Ozone deposition modelling in a Portuguese coastal zone

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Abstract

The deposition of pollutants from the atmosphere to ecosystems is the cause of some present environmental problems: acidification, eutrophication and, indirectly, ground level ozone. Related with these issues is the critical loads/levels concept, widely accepted in Europe as basis for pollution control strategies. The knowledge of atmospheric pollutants deposition on ecosystems is needed to set up this methodology.

This paper presents the parameterisation done in the deposition module of the system of models MAR IV which is adequate to simulate the transport, dispersion and removal of pollutants, including ozone production for mesoscale application. The ozone surface resistance (Rc) parameterisation was applied to Lisbon region and the model’s performance was assessed with ozone deposition experimental data observed in the study area during the fieldwork LisbEx 97. The influence of parameterisation became evident with the good fit between modelled results and measured data.

Based on an empirical method described by the Stockholm Environmental Institute report a Critical Load map, for non-forested areas, was calculated for Portugal. The methodology is based on the kind of soil and its buffer capacity to acid compounds. The results show that around 70% of the country is in sensitive areas reinforcing the need for the application of this concept.

1 Introduction

The total deposition is defined as the contribution of three depositions processes, the dry, wet and occult deposition [1]. The wet and dry deposition is passible of
measure as well as numerical calculation and gives the amount of pollutants entering in the ecosystems, per unit area and time.

The development of the dry deposition processes for atmospheric chemical models requires parameterisations in their formulation. This parameterisation is based in measurements done both in laboratory, using enclosure methods, and in pollutants flux measurements field campaigns.

The critical load/level concept has been worked out since the 1980's and is based on a dose-effect relation. It assumes that different ecosystems have different capacities to receive atmospheric pollutants without dangerous modifications that can introduce changes into the ecological equilibrium or direct damage to the vegetation. The maximum pollutant quantity that each system can handle without consequences is called "critical load" or "critical level" depending if the pollutants are considered to have cumulative effects (like acidity and eutrophication) or direct effects (like the effect of ozone on vegetation) [2].

2 Atmospheric deposition and critical loads

The Gothenburg Protocol for Acidification, Eutrophication and Ozone reduction includes the critical load concept into a broad integrated evaluation methodology. Figure 1 shows the critical load/level concept application and the role of critical load/level maps on the development and implementation of pollution control strategies.

Figure 1: Critical loads and abatement strategies (adapted from UBA [3]).
Concerning the regional effects of atmospheric pollution it is necessary to analyse the results of two evaluation processes:

- To determine the ecosystems sensitivity to atmospheric pollution through the implementation of critical load maps;
- To evaluate atmospheric pollutants levels in space and time through the analysis of air pollutants concentration and deposition maps.

The methods applied to the critical loads calculation relays on simple estimations resulting from empirical data, balance and dynamical models [4].

The application of numerical simulations for the air quality studies is a fundamental tool for the development of adequate management policies. But the numerical tool application and evaluation implies air quality data measured in field campaigns. In this work attention was drawn to the Portuguese coastal zone, namely the Lisbon region.

3 Ozone deposition modelling

Concerning air pollutants deposition maps, a model system – MAR IV system, was applied to a coastal zone, including the Great Lisbon Area.

3.1 Study area

Lisbon’s domain is a 200 x 200 km² area centered on the city of Lisbon (Figure 2). Lisbon is build near the Tagus estuary (320 km²) on a coastal zone with a complex coastline associated to a gently rolling terrain and multiple hills reaching more than 400 m above sea level (ASL) (Montejunto 666 m and Sintra 528 m). To the South the coastline still sinuous and the domain is dominated by the Sado estuary (more than 135 km²) and Arrábida hill (501 m). To the interior, the Tagus and Sado river valleys are the major orographical features.

3.2 MAR System

The numerical simulation was carried out by the application of the model system MAR IV [5]. The MAR IV system is made up of two mesoscale models, the System Application International Mesoscale Model (SAIMM) and the photochemical Urban Airshed Model (UAM).

In the UAM, dry deposition is assumed to occur in a two-step process: the transfer of pollutants through the atmosphere to the surface and the uptake of the pollutants by vegetation and other materials at the surface. This process involves a resistance to mass transport ($R_m$) and a resistance to surface removal ($R_c$)

$$ R_d = R_m + R_c $$  \hspace{1cm} (1)

The transport resistance is estimated from theoretical considerations of turbulent transfer in the atmospheric boundary layer.
It is assumed an equal transfer processes of mass and momentum in the atmospheric boundary layer (ABL), resulting:

\[ R_m = \frac{u(z)}{u^2} + \left(2.2 u_*^{-1/3}\right) u_*^{-1} \]  \quad (3)

The surface resistance is obtained from experimental data on the uptake of pollutants by various surface features [6].

3.3 Numerical simulation

Simulations were performed for the simulation domain for a typical summer synoptical circulation characterised by an extension of the Azores anticyclone over the northern part of the Iberian Peninsula and to the location of a low pressure system to the west of the British Islands and initialised with a clean air condition.

The MAR IV system was applied to the study area with an horizontal resolution of 4 x 4 km². Four different \( R_c \) values were used in the photochemical model application (Table 1).

A literature value, obtained in a chamber specifically designed for the study of gaseous exchanges, was used [7]. In the other applications \( R_c \) values measured at Baldios during the LisbEx 97 air quality campaign [8], were used. It were considered the average, maximum and minimum values for a typical day of the field campaign. This parameterisation was evaluated with deposition fluxes measured at Baldios station in the referred day.
Table 1: Surface resistance (Rc) values used in the simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>h m⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>Literature</td>
<td>53</td>
<td></td>
</tr>
<tr>
<td>Average</td>
<td>1041</td>
<td></td>
</tr>
<tr>
<td>Minimum</td>
<td>382</td>
<td></td>
</tr>
<tr>
<td>Maximum</td>
<td>3061</td>
<td></td>
</tr>
</tbody>
</table>

3.4 Results

In Figures 3 and 4 are presented the ozone deposition fields together with the surface wind fields at 17 h. This spatial-temporal analysis example is done for simulations with literature value and measured values. At this hour the sea breeze is fully developed and the deposition fields present the same dispersion pattern over the simulation domain.

The comparison between the two figures confirms Rc influence in the ozone model mass balance. In fact, the deposition fields are less expressive, in numerical value and dispersion patterns, where there are the higher ozone concentrations.

Figure 3: Ozone deposition and wind fields at 10 m at 17 h for Rc literature value (adapted from Valinhas, [9]).
Figure 4: Ozone deposition and wind fields at 10 m at 17 h for $R_c$ mean value obtained during LisbEx 97 (adapted from Valinhas, [9]).

### 3.5 Sensivity analysis

The comparison between numerical results and observed deposition fluxes was done by a point quantitative error analysis methodology [10] where skill is demonstrated when: $S \approx S_{\text{obs}}$, $E < S_{\text{obs}}$, $E_{\text{ub}} < S_{\text{obs}}$. $S$ and $S_{\text{obs}}$ are the standard deviations for numerical and observed values, respectively, the parameter $E$ is the root mean square error (rmse) and $E_{\text{ub}}$ is rmse after a constant bias is removed.

Table 2 presents the results where $R_c$ literature values application has a poor performance. From $R_c$ measured values parameterisation, the minimum value presents best results showing a good correspondence with observed data.

Table 2: Error analysis of model predicted ozone fluxes deposition for Baldios.

<table>
<thead>
<tr>
<th>Applications</th>
<th>$S/\text{Sobs}$</th>
<th>$E/\text{Sobs}$</th>
<th>$E_{\text{ub}}/\text{Sobs}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Literature</td>
<td>5.91</td>
<td>11.17</td>
<td>5.41</td>
</tr>
<tr>
<td>Average $R_c$</td>
<td>0.30</td>
<td>1.95</td>
<td>0.92</td>
</tr>
<tr>
<td>Maximum $R_c$</td>
<td>0.10</td>
<td>2.52</td>
<td>0.97</td>
</tr>
<tr>
<td>Minimum $R_c$</td>
<td>0.84</td>
<td>1.00</td>
<td>0.98</td>
</tr>
</tbody>
</table>

Ozone deposition fluxes show a better agreement with measured values for $R_c$ parameterisation. Nevertheless, this validation methodology should be done with
more deposition data, meaning more field campaigns about atmospheric pollutants deposition.

4 Portugal Critical Load Map

The work presented with the numerical simulation was important for the deposition module development and its application to a region of interest. The methodology presented for the critical load map has a global concept.

The critical load map over Portugal was constructed based on the Stockholm Environment Institute (SEI) methodology [11], which indicates that the best method for calculation critical loads on a coarse grid is the one based on the soil neutralising capacity, although vegetation and climate are considered important parameters influencing the ecosystems response to acid deposition. Nevertheless, the available information concerning these parameters is considered to be scarce.

Concerning soil processes that influences soils buffer capacity two are of major importance: minerals meteorization (the most important one) and interchange of cations within the soil, measured as Cations Interchange Capacity (C.I.C).

Based on the SEI's work, five-soil sensitivity classes were defined according with soil type, base saturation and CIC average value. The soil classes were defined by FAO scheme for the European Soils Map [11] (Table 3).

<table>
<thead>
<tr>
<th>Soil Sensitivity Class</th>
<th>1 - More sensitive</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5 - less sensitive</th>
</tr>
</thead>
<tbody>
<tr>
<td>Less than 25</td>
<td>Between 25 and 50</td>
<td>Between 50 and 100</td>
<td>Between 100 and 200</td>
<td>More than 200</td>
<td></td>
</tr>
</tbody>
</table>

Then, the Portuguese soil types (Figure 5) were classified according to soil sensitivity classes defined in the previous table. This classification was applied to the Portuguese case resulting in the critical loads map for acidity presented in Figure 6. The results show that around 70% of the country is in sensitive areas. The former value reinforces the need of a better atmospheric deposition modelling.
Figure 5: Portugal soils map (adapted from Valinhas [9]).

Figure 6: Portugal critical loads map (adapted from Valinhas [9]).
5 Conclusions

A parameterisation of the deposition module of the system of models MAR IV was done. This system is adequate to simulate the transport, dispersion and removal of pollutants, including ozone production for mesoscale application. The surface resistance parameterisation was applied to Lisbon region and the model's performance was assessed with deposition experimental data observed in the study area. The comparison between ozone concentration fields and deposition fields shows a clear response of the model to the surface resistance parameterisation. In fact, the influence of this variable in ozone model mass balance is consistent with the ozone fields presented for the two numerical applications.

An empirical method was applied to estimate critical loads for acidity for continental Portugal. The results show that around 70% of the country is in sensitive areas reinforcing the need for the application of this concept. The possibility of new parameterisations applications in the deposition module of MAR IV as well as the need of more experimental data on surface resistance leaves an open door to more research work. The development of the deposition modelling is an important task in the critical loads concept providing other features in this subject.

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