guiding policy makers towards a structured economic development. For these reasons the LEAQ project is focused on the optimisation operational mode. The ultimate goal is to apply the LEAQ model to other target regions or cities. The LEAQ model aims at solving the following problem: Find the optimal energy arrangement which complies with a given ambient ozone level standard.

The LEAQ model consists of two sub-models, the energy model ETEM and the Air quality model, AUSTAL2000-AYLTP. The two models are coupled by an optimisation routine called OBOE, Figure 1.

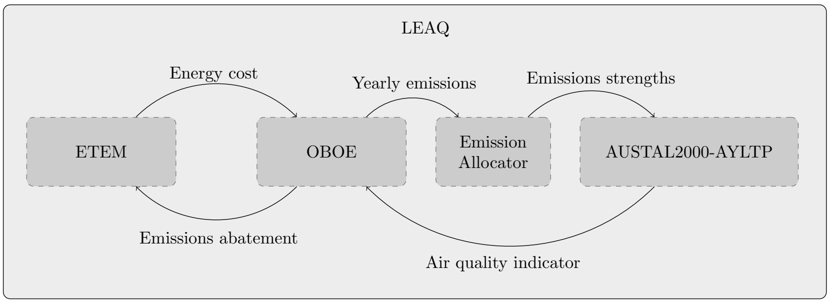


Figure 1: Overview of the integrated assessment LEAQ model, showing the two sub-models, ETEM and AUSTAL2000-AYLTP.

The models are connected by a common variable or by a module which “translates” the information from one model to the other. A first guess of yearly emissions is defined and then disaggregated spatially and temporally by the emission allocator, which in turn uses the emission time series to feed the air quality model in order to compute concentrations. This algorithm path assumes the LEAQ model is run in simulation mode. However in the optimization mode the sequence continues and the meta-model provides feedback to the energy model. The OBOE module checks if the air quality index breaches an air quality limit. In this context, the air quality limit, can be a legislative value or a long term objective. In this application we are most interested in ozone levels as the air quality indicator due to the complex relation between the precursor emissions and the ozone formation. If the air quality index breaches a given limit the meta-model proposes new lowered emission constraints. This procedure is repeated until the air quality levels satisfy the limit. Once the air quality compliance is assured, the constraint forces ETEM to choose less polluting technologies, which normally leads to a rise in the cost. ETEM then optimizes the energy shares to arrive at the least-cost energy arrangement that complies with a given air quality objective.

So far many developments have been made in the field of air pollution. Larger efforts have been put into developing scientific research oriented models, but also forecasting, regulatory and policy support models. Nevertheless few have been specifically developed for the coupling approach inherent to an integrated assessment modelling. Even more rare is to find studies where models have been run in its full mode in an optimization environment.

There are nowadays well validated models that can simulate ozone photochemistry with accuracy. Nevertheless, such models demand high computational resources, Carnevale et al. [2008]. The optimization framework involves many evaluation runs and thus the integrated assessment structure must be built strategically. In the known attempts of using integrated assessment air quality models in optimization mode, it is typical to apply reduction techniques. The reason for this is that air quality models are generally CPU time intensive. Amongst the most used reduction techniques are, linearisation, source-receptor matrices or model reduction.

**Linearisation** The Linearisation technique has been used by Shih et al. [1998], where first a response surface - isopleth - is generated. The isopleth relates the ozone concentration levels to the $NO_x$ and VOCs emissions, that are useful to evaluate precursor emission reductions. A mathematical program approximates the response surface. This is a very fast technique that allows the incorporation into an optimised decision making model. Amann et al. [2011] assumes a linear relationship between $NO_x$ and VOCs emissions and an ozone based air quality indicator.

**Source-receptor matrices** Source-receptor matrices store information about the contribution of emissions by a source to the concentration levels in a receptor point. They can be used in emission reduction policy studies, where they yield the change of concentration per change in emissions. Oxley et al. [2009] makes use of this technique to calculate the reduction in the concentration of SO$x$, NH$3$, $NO_x$ and PMs. Nevertheless secondary aerosol chemistry has been ignored and uniform vertical mixing have been assumed to lighten the computational resources. Reis et al. [2005] also applies this technique in a optimization integrated assessment study. In the same way, Carnevale et al. [2008] built source-receptor matrices based on artificial neural networks. It has been also used in other policy studies, although not in an optimization framework Muller and Mendelsoh [2006].

**Model reduction** is a Technique used by Carlson et al. Carlson et al. [2004], in which the model TAPOM is reduced to its simpler form TAPOM-Lite by assuming a linear relationship between the $NO_x$ and VOCs concentrations, with no turbulence nor topography. Previously Venkatram et al. [1994] had tried a model reduction using semi-empirical relations.

## 3 THE AIR QUALITY MODEL - AUSTAL2000-AYLTP

Carnevale et al. [2008] points out the need to develop innovative solutions that can reproduce the complex relations between ozone and its precursors, and at the same time remain simple to keep the uncertainties at a minimum level.

We have extended the work of Carlson et al. [2004] introducing the effects of turbulence and topography and resolving photochemistry spatially. The AUSTAL2000-AYLTP is the air quality model that has been built for the LEAQ meta-model. It uses the Lagrangian particle model for German regulation on air quality control, AUSTAL2000, Janicke and Janicke [2004], as a transport core calculator. The selection of the core model is explained in Aleluia Reis et al. [2009]. The Lagragian approach avoids the numerical diffusion errors which are generally associated with the numerical schemes used in the Eulerian approach. Furthermore Lagrangian models are know to be fast transport calculators. On the other hand, non-linear chemical reactions are very difficult to implement in this type of models (Nguyen et al. [1994]; Alessandrini and Ferrero [2009]). However linear and quasi-linear transformations (VDI [2000]) can be implemented. In the Asymptotic Level Transport Pollution (AYLTP) chemical module we implement quasi-linear relationships yield by a Look-up table (LUT).

### 3.1 Methodology

A set of variables, which are important drivers of the ozone behaviour, have been chosen to be the most significant, including zenith angle ($\theta$), relative humidity ($RH$), temperature ($T$), $NO_x$, VOC and $O_3$ concentrations. A probable interval of variation has been defined for each of these variables. We then use the box model, OZIPR (Gery and R.R. Crouse [1990]), to compute all the possible combinations of the variable's intervals and store the resulting final concentrations. The final concentration is used to calculate the reaction coefficient $Ks$, for all the pollutants $p$, according to:

$$Ks_p(c_p(t), T, RH, \theta) = \frac{c_p(t+1, c_p(t), T, RH, \theta) - c_p(t)}{c_p(t) \cdot \Delta t}, \; p \in \{1, 2, 3\}, \quad (1)$$

where the concentration of the pollutant $c_p$ in time $t + 1$ is the resulting concentration after $\Delta t$, which is given by OZIPR model. The initial concentrations are calculated using AUSTAL2000-AYLTP and the meteorology is an input of the model. This approach assumes perfect mixing inside the cells and a constant reaction coefficient during the time step. All the resulting reaction coefficients are stored in the LUT, and starting combination values of the variables are used to order the results by indexation. It is worth noting that the zenith angle ($\theta$) is actually represented by the variable "hour of the day". The use of "hour of the day" is less misleading since during one day the solar angle can take the same value in the mooring and in the afternoon. Hence using directly "hour of the day" variable simplifies the indexing of the results in the LUT. AUSTAL2000 has been adapted to read the $Ks$ value in the LUT and use it in the calculation of the Concentrations. For the cell $(i, j, k)$ in the space $S = \{i \in 1, \ldots, Nx; j \in 1, \ldots, Ny; k \in 1, \ldots, Nz\}$, where $Nx, Ny, Nz$, are the number of cells in each direction, the concentrations $c_p$ are updated in AUSTAL2000 as follows:

$$c_{p,i,j,k}(t+1) = c_{p,i,j,k}(t) + Ks_p(c_p(t), T, RH, \theta) \cdot c_p(t) \cdot \Delta t, \; \forall p \in \{1, 2, 3\}; \forall (i, j, k) \in S, \quad (2)$$

where $c_{p,i,j,k}(t)$ corresponds to the photochemistry modified concentration. The new concentration is then transformed into mass and distributed equally over the particles in the cell.

The use of quasi-linear coefficients allows the fast simulation of ozone production/depletion in the AUSTAL2000 Lagrangian model. We assume that under a certain number of restricted conditions a linear reaction rates holds. These conditions are imposed by the meteorological and concentration variables. The LUT in indexed according to the its 6 variables, and yields the resulting $O_3$, $NO_x$ and VOC coefficients, thus the matrix as 9 dimensions. Figure 2 shows a 3-D sub set of the a LUT for two different hours of the day. The model performs a search on the initial point *(i)*, in Figure 2, and looks for the result of that simulation a time step after *(f)*. In Figure 2 the time step is defined as seven hours to ease the visualization. Normally the time step for the calculation of the LUT is set to 10 minutes or one hour. The reaction coefficients are calculated using the information of *(i)* and *(f)* according to Eq. 1.

Luxembourg is a particular case study due to its very small dimensions and its position. It is a central and very small country in the border with France, Belgium and Germany. Although Luxembourg has important emission levels mainly from traffic and aluminium and steel industry, the contribution from the countries at the border is not negligible as it can change the VOC/$NO_x$ ratio. ETEM only includes Luxembourg's national emissions and therefore the emission measures can only control the additional concentration load coming from Luxembourg. Nevertheless, for compliance with legislation limits the contribution of transboundary can be added though the background concentrations. This is achieved by adding the background concentrations to the additional load, using the same methodology used in AUSTAL2000 [Janicke and Janicke, 2004].

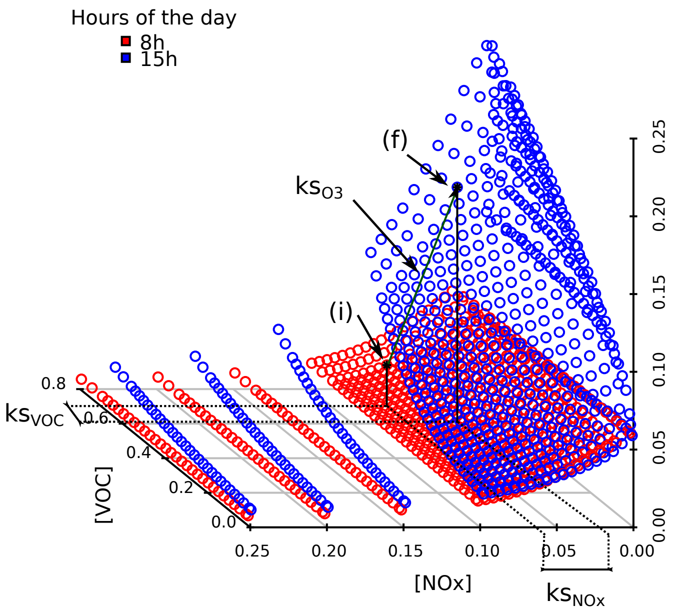


Figure 2: Subset of the LUT for two different hours, 8 and 15 hours of the day. The ozone and $NO_x$ concentrations are in ppm and the VOC concentrations are in ppmC. Point *(i)* represents a possible initial point at 8 hours, and *(f)* represents the resulting ozone concentration (ppm) 7 hours later. The reaction coefficients $Ks_{NOx}$, $Ks_{VOC}$ and $Ks_{O3}$ are calculated according to Eq. 1.

**The LUT results.** The implementation of the LUT is an important factor to reduce the calculation time, because AUSTAL2000 does not have to carry out the chemical calculations. It reads values from a file. The CPU times for a one day simulation with one hour time step, are presented in Table 3.1. The model has been run with and without the photochemical module, to assess the CPU time incremented by the implementation of the module. The results show a that the photochemical module, using LUT, introduces extra time. However the time becomes more marginal as the number of cells increase. This happens because the module requires some overhead time to read the LUT, that becomes less important when the number of cells increase.

| Team | Number of cells | CPU time (min.) |
|---|---|---|
| with LUT | 120 | 9.3 |
| with LUT | 480 | 9.6 |
| without LUT | 120 | 4.6 |
| without LUT | 480 | 7 |

The loss of accuracy inherent to this approach is acceptable given the reduction of CPU time. The model results have been compared to observations in [Reis et al., 2012].

## 4 Conclusions and future work

The LEAQ integrated assessment model works on an optimization framework. Therefore a fast air quality model needed to be developed. We have implemented a fast photochemical module on the Lagrangian model AUSTAL2000, using LUTs and a quasi-linear reaction coefficients. We conclude that the use of quasi-linear coefficients eases the implementations of non-linear relations in Lagrangian models. This implementation requires, simply, the addition of a multiplication coefficient on the concentration equation. This method only takes into account slow ozone formation processes and therefore represents an approximation to reality. The air quality results are based on the total emissions from the energy model for each economic period, typically a time horizon of 30 years and periods of one to five years. Hence LEAQ has inherently large uncertainties associated with long time scales and approximations are therefore acceptable.

Moreover the fact that coefficients have been pre-calculated saves time, since the AUSTAL2000 does not have to carry out the chemical calculations, but instead it reads values from a file. We conclude that the CUP time required for the air quality model is acceptable for this optimization framework.

AUSTAL-AYLTP must be subject of further validation, notably a comparison with other more complex photochemical models.

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