

Integrated assessment modeling in Spain

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ABSTRACT

This paper shows the current state of the integrated modeling system being implemented in Spain. The system developed by the Technical University of Madrid (UPM) basically includes two major components; the emission projection system and the air quality modeling system. Emission information is one of the main sources of uncertainty in air quality modeling. This issue is also relevant to the analysis of the possible alternatives to improve air quality in a given region in future years as a result of the implementation of control strategies. Emission processing and generation of input files for the eulerian chemical-transport model is based on the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. The adaptation of this software tool to Spain is briefly discussed and some examples are provided through a case study in the Iberian Peninsula. In addition, the utility and capabilities of the modeling framework are illustrated by showing some results regarding future-year ozone simulations in Spain.

INTRODUCTION

The development of effective environmental policies is needed in order to meet regulatory standards and international legislation and agreements in the future. The design, assessment and comparison of control strategies require the support of an integrated modeling system. For instance, the development of ozone control strategies requires the understanding of the complex nonlinear processes governing tropospheric ozone levels. Urban and regional air quality is determined by emission of ozone precursors, complex chemical reactions, physical transport and diffusion and deposition phenomena. The ozone dynamics involves processes extending over multiple spatial and temporal scales and complicated relationships with other atmospheric issues such as aerosols or acidification.

According to Harris¹ “Integrated Assessment implies that the science is exemplary and that it is being done in the context of social and economic forces at work in society. Science is being used to generate both explanations and policy options”. Under this point of view, an integrated modeling system must be based on the most up-to-date science, but it also needs to consider other relevant inputs. A system capable of supporting the assessment and comparison of environmental policies and control strategies must be able to evaluate nation-wide future atmospheric emission levels under different emission scenarios taking into account a variety of activity patterns, alternative fuel usage and technological reduction and regulatory options. Air pollution control (as well as greenhouse effect mitigation) usually entails significant economic and social costs and, therefore, the risk of

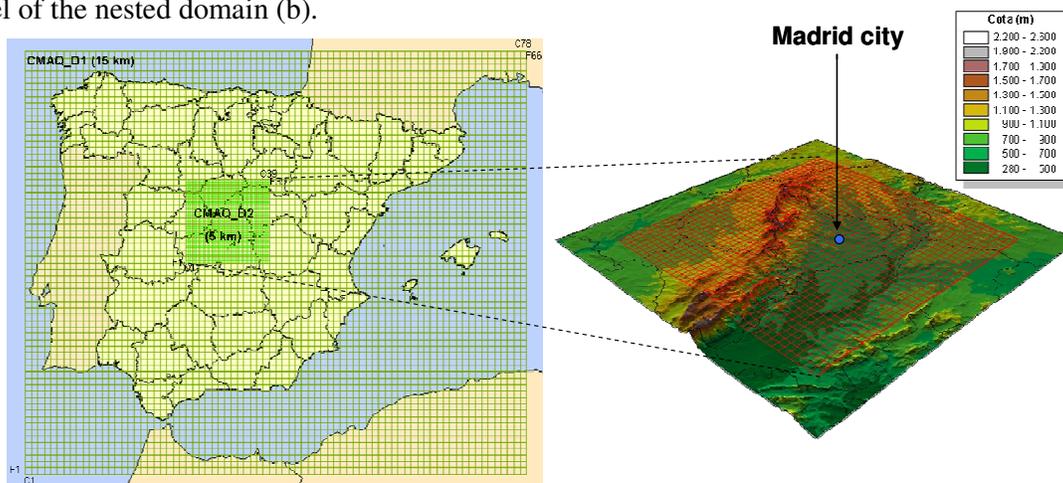
error when designing abatement measures should be reduced as much as possible. This is the reason why the integrated modeling system must include the support of numerical air quality models.

The Technical University of Madrid (UPM) is currently developing and implementing an integrated modeling system for Spain. The system is based on two major components.

- 1) Spain's Emission Projections (SEP)^{2,3} model. Emissions for the main atmospheric pollutants and greenhouse gases are available up to 2020. These emissions are based on individual, highly-detailed projections for nearly 300 emission categories according to the Selected Nomenclature for Air Pollution (SNAP) classification. National figures are obtained through an integration methodology that guarantee full consistency among individual projections and complete agreement with the National Atmospheric Emission Inventory (SNAEI)⁴ estimates for past years. A piece of software called EmiPro² has been developed to implement the SEP's methods and support the QA/QC process in emission projections. This tool also assists report generation, including mapping to other nomenclatures relevant in the framework of the Clean Air For Europe (CAFE) program and comparison with other European models (RAINS, PRIMES, etc.)
- 2) An air quality modeling system for the Iberian Peninsula based on MM5/WRF, SMOKE and CMAQ models. It includes the adaptation of the SMOKE system to European conditions and the integration of the SNAEI and SEP's databases as inputs to the emission preparation for modeling process.

This paper is focused on the second component and specifically on the procedures needed to adapt emission official estimates in order to match the requirements of the chemical-transport model selected. In the following section, the methodology developed to adapt the SMOKE system to European Conditions is summarized and the main stages involved in the process of emission preparation for modeling are discussed. For the sake of clarity, some practical examples and results are shown. The results are taken from a case study involving two nested modeling domains (Figure 1) over the Iberian Peninsula and the Greater Madrid Area (GMA) for the year 2010.

Figure 1. D1 and D2 (15 and 5 km resolution respectively) modeling domains (a). Digital Elevation Model of the nested domain (b).



EMISSION PREPARATION FOR MODELING

Beside emission estimation itself, emission inventory preparation is a critical stage in air quality modeling. Many authors have clearly shown that emission input to Air Quality Models (AQMs) is one of the main sources of uncertainty^{5,6}. This issue is also important from the point of view of the analysis of the possible alternatives to improve air quality in a given region in future years as a result of the implementation of pollutant emissions abatement strategies⁷.

In Spain the most comprehensive and reliable source of information concerning emissions is the SNAEI, based on the CORINAIR methodology⁸. As for future year emission estimations, the best available source of information is the SEP model. These projections cover the main atmospheric pollutants up to 2020 and are fully consistent with the SNAEI. In addition, emission and projection estimates from EMEP⁹ have been used to incorporate non-Spanish emissions inside the domains of interest. However, this information must be processed and extended in order to meet the requirements of the chemical-transport model. The AQM basically needs gridded emission data with hourly resolution in terms of the species involved in the chemical mechanism selected for the simulation.

All the procedures and transformations needed to provide that information in the format expected by the AQM are undertaken through the Sparse Matrix Operator Kernel Emissions (SMOKE)^{10,11} system (version 2.1.)¹². The SMOKE system was developed by the MCNC Environmental Modeling Center (EMC) to allow emissions data processing methods to integrate high-performance-computing sparse matrix algorithms. This software is based on a parallel approach to emissions processing and was redesigned and improved with the support of the US EPA, for use with EPA's Models-3 Air Quality Modeling System. Despite the system being strongly US-oriented, its flexibility allows the application of SMOKE to European Conditions¹³.

Basic approach

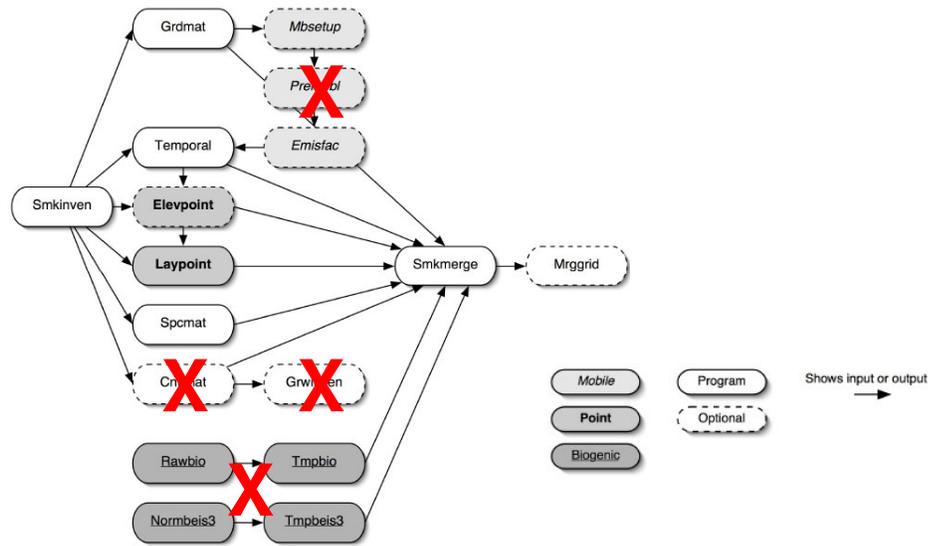
More than modifying the model, the approach is based on the development of an interface between the US National Emission Inventory¹⁴ and EU CORINAIR datasets and procedures.

In order to guarantee consistency with CORINAIR methods, SMOKE has been applied strictly for emission processing, i.e. the models included for emission computations for biogenic sources¹⁵ and mobile sources¹⁶ have not been used as illustrated in Figure 2. Following the CORINAIR criteria, all the sources have been grouped into area and point sources (Large Point Sources, LPS). Biogenic and mobile sources are considered in this study as special sources inside the area category. The process line related to emission projections is not used since detailed future year emissions are provided as separate inventories.

Codes

The adaptation of the SMOKE modeling system to Spain involves the translation of Source Classification Codes (SCC) into SNAP codes and the incorporation of the geographic codes according to the European administrative classification; Nomenclature of Territorial Units for Statistics (NUTS).

Figure 2. Information flow through SMOKE core programs. The crosses indicate the processor is not used. Apadanted from Houyoux et al., 2004.



Emissions inventories and projections are processed at the highest possible detail, which means the third hierarchical level (or activity level) of the EU SNAP 6-digit categories⁸. The highest level of the SNAP classification (Group level), comprises of 11 divisions reflecting the largest categories of anthropogenic and natural activities, as shown in Table 1. SMOKE, though, is design to cope with SCC categories, a four-level nomenclature. Under this hierarchical scheme, area and point sources are represented by 10 and 8-digit codes respectively. The SCC-like codes are generated by adding a fixed code (4 and 2-digit respectively) at the end of the original SNAP code. This approach allows keeping the advantages of SMOKE hierarchical cross-reference system, and makes possible to handle a given SNAP activity as both, area and point source simultaneously.

Table 1. Groups considered within SNAP-97 nomenclature

Group	Name
SNAP-1	Combustion in energy and transformation industries
SNAP-2	Non-industrial combustion plants
SNAP-3	Combustion in manufacturing industry
SNAP-4	Production Processes
SNAP-5	Extraction and distribution of fossil fuels and geothermal energy
SNAP-6	Solvent and other product use
SNAP-7	Road transport
SNAP-8	Other mobile sources and machinery
SNAP-9	Other mobile sources and machinery
SNAP-10	Agriculture
SNAP-11	Other sources and sinks

As for administrative division codes, SMOKE is meant to deal with the US 6-digit integer codes for the identification of Country, State and County, which is easily adaptable to the European NUTS hierarchical system. In the particular case of Spain geographic codes would consist on the union of the relevant codes for Country, Autonomous Region and Province. Code definitions and correspondences are defined in the intermediate inventory databases and are consistently applied all over the SMOKE system as well as the Geographic Information System (GIS).

Formats

Information flows inside SMOKE are based on the I/O API Network Common Data Form (netCDF) adapted gridded format, which is automatically generated for intermediate files. Input information can be provided via pre-gridded I/O API files, but input information mainly consists of ASCII (list-directed or column-specific) files. Special attention must be paid to inventory files (\$ARINV and \$PTINV). SMOKE can incorporate input information regarding emissions through a variety of formats, but some of them are very specific to the US and can not be reproduced for Europe. For this study, the Inventory Data Analyzer (IDA) format has been adopted. Inventory files according to this format contain some information unneeded or disregarded by SMOKE. Only the relevant information is provided.

Emissions

Emission estimates for modeling are taken from the CORINAIR database, which includes all the information in the SNAEI. Intermediate inventory databases in Figure 3 (SMOKE_AR and SMOKE_PT) are the key element to extract the relevant information from the CORINAIR database and to process it to generate the fields needed in the SMOKE inventory files, as illustrated in the flowchart.

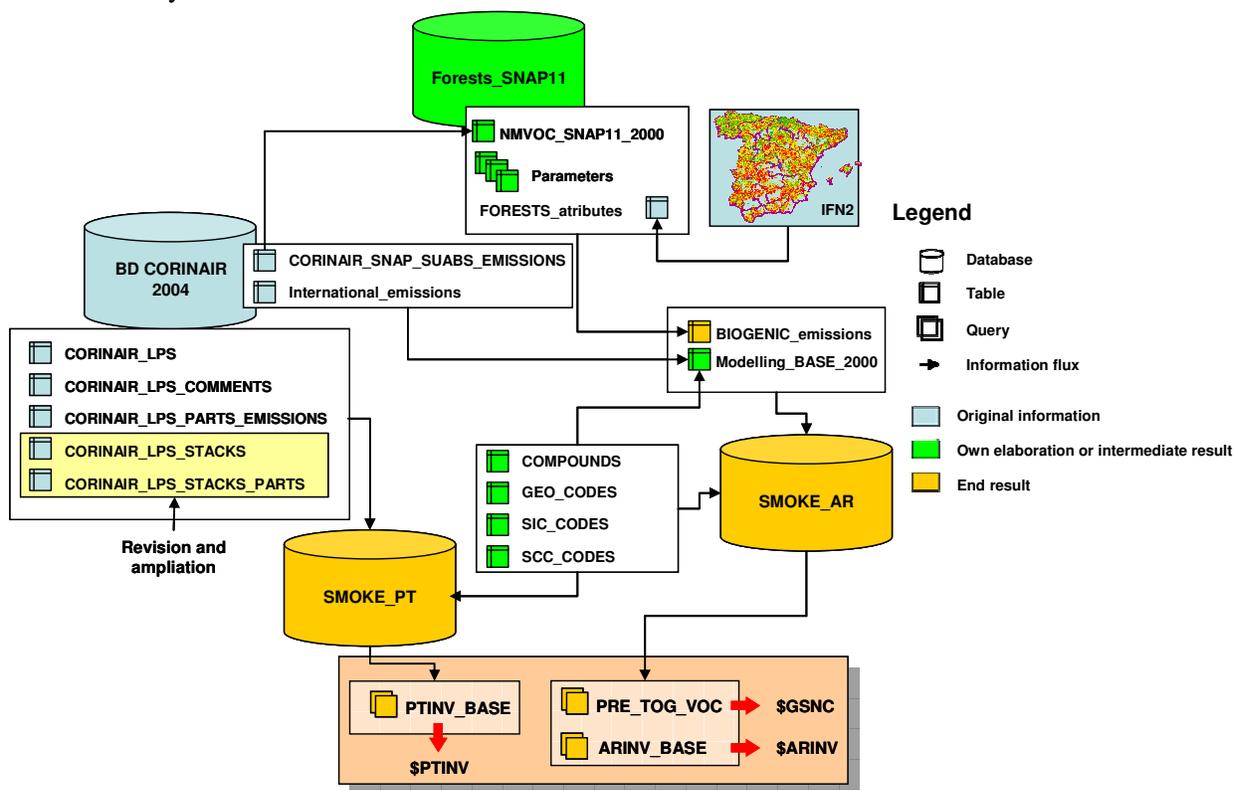
The inventory for point sources has been developed using all the information available in the SNAEI database regarding LPS location (geographic coordinates), number of stacks and stack parameters (height and exit area, temperature and vertical speed or flow of exit gases). Among the LPS are included all the facilities belonging to the main industrial activities, such as power plants, oil refineries, sulphuric and nitric acid plants, integrated iron and steel plants, paper and pulp plants, etc.

The SNAEI database, produced by the Ministry of Environment, has been checked and extended in order to fill the gaps in the data and the restore missing relationships between stacks and emissions at part level. The emissions from point sources are quantitatively very important; for example, LPS emissions represented the 74.2% of total national SO₂ and 23.9% of NO_x in the year 2000. For the year 2010, specific projections at activity level have been computed and incorporated into the corresponding point sources inventory. In addition, some new point sources have been included, accordingly to the new developments envisaged by official national and regional plans.

Plume rise computation for all the point sources has been performed inside SMOKE using the meteorological outputs from MM5. The algorithms employed are based on various equations from Briggs¹⁷. This results in the allocation of the emissions according to the vertical structure of the model taking into account plume buoyancy and momentum as well as mixing depth and atmospheric stability conditions. This approach to LPS emissions processing showed that a large fraction of the

emissions are located at heights around 500-1000 meters above ground level. Therefore, the importance of addressing this kind of sources properly is clearly stated.

Figure 3. Emission databases and main tables involved in the generation of inventory input files to the SMOKE system



The remaining sources are regarded as area sources. Nevertheless, some of them present specific features that require a particular processing. The first type of these special area sources is road transport. Despite that SMOKE integrates the MOBILE software¹⁶ to compute and process this sort of emissions, the CORINAR methodology relies on the COPERT software¹⁸ for this issue. In order to guarantee the consistency with the SNAEI, the emissions for all pollutants from road traffic have been estimated using this tool developed by the European Environmental Agency, both for past and future.

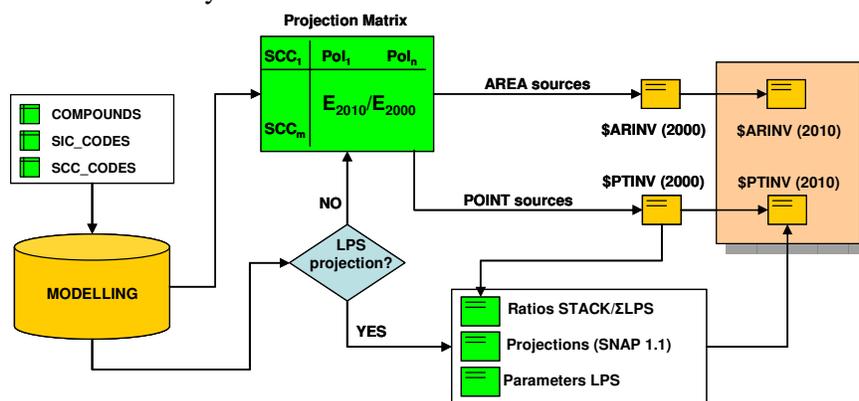
Some of the off-road mobile sources have peculiarities that have led to the development of specialized processing approaches. Specific methods have been implemented to incorporate the emissions from ships and aircrafts (during landing and take off cycles).

Finally, emissions from biogenic sources, basically VOC from forests (around 50% of total national VOC emissions), have been derived from the Forestry National Inventory¹⁹ (IFN2). The computation methods provided for these sources in the CORINAIR methodology have been integrated into the GIS²⁰. An interface between the GIS databases and the inventory for area sources in SMOKE has been developed. Although the results differed significantly from the SNAEI estimations, the emissions of isoprene, monoterpenes and other volatile organic compounds have been readjusted to match the SNAEI figures at national level.

Emission projections

Future-year inventories have been derived from the SEP model. These emission projections are based on the same methodological basis than the SNAEI. The way in which emission projections were calculated for a particular activity was determined by the methodology used for the compilation of SNAEI. In most of the cases for the Spain's calculations, the same approach used in the national inventory (i.e. bottom-up or top-down) and the same sources of information are adopted, which ensure the consistency with historical datasets. However, in certain cases an improved approach could be implemented, e.g. when more detailed information on a specific sector not included in SNAEI has become available. The original estimates have been adapted for modeling purposes (details can be found in Borge et al., 2005²). Once the emission projections have been modified, a projection matrix is created and applied, similarly to the CNTLMAT processor inside SMOKE, as illustrated in Figure 4.

Figure 4. Generation of future year inventories for SMOKE.



As an example, emissions estimates for the year 2010 presented in Figure 5 are taken from the SEP BASE scenario, which is intended to provide national emission projections according to the baseline scenario defined in the CAFE Programme. It provides estimates for national emissions under many of the implemented policies and measures for reducing emissions through technology improvements and dissemination, demand-side efficiency gains, more efficient regulatory procedures, and shifts to cleaner fuels. This scenario has also been defined taking into consideration all sectoral plans and measures (enacted and in force) published by official organizations and the national sectoral legislation. Thereby, it outlines a likely range for the future emissions of air pollutants and greenhouse gases up to 2020.

International emissions

Mesoscale modeling usually involves emissions from more than just one country. Several National Inventories could be treated exactly in the same way explained before (SMOKE inventory files accept up to 10 different country codes), but for this case study, emissions from Portugal and France have been incorporated via a simplified method in which emission computation and spatial allocation are performed simultaneously. This is done through a mass-conservative, GIS-

interpolation process of EMEP gridded emissions. EMEP grid definition is based on a Polar Stereographic projection; before performing the overlapping process, it must be converted into the Lambert Conformal system adopted for the modeling system, as illustrated in the example of Figure 6. In this case, emission projections for 2010 are also retrieved from the EMEP expert emission database (WebDad 2005).

Figure 5. Emissions for modeling by SNAP group (tonnes). Comparison of 2000 and 2010 Spain’s emissions in the mother domain.

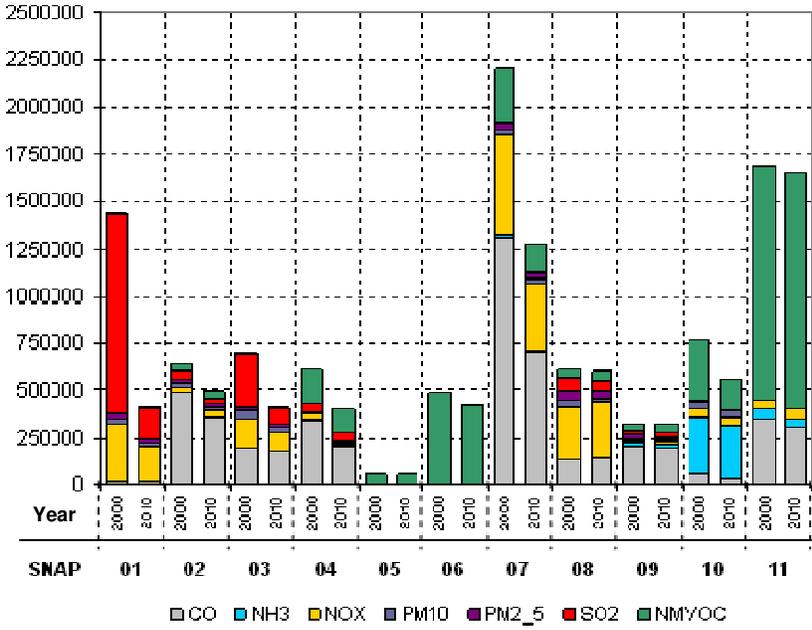
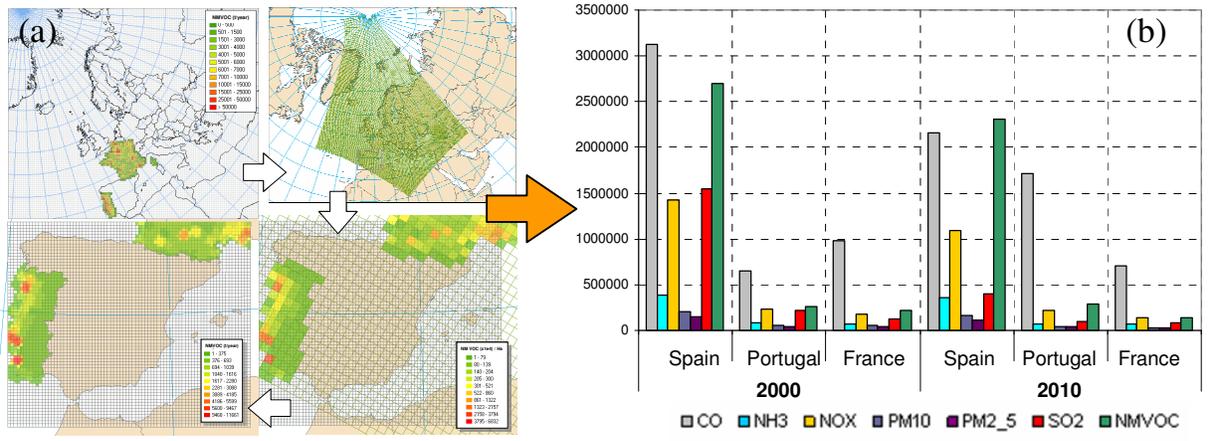


Figure 6. Interpolation process of non-Spanish emissions into the modeling domain (a). Total emissions inside the mother domain and comparison with Spanish emissions for 2000 and 2010 (b). Figures in tons.



Chemical speciation

The chemical speciation step consists of the transformation of generic inventory compounds, such as NO_x , VOC and $\text{PM}_{2.5}$ into the chemical mechanism species. The conversion into the model species is carried out using cross-reference tables that link the speciation profiles with the SNAP activities in both inventories (area and point sources). This procedure has been done considering the Carbon Bound IV mechanism (CB4)^{21,22}. This is one of the most widely used models for simulating tropospheric chemistry, mainly because it has been used for regulatory modelling studies in the USA during the last decade. Although this is probably not the most updated and comprehensive mechanism available, it is the best documented one and there is a large amount of information about chemical speciation profiles for VOC and $\text{PM}_{2.5}$. Most of the references used to perform the conversion into the mechanism species come from the US EPA²³. In addition, some references from the EMEP/CORINAIR guide book have been incorporated depending on their availability.

The generation and linkage of synthetic chemical profiles is supported by an interface based on a mapping between EPA SSC and EU SNAP categories. USEPA's VOC speciation profiles are actually expressed in terms of Total Organic Gases (TOG) and, therefore, activity-specific factors for VOC to TOG conversion are needed. In practice, these factors are computed as the ratio between $\text{NMVOC}/(\text{NMVOC}+\text{CH}_4)$ in the intermediate databases (Figure 3). SMOKE is provided with these activity-specific factors through the VOC-to-TOG conversion file (\$GSCNV).

Up to 87 chemical profiles for VOCs and 54 for $\text{PM}_{2.5}$ were developed and applied for this case study. Following USEPA defaults, a constant non-specific NO/NO_x ratio of 0.9 has been assumed for all the categories emitting nitrogen oxides.

Temporal allocation

The next step in the emission preparation for modeling is the temporal allocation of the emissions. This stage is also based on the linkage between cross-references files and profiles for each SNAP activity and pollutant. Suitable monthly, daily and hourly profiles have been generated in order to provide a realistic temporal allocation of the emissions to the chemical-transport model. Hourly distribution of annual emission estimates was carried out through the application of 208 monthly profiles, 48 weekly profiles and 212 diurnal profiles.

Each diurnal profile actually includes two different emission patterns, applicable for weekdays and weekends. Domain-specific holidays calendar were provided to SMOKE (via the \$HOLIDAYS file) to take into account the effect of national and regional holidays. The dates included in these files are processed as if they were a Sunday.

All temporal profiles are treated by the TEMPORAL processor as local profiles, which allows the user to provide temporal profiles according to the time zones declared in the \$COSTCY file for the administrative divisions included in the modeling domain. For this application, all temporal references, as well as model outputs, are referred to UTC. The automatic daylight saving option implemented in SMOKE was switched off since it is not applicable to time zones east of the Greenwich meridian.

Spatial allocation

The last stage of the process consists of the spatial allocation of the emissions from area sources. The geographic allocation is carried out by using surrogate data. For the case study presented in this paper, 24 different surrogates (listed in Table 2) have been generated for both the 15 km and the 5 km meshes, so that all the emissions can be properly linked to each of the cells of the CMAQ_D1 and CMAQ_D2 domains. The elaboration of surrogate data is supported by the GIS and is based on the process of infrastructures and land use covers. Most of this information has been extracted from the CORINE Land Cover 2000²⁴. It should be noted that the allocation procedure starts from the geographical disaggregation considered in the SNAEI, i.e., the sum of cell ratios for a given surrogate is equal to one over any province (NUTS-3 level).

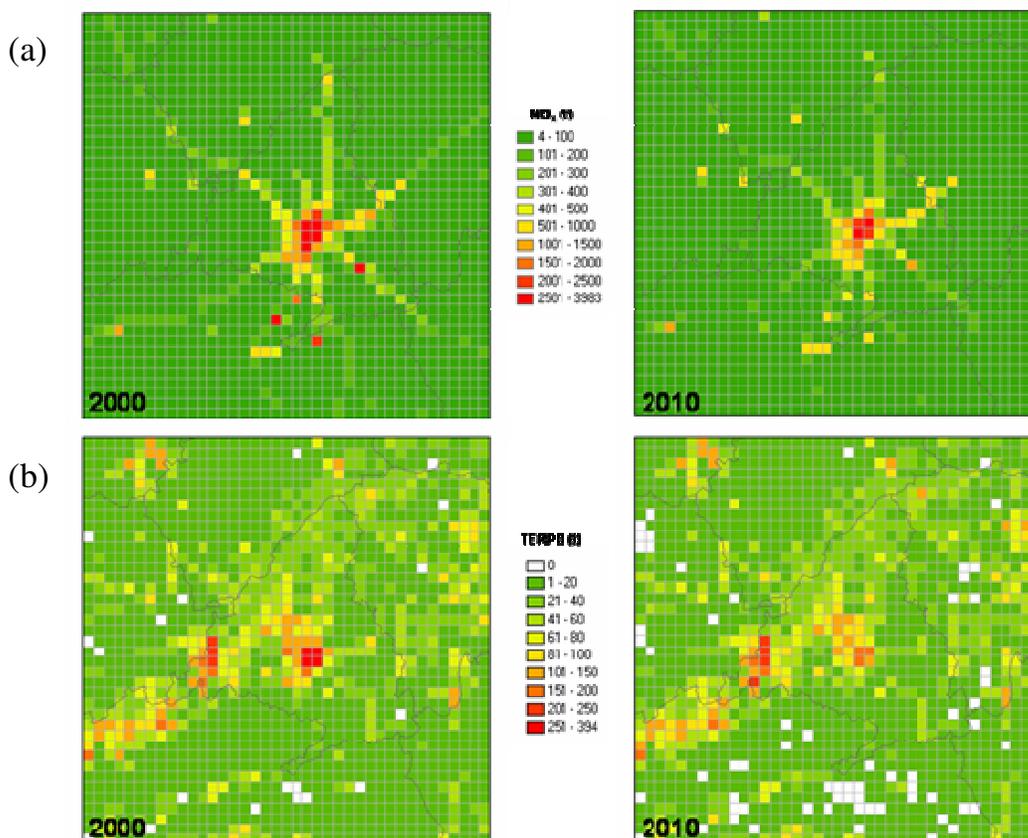
Table 2. Spatial surrogate datasets developed for the case study

#	Spatial surrogate	#	Spatial surrogate
1	Highways	13	Petroleum pipeline
2	Rural roads	14	ISOP (from forests)
3	Industrial and commercial units	15	MONO (from forests)
4	Railroads	16	OVOC (from forests)
5	Urban population	17	Agriculture
6	Population (fallback surrogate)	18	Permanent crops
7	Pasture	19	Arable land
8	Forestry	20	Rice fields
9	Construction sites	21	Horticulture
10	Mineral extraction sites	22	Sea
11	Dump sites	23	Portugal
12	Natural gas pipelines	24	France

The allocation of aggregated emissions is obtained by merging spatially resolved emissions from all the activities present in a given domain. The Figure 7 shows some examples for the nested domain covering the GMA. The largest share of nitrogen oxides total emissions from area sources is due to road traffic. Consequently, the Madrid radial highway system can be clearly distinguished in Figure 7a. However, some of the cells with higher emission rates are related to industrial facilities not considered in the SNAEI as point sources. Emissions belonging to some of these activities have been allocated through the area-to-point algorithm implemented in SMOKE, originally intended to allocate emissions from airports. In some cases, this was found to produce some biases in the results of the air quality model for pollutants such as ozone or fine particles.

Emission pattern in Figure 7b is completely different, since monoterpenes emissions are strongly influenced by biogenic sources. Anthropogenic emissions of these compounds are expected to decline in the future.

Figure 7. Spatial allocation of NO_x (a) and monoterpenes (b) in the nested domain (tonnes/year).



RESULTS

The system to support integrated modeling activities in Spain must be considered as a work in progress. Costs and optimization modules are still under development and the whole system (emission projections, emission processing methods, AQM) is currently being updated and upgraded. However, some preliminary results are available from the case study presented.

As an example, Spain's compliance of the European Directive 2002/3/EC 2002²⁵ is evaluated. Figure 8 illustrates the results for the target value for the protection of vegetation. According to the ozone Directive mentioned before the AOT40 calculated from 1h values from May to July should not exceed 18000 $\mu\text{g}/\text{m}^3\cdot\text{h}$ (9 ppm·h). This index has been computed from the outputs of the CMAQ model^{26,27} for the year 2010.

Focusing on the nested domain, it can be seen how according to the model predictions for 2010, ozone levels in the Greater Madrid Area under the BASE scenario of the SEP mode would not match the requirements of the ozone Directive (2002/3/CE). In other words, expected reductions shown in Figure 5 will not be enough to guarantee the protection of forests and crops. Similarly, in some areas of the region the target values for 8-hour ozone average concentration would be successfully achieved (not shown). However, in most of the city and its surroundings, where most of the population is concentrated, the exposure levels to ozone would not be compatible with the fulfillment of the target value established for the protection of human health.

Figure 8. Modeled ozone AOT40 for 2010.

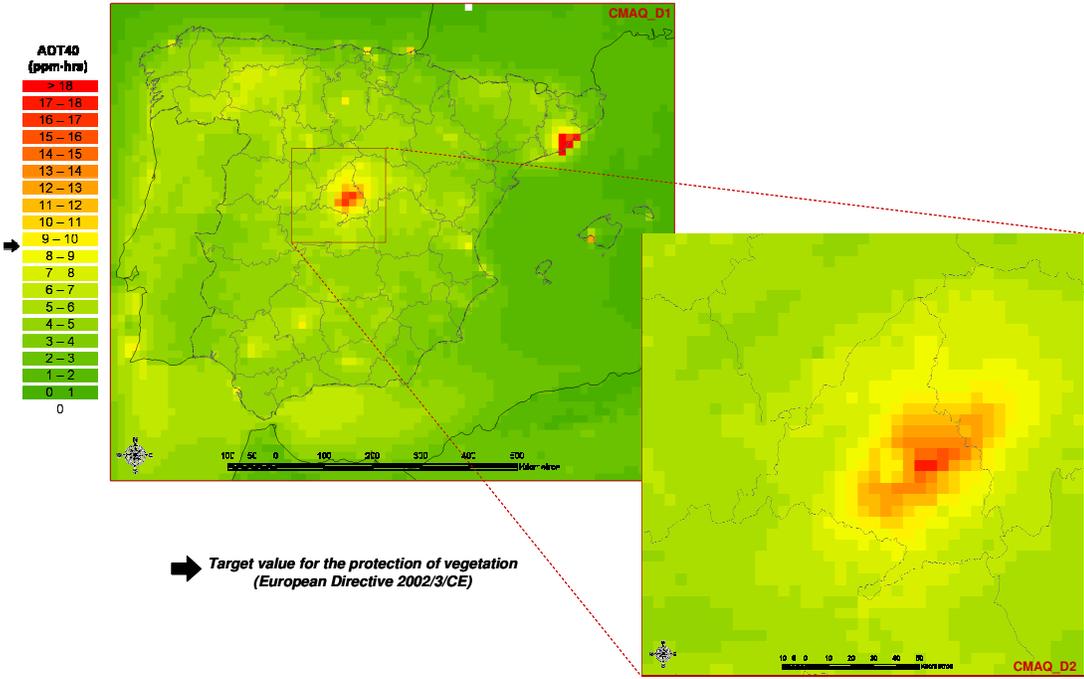
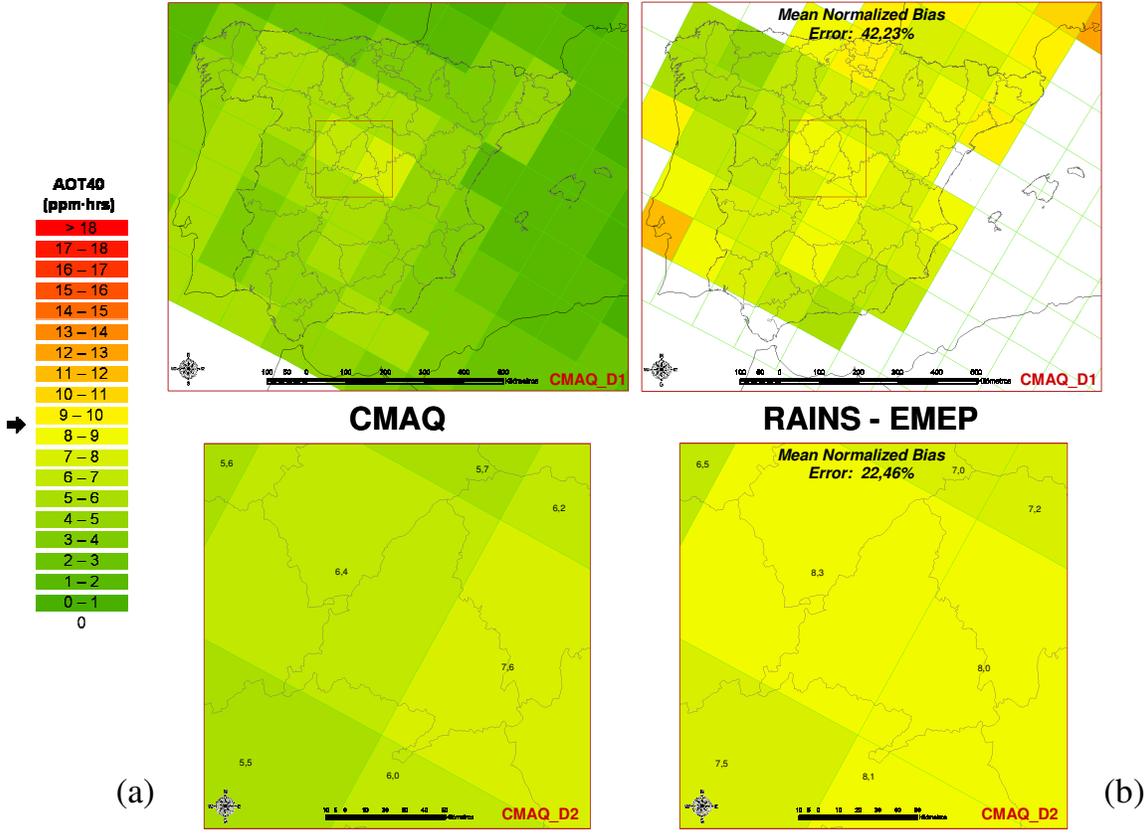


Figure 9. Modeled ozone AOT40 for 2010. CMAQ (a) Vs RAINS-EMEP (b)



The Spain's Ministry of Environment and the UPM are working on the development of emission scenarios compatible with both, the fulfillment of national emission ceilings and the achievement of future air quality standards. Such scenarios are based on cost-effective emission abatement measures. It should be noted that emission preparation for modeling is not only a critical stage from the point of view of model performance, but it also provides valuable information to assist the decision-making process and the design of such environmental plans and reduction strategies.

Another utility of the system is to provide a reliable, state-of-the-science, high-resolution, modeling platform that could complement to European-scale impact assessment modeling. As an example, Figure 9 illustrates the comparison of the RAINS-EMEP modeling system (150 km resolution) and the national system. Modeled ozone AOT40 results from the CMAQ model in Figure 9 are derived from those in Figure 8. Although average AOT40 values predicted by RAINS-EMEP are higher, no exceedences of the target value are observed at such a gross scale. This comparison highlights the influence of the reference scale and gives clear evidence that the consideration of national modeling results in the decision-making process is needed to optimize the setting and achievement of health and environmental targets.

CONCLUSIONS

The main components of the integrated assessment modeling system under development in Spain are shown and some results are discussed. Although the system is being upgraded, the methodology has been tested successfully and some promising results have been obtained.

The emission subsystem is one of the most important components of the modeling framework. Emission information is taken from the SNAEI and the SEP, which constitute the official Spain's atmospheric emissions estimates for past and future years respectively. This information however, must be processed to produce model-ready emission inputs according to the CMAQ model requirements. This adaptation process, usually referred to as emission preparation for modeling, is performed by the SMOKE system. This is a powerful tool but is strongly US-oriented. However, it has been found flexible enough to accommodate and process European emission inventories based on the CORINAIR methodology and it has been successfully applied to Spain. Actually, the main constraints in the application of the SMOKE system are related to the lack of meaningful information regarding chemical speciation or allocation patterns. Therefore, future efforts must be oriented to the improvement of the ancillary information regarding these issues.

Besides generating emission input information for the CMAQ model, this software provides a valuable platform for emission scenario analysis and may assist in the definition and design of abatement measures and environmental strategies.

KEY WORDS

Integrated assessment modeling
Air quality
SMOKE
Emission preparation for modeling

ACKNOWLEDGEMENTS

The authors would like to thank the Environment Ministry of Spain for funding the project and the staff from the “Dirección General de Calidad Ambiental” for their collaboration.

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