DEVELOPMENT AND IMPLEMENTATION OF AN AIR QUALITY
INTEGRATED ASSESSMENT MODELLING SYSTEM FOR THE IBERIAN PENINSULA

presented in June, 2015
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for obtaining the Doctorate in Chemical Engineering
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Madrid, Spain, 2015
La salud del mundo está hecha un asco.
“Somos todos responsables”
claman las voces de la alarma universal,
y la generalización absuelve:
si somos todos responsables,
nadie es.

—Las cinco frases que hacen crecer la nariz de Pinocho
Eduardo Galeano

A mis queridos padres.
Acknowledgements

When the construction and development of AERIS was first offered to me back in 2011, it sounded totally unappealing. After three years of intense work the model is now ready and available, and this would not have been possible without the help of many people that participated directly or indirectly: I would like to say “thank you” to all of them. The first person that believed in my capability to make this model a reality was Dr. Rafael Borge, whose previous tenacious work provided me with a fully-operative air quality model and who opened me for three whole years the doors of his laboratory. Professionally and personally I owe him a lot, so I hope this dissertation constitutes a decent recognition to his work. I would also like to thank Dr. Julio Lumbreras for his experience, know-how, advice and orientation since the early stages of this work. Without his participation in AERIS, this doctoral dissertation would not have been ready by now. I am also very grateful for the trust, the compromise and the motivation that Dr. María Encarnación Rodríguez placed in my work, as well as the new knowledge fields she opened for me. In the current economic situation, the three professors provided me with full and constant economic support.

I want to extend a special “thank you” to my work colleagues at the Environmental Modeling Laboratory of the Technical University of Madrid: David de la Paz, Juan Manuel de Andrés and Javier Pérez. Their help, advice and company made my work a lot easier. I also thank Dr. Adolfo Narros for his help and diligence regarding the administrative aspects of the dissertation, as well as Katerina Foteinopoulou and Nikos Karagiannis for their company and friendship.

The creation of AERIS would not have been possible without the effort of many people that I have not personally met. I am especially grateful with the Mitigation of Air Pollution and Greenhouse Gases program of the International Institute of Applied Systems (IIASA), whose reports on the methodology of GAINS greatly allowed me to extend the modules of AERIS under my own perspective. I also acknowledge the United States Environmental Protection Agency that supports and makes available the CMAQ modeling system through the Community Modeling and Analysis System (CMAS); the Spanish and Portuguese Ministries of the Environment and EMEP for making available the emission datasets and monitoring data used throughout this work; Dr. Maximilian Posch and Dr. Jean Paul Hettelingh of the Coordination Centre for Effects for providing the VSD model for estimating critical loads on soils; Dr. Panos Panagos for making available the SPADE and MEUSIS databases on European soils; Dr.
Acknowledgements

Chad Monfreda of the University of Minnesota for providing the shapefiles with crop covers and yields; Dr. John Douros of the Aristotle University of Thessaloniki for his advice; Dr. Niko Karvosenoja of the Finnish Environment Institute and Dr. Rob Maas of RIVM for their fruitful contributions to the thesis; and Dr. Marialuisa Volta of the University of Brescia for making the documentation of the Opera and APPRAISAL projects publicly available. I am especially grateful with CONACyT (Mexico), which partially funded my doctoral dissertation.

On a more personal perspective, I would like to express my gratitude to my friends Rubén Vásquez and Margarita Hernández for being the persons who initiated me into research and who encouraged me to follow postgraduate studies. Naturally the help and support that my family provided was essential for me to carry on with my career. I would like to thank my parents, Michel Gérard and Patricia for their unconditional support, love and empathy and for understanding my success as their own. Finally, I would like to thank Stephanie for her love, acceptance, support and sense of humor, but above all, for being there.

Madrid, Spain - January 9th, 2014

M. V.
Abstract

Improving air quality is an eminently inter-disciplinary task. The wide variety of sciences and stakeholders that are involved call for having simple yet fully-integrated and reliable evaluation tools available. Integrated Assessment Modeling has proved to be a suitable solution for the description of air pollution systems due to the fact that it considers each of the involved stages: emissions, atmospheric chemistry, dispersion, environmental impacts and abatement potentials. Some integrated assessment models are available at European scale that cover each of the before mentioned stages, being the Greenhouse Gas and Air Pollution Interactions and Synergies (GAINS) model the most recognized and widely-used within a European policy-making context. However, addressing air quality at the national/regional scale under an integrated assessment framework is desirable. To do so, European-scale models do not provide enough spatial resolution or detail in their ancillary data sources, mainly emission inventories and local meteorology patterns as well as associated results.

The objective of this dissertation is to present the developments in the design and application of an Integrated Assessment Model especially conceived for Spain and Portugal. The Atmospheric Evaluation and Research Integrated system for Spain (AERIS) is able to quantify concentration profiles for several pollutants (NO\textsubscript{2}, SO\textsubscript{2}, PM\textsubscript{10}, PM\textsubscript{2.5}, NH\textsubscript{3} and O\textsubscript{3}), the atmospheric deposition of sulfur and nitrogen species and their related impacts on crops, vegetation, ecosystems and health as a response to percentual changes in the emissions of relevant sectors. The current version of AERIS considers 20 emission sectors, either corresponding to individual SNAP sectors or macrosectors, whose contribution to air quality levels, deposition and impacts have been modeled through the use of source-receptor matrices (SRMs). These matrices are proportionality constants that relate emission changes with different air quality indicators and have been derived through statistical parameterizations of an air quality modeling system (AQM). For the concrete case of AERIS, its parent AQM relied on the WRF model for meteorology and on the CMAQ model for atmospheric chemical processes. The quantification of atmospheric deposition, impacts on ecosystems, crops, vegetation and human health has been carried out following the standard methodologies established under international negotiation frameworks such as CLRTAP. The programming structure is MATLAB ® -based, allowing great compatibility with typical software such as Microsoft Excel ® or ArcGIS ®
Acknowledgements

Regarding air quality levels, AERIS is able to provide mean annual and mean monthly concentration values, as well as the indicators established in Directive 2008/50/EC, namely the 19th highest hourly value for $NO_2$, the 25th highest daily value and the 4th highest hourly value for $SO_2$, the 36th highest daily value of $PM_{10}$, the 26th highest maximum 8-hour daily value, $SOMO_{35}$ and $AOT_{40}$ for $O_3$. Regarding atmospheric deposition, the annual accumulated deposition per unit of area of species of oxidized and reduced nitrogen as well as sulfur can be estimated. When relating the before mentioned values with specific characteristics of the modeling domain such as land use, forest and crops covers, population counts and epidemiological studies, a wide array of impacts can be calculated. When focusing on impacts on ecosystems and soils, AERIS is able to estimate critical load exceedances and accumulated average exceedances for nitrogen and sulfur species. Damage on forests is estimated as an exceedance of established critical levels of $NO_2$ and $SO_2$. Additionally, AERIS is able to quantify damage caused by $O_3$ and $SO_2$ on grapes, maize, potato, rice, sunflower, tobacco, tomato, watermelon and wheat. Impacts on human health are modeled as a consequence of exposure to $PM_{2.5}$ and $O_3$ and quantified as losses in statistical life expectancy and premature mortality indicators.

The accuracy of the IAM has been tested by statistically contrasting the obtained results with those yielded by the conventional AQM, exhibiting in most cases a good agreement level. Due to the fact that impacts cannot be directly produced by the AQM, a credibility analysis was carried out for the outputs of AERIS for a given emission scenario by comparing them through probability tests against the performance of GAINS for the same scenario. This analysis revealed a good correspondence in the mean behavior and the probabilistic distributions of the datasets. The verification tests that were applied to AERIS suggest that results are consistent enough to be credited as reasonable and realistic. In conclusion, the main reason that motivated the creation of this model was to produce a reliable yet simple screening tool that would provide decision and policy making support for different “what-if” scenarios at a low computing cost. The interaction with politicians and other stakeholders dictated that reconciling the complexity of modeling with the conciseness of policies should be reflected by AERIS in both, its conceptual and computational structures. It should be noted however, that AERIS has been created under a policy-driven framework and by no means should be considered as a substitute of the ordinary AQM.
Resumen

La mejora de la calidad del aire es una tarea eminentemente interdisciplinaria. Dada la gran variedad de ciencias y partes involucradas, dicha mejora requiere de herramientas de evaluación simples y completamente integradas. La modelización para la evaluación integrada (integrated assessment modeling) ha demostrado ser una solución adecuada para la descripción de los sistemas de contaminación atmosférica puesto que considera cada una de las etapas involucradas: emisiones, química y dispersión atmosférica, impactos ambientales asociados y potencial de disminución. Varios modelos de evaluación integrada ya están disponibles a escala continental, cubriendo cada una de las etapas antes mencionadas, siendo el modelo GAINS (Greenhouse Gas and Air Pollution Interactions and Synergies) el más reconocido y usado en el contexto europeo de toma de decisiones medioambientales. Sin embargo, el manejo de la calidad del aire a escala nacional/regional dentro del marco de la evaluación integrada es deseable. Esto sin embargo, no se lleva a cabo de manera satisfactoria con modelos a escala europea debido a la falta de resolución espacial o de detalle en los datos auxiliares, principalmente los inventarios de emisión y los patrones meteorológicos, entre otros.

El objetivo de esta tesis es presentar los desarrollos en el diseño y aplicación de un modelo de evaluación integrada especialmente concebido para España y Portugal. El modelo AERIS (Atmospheric Evaluation and Research Integrated system for Spain) es capaz de cuantificar perfiles de concentración para varios contaminantes \( \text{NO}_2, \text{SO}_2, \text{PM}_{10}, \text{PM}_{2.5}, \text{NH}_3 \) y \( \text{O}_3 \), el depósito atmosférico de especies de azufre y nitrógeno así como sus impactos en cultivos, vegetación, ecosistemas y salud como respuesta a cambios porcentuales en las emisiones de sectores relevantes. La versión actual de AERIS considera 20 sectores de emisión, ya sea equivalentes a sectores individuales SNAP o macrosectores, cuya contribución a los niveles de calidad del aire, depósito e impactos han sido modelados a través de matrices fuente-receptor (SRMs). Estas matrices son constantes de proporcionalidad que relacionan cambios en emisiones con diferentes indicadores de calidad del aire y han sido obtenidas a través de parametrizaciones estadísticas de un modelo de calidad del aire (AQM). Para el caso concreto de AERIS, su modelo de calidad del aire “de origen” consistió en el modelo WRF para la meteorología y en el modelo CMAQ para los procesos químico-atmosféricos. La cuantificación del depósito atmosférico, de los impactos en ecosistemas, cultivos, vegetación y salud humana se ha realizado siguiendo las metodologías estándar establecidas bajo los marcos internacionales de negociación, tales como CLRTAP. La estructura de programación está basada en MATLAB®,
Acknowledgements

permitiendo gran compatibilidad con software típico de escritorio como Microsoft Excel® o ArcGIS®.

En relación con los niveles de calidad del aire, AERIS es capaz de proveer datos de media anual y media mensual, así como el 19º valor horario más alto para NO\textsubscript{2}, el 25º valor horario y el 4º valor diario más altos para SO\textsubscript{2}, el 36º valor diario más alto para PM\textsubscript{10}, el 26º valor octohorario más alto, SOMO\textsubscript{35} y AOT\textsubscript{40} para O\textsubscript{3}. En relación al depósito atmosférico, el depósito acumulado anual por unidad de area de especies de nitrógeno oxidado y reducido al igual que de azufre pueden ser determinados. Cuando los valores anteriormente mencionados se relacionan con características del dominio modelado tales como uso de suelo, cubiertas vegetales y forestales, censos poblacionales o estudios epidemiológicos, un gran número de impactos puede ser calculado. Centrándose en los impactos a ecosistemas y suelos, AERIS es capaz de estimar las superaciones de cargas críticas y las superaciones medias acumuladas para especies de nitrógeno y azufre. Los daños a bosques se calculan como una superación de los niveles críticos de NO\textsubscript{2} y SO\textsubscript{2} establecidos. Además, AERIS es capaz de cuantificar daños causados por O\textsubscript{3} y SO\textsubscript{2} en vid, maíz, patata, arroz, girasol, tabaco, tomate, sandía y trigo. Los impactos en salud humana han sido modelados como consecuencia de la exposición a PM\textsubscript{2.5} y O\textsubscript{3} y cuantificados como pérdidas en la esperanza de vida estadística e indicadores de mortalidad prematura.

La exactitud del modelo de evaluación integrada ha sido contrastada estadísticamente con los resultados obtenidos por el modelo de calidad del aire convencional, exhibiendo en la mayoría de los casos un buen nivel de correspondencia. Debido a que la cuantificación de los impactos no es llevada a cabo directamente por el modelo de calidad del aire, un análisis de credibilidad ha sido realizado mediante la comparación de los resultados de AERIS con los de GAINS para un escenario de emisiones determinado. El análisis reveló un buen nivel de correspondencia en las medias y en las distribuciones probabilísticas de los conjuntos de datos. Las pruebas de verificación que fueron aplicadas a AERIS sugieren que los resultados son suficientemente consistentes para ser considerados como razonables y realistas. En conclusión, la principal motivación para la creación del modelo fue el producir una herramienta confiable y a la vez simple para el soporte de las partes involucradas en la toma de decisiones, de cara a analizar diferentes escenarios “y si” con un bajo coste computacional. La interacción con políticos y otros actores dictó encontrar un compromiso entre la complejidad del modelado medioambiental con el carácter conciso de las políticas, siendo esto algo que AERIS refleja en sus estructuras conceptual y computacional. Finalmente, cabe decir que AERIS ha sido creado para su uso exclusivo dentro de un marco de evaluación y de ninguna manera debe ser considerado como un sustituto de los modelos de calidad del aire ordinarios.
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1 Introduction

1.1 Environmental Modeling

1.1.1 Overview

The history of humankind is a continuing record of interactions between peoples’ efforts to improve their life quality and the ability of the environment to sustain such well-being levels. During the last two decades, the increasing interest of the human system to impact the environment minimally while keeping the attained growth and welfare levels stresses out the need of having a correct description of the systems and its interactions (Janssen, 1998).…

The description of both, the natural and human systems, depends intrinsically on their complexity and their relevance. Natural systems are much more difficult to model than human or engineered systems, especially because of the intense dynamic and multidimensional interactions that are of physical, chemical and biological nature. Another issue is that the interactions they exhibit may occur in more than one medium, being each spatially heterogeneous (Jakeman and Letcher, 2003).…

**Environmental issues** are usually a consequence of a complex series of interactions among physical and human systems that demand analytical skills beyond those of a single discipline. In order to correctly describe these problems and fully understand them, researchers have worked together to formulate and build integrated tools that would analyze and represent the known interactions underway. A thorough understanding of an environmental problem encompasses disciplines such as physics, biology, ecology and economy. The fact of environmental sciences being inter-disciplinary makes integration between knowledge fields almost indispensable in order to understand the dynamics of complex systems. Furthermore, experimenting in environmental sciences is often difficult due to the large spatial and temporal scales in which phenomena occur which impede the replications of the experiments (Quesnel et al., 2009).…
Chapter 1. Introduction

In the light of the above, environmental sciences often rely on models in order to perform virtual experiments. Broadly, a model is a simplification of reality. People in everyday life think and communicate in terms of models, since they are representations that help to understand a series of phenomena under an intuitive and addressable perspective (Hordijk and Kroeze, 1997). In a more strict sense, models may include for example, (i) data models that are representations of measurements and experiments; (ii) qualitative, conceptual models as verbal or visual descriptions of systems and processes; (iii) quantitative numeric models that are formalizations of the qualitative models; (iv) mathematical methods and models used to analyze other models and to interpret the results; and (v) decision making models that transform values and knowledge into actions (Parker et al., 2002).

In general, models are tools designed to allow a given variable to vary within a practical range to attain outcomes. Simulation, to this respect, is a way of fully exploring the effects of the variation of scenarios and its variables in terms of indicators of system response. This will be translated into a better understanding of the interdependencies between the model variables and their influence on the outcomes. However, modeling an environmental issue in order to generate a model or to produce relevant model-derived data involves a series of steps that need to be correctly fulfilled: (i) refining the research questions; (ii) identifying the system to be studied; (iii) assembling a research tool in the form of an “integrated modeling framework”; (iv) deriving results that are scientifically and policy relevant; (v) and identifying gaps in knowledge and priorities for further research (Alcamo et al., 2002).

1.1.2 The modeling process

Refsgaard et al., (2007) state that any modeling study should involve several parts or actors that would participate in different extents and magnitudes. Usually, modeling efforts include four different types of actors:

- **A manager**, which is the person or organization responsible for the management or protection of any resources (air, water, land, etc.) and therefore, of the modeling study and its outcome. In other words, it is the problem owner.

- **A modeler**, which is the person or organization that develops the model and works it, assembling the modeling study. Usually if the modeler and the manager belong to different organizations, their roles will be situated typically under a consultant-client framework.

- **A reviewer**, which is the person that conducts any kind of external review of a modeling study. The review may be more or less comprehensive depending on the requirements of the particular case. The reviewer is often appointed by the manager for support to match the modeling capability of the modeler.
1.1. Environmental Modeling

- Stakeholders/public, being an interested party with a stake in the management issue, either in exploiting or protecting the resource. Stakeholders might include the following categories: competent resource authorities, interest groups and general public.

From a conceptual point of view, the modeling steps defined previously by Alcamo et al., (2002) carried out during a modeling exercise can be described and grouped in five relevant stages that occur chronologically and whose correct development will result in high-quality system descriptions.

1. **Model study plan.** The objective of this step is to answer a series of questions required as any starting point for any modeling practice. *Why is modeling required for this particular study? What is the overall modeling approach and which work should be carried out? Who will do the modeling work? Who should do the technical reviews? Which stakeholders/public should be involved and to what degree? What are the resources available for the project?* At this stage, the manager should describe thoroughly the problem and its context as well as the available data. It is also a very important, yet overlooked task to analyze the various requirements of the modeling study in terms of the accuracy of the modeling results. An acceptable level of accuracy will vary from case to case and must be seen in terms of the relevance of the results.

2. **Data and conceptualization.** This step involves the modeler gathering all the relevant knowledge about the problem to be studied and develop an overview of the processes and the interactions that exist in order to conceptualize the system to be modeled in sufficient detail. Special consideration should be given to the spatial and temporal detail required of a model, to the system dynamics, to the boundary conditions, and to how the model parameters can be determined from the available data. Modeling processes in alternative ways or with different levels of detail in order to enable assessments of model structure uncertainty should be evaluated as well. The availability of existing computer codes that can successfully address the model should be considered.

3. **Model set-up.** Setting up the model means to transform the conceptual model into a language-specific model that can be run in the selected computer code. A major task in model setup is the processing of data in order to prepare the input files necessary for executing the model. The model in some cases may be run within a graphical user interface (GUI) where many tasks have been automated.

4. **Calibration and evaluation.** This stage is related with the analysis of the model that was previously constructed, first by its calibration and then by the validation of its performance against independent field data. It also involves the estimation of the reliability of the model simulations for the selected application through uncertainty analysis. The obtained results should be described so that the scope of the model use and its associated limitations are documented and explicated.
5. **Simulation and assessment.** Finally, the modeler must use the calibrated and validated model to execute simulations that meet the objectives and requirements of the model study. According to these objectives, these simulations may result in relevant information that can be used in subsequent decision making or to improve understanding about a specific area. It is important to keep in mind the uncertainty degree of the model predictions in order to reach a decision about any aspect.

As it has been previously suggested, the entire modeling process bears an inherent amount of **uncertainty** throughout all of its stages. In general, the total uncertainty associated to the output data obtained from the modeling exercise, is a result of the uncertainty propagation considering a series of sources that occur at each of the before mentioned modeling stages. The type of uncertainty can be described in terms of its nature, being of eminently two types, epistemic uncertainty and stochastic uncertainty. Epistemic uncertainty is related with the imperfect knowledge degree upon which the construction of the model has relied, while stochastic uncertainty or ontological uncertainty is the uncertainty associated with inherent variability (e.g. climate). While epistemic uncertainty is reducible by incorporating new state-of-the-art knowledge, stochastic uncertainty is non-reducible. Yet what often seems to occur is that uncertainty on a certain issue is usually caused by both, epistemic and stochastic uncertainties. There is an additional contribution to the total uncertainty associated with the quality of the used data. Walker et al., (2003) and Refsgaard et al., (2007) agree that uncertainty may originate from a series of sources:

1. **Context and framing.** Models are usually determined at the initial stage of the study where the problem is identified and the focus of the model study selected as a confined part of the overall problem. This includes the external economic, environmental, political, social and technological circumstances that compose the problem in its entire context.

2. **Input uncertainty regarding external driving forces.** These forces may be either within or without the control of the manager. They include the system data that drive the model such as land use maps, pollution sources and climate data that have been incorporated.

3. **Model structure uncertainty**, defined as the conceptual uncertainty caused by the incomplete understanding and simplified descriptions of modeled processes as compared to reality.

4. **Model technical uncertainty**, arising from the uncertainty related to the computer implementation of the model, due to numerical approximations, resolution in space and time or bugs in the software.
1.2 Integrated Assessment Modeling

Integrated assessment models (IAM) are models or tools that aim to describe quantitatively and as much as possible the cause-effect relationship of events, cross-linkages and interactions between issues for a given problem. More specifically, IAMs are designed to analyze phenomena from a holistic perspective. Under this scope, integrated assessment modeling is more than just a modeling exercise; it is in a broader sense, a methodology likely of being used for gaining insight over an array of environmental problems spanning over a wide variety of spatial and temporal scales (Janssen, 1998; Parker et al., 2002).

Unlike many modeling efforts, integrated assessment modeling does not pretend to offer a comprehensive picture of all the relevant processes of a complex reality. It is precisely the interpretative and instructive value of an IAM that is far more important than its predictive capability. Being this so, it is evident that an IAM should be considered an interpretative tool, whereby its predictive value is rather low (Wynne and Shackly, 1994). In spite of the aforementioned, IAMs enable the inclusion of system interactions and feedback mechanisms that yield insights that scattered information cannot offer. This provides useful indications of the potential range and magnitude of the studied phenomena. Moreover, these models are outstanding means of communication between scientists and exponents of all kinds of disciplines; they also foster communication between scientists and decision makers (Morgan and Dowlatabadi, 1996). To this respect, Rotmans and van Asselt (1996) have defined two main goals for integrated assessment modeling: (i) it should add value compared to insights derived from disciplinary research and (ii) it should provide decision makers with useful information.

Constructing an integrated assessment model is a resource-intensive activity that is almost always tailored to the needs of the described system and the chosen impacts. This fact will ultimately condition the modeling effort, since every environmental problem has its own physical characteristics and may respond differently to affecting factors and causes. Furthermore, the resulting effects are unlikely to be the same. Additionally, any Integrated Assessment Modeling exercise should reconcile the problem-specific ecological, social and economic values in the decision making process (Alcamo et al., 2002; Jakeman and Letcher, 2003).

It is almost unconceivable to carry out a complete and sound environmental assessment or modeling effort without some kind of reference to stakeholders or their involvement in the process. The general trend nowadays is to make them part of the modeling process, which usually brings decisions that are implemented with less conflict and more success (Voinov and Bousquet, 2010). In order to attenuate the profound divergence in criteria between scientists and policy makers, the generated scientific information meant to be used in a decision making process has to be (i) relevant to answering the specific policy questions, (ii) readily accessible
Chapter 1. Introduction

and understandable by decision makers, (iii) acceptable in terms of accuracy and trustworthiness, (iv) compatible and usable in specific decision making contexts and (v), provided in a timely fashion (Johnston et al., 2011). The aforementioned highlights that the study of the science-policy interface is an issue of great importance in integrated assessment modeling (Hinkel, 2009).

Intrinsically, IAM is closely related to policy modeling. Policy modeling is defined as a series of academic or empirical research projects carried out under several theoretical frameworks as well as quantitative or qualitative models and techniques in order to evaluate analytically the past (causes) and future (effects) of any policy on society, anywhere and anytime. Integrally, this definition implies that policies are theoretical and technical instruments that are formulated to solve specific problems affecting societies directly or indirectly across different periods of time and geographical spaces (Ruiz-Estrada, 2011). IAM is currently a problem-focused area of research, often being project-based and undertaken on a demand-pull or stakeholder needs basis. These projects are undertaken to address specific sustainability or environmental management issues, in contrast to other types of research that are often science-driven and focused on providing complex systems descriptions and prescriptions for decision makers (Parker et al., 2002).

After a model is delivered as a finished product to the concerned stakeholders, modelers should be able to respond to two basic questions: (i) can we comprehend what we have done with the model sufficiently, as to interpret the results in ways that will be understandable to the professional scientists and communicable to an audience of scientifically-lay stakeholders? And (ii) how valid, trustworthy, reliable and reasonable has the model been as it has evolved throughout the modeling process? In every case, a quality check on the results provided by the model should be carried out. To this respect, an evaluation on the quality of the approved constituent hypotheses should be made. Moreover, its behavior should be compared to that of the real system as to answer whether it fulfills its designated tasks or serves for its intended purpose (Parker et al., 2002).

The system being modeled should be well defined in terms of its physical, socioeconomic and institutional boundaries. It is critical to keep the level of integration of issues and disciplines manageable. Error accumulation through scales and databases needs to be successfully addressed methodologically too (Jakeman and Letcher, 2003). In the same line, scale is an important issue to consider since IAMs are usually designed at one scale although the support these models provide is needed at a smaller (local or catchment) one (Collins et al., 1999; Warren and ApSimon, 1999; Parker et al., 2002). Scales are defined as the spatial extension over which the model is run (the domain) as well as the time and space step (the discretisation) of the model. The selection of a spatio-temporal scale for the different subsystem components of an integrated assessment problem is one of the key considerations for a credible
1.2. Integrated Assessment Modeling

IAM. Scale should be chosen always fine enough to capture the required level of variability of the system response but not finer than is warranted by the availability and quality of input data. The specific breakdown of a system into its subsystem components depends upon the management questions being asked and the nature of the available knowledge. In many cases it has been demonstrated that if scaling properly, modeling complexity might decrease dramatically (Jakeman and Letcher, 2003). A hierarchical-modular approach can be used so that the complexity in certain modules might not appear in higher hierarchical levels and thus simplify analysis and the interpretation of results.

Beside the fact that an IAM should be constructed upon a solid conceptual framework, the crucial stage during the entire modeling process is the materialization of the model as a computer application. Since modeling usually means the formalization of any research questions into mathematical problems, it should also involve the implementation of a numerical algorithm on a computer because usually such problems do not have an analytical solution. This involves choosing a computer platform, a programming language, a compiler, a design an efficient coding which would yield an executable computer model as a final result.

Ideally, IAMs must be designed to cover all the interacting processes that cause a problem. In practice, the casual structure with its many feedbacks need to be simplified depending on the specific perspective taken and the resources available. Over the last two decades, IAMs have become increasingly complex requiring every time more drivers, processes, subsystems and feedbacks that need to be represented. On the other hand, it is widely recognized that IAMs must be structurally flexible to respond quickly and efficiently enough to any new question raised. Likewise, the idea of a modular approach in which such a diverse expertise is brought together is gaining acceptance (Hinkel, 2009).

Integrated assessment models are becoming every time more sophisticated in terms of their software architecture in order to cope with the complexity of the problems they intend to solve. Moreover, since integrated assessment spreads over a wide range of disciplines, the applied software tools must support a wide range of methodologies and techniques. Regarding software and IAM construction, a modeling framework must be selected and defined in terms of a set of software libraries, classes, components, which can be used to assemble and deliver any decision support systems. These frameworks need not be complex programming languages nor require robust computational resources. Some of them are available as commercial packages such as MATLAB® for scientific computing, or GAMS® and AMPL® for management science and operation research applications (Rizzoli et al., 2008). Moreover, decision support by stakeholders highlights the need of having solid scientific models embedded in user-friendly applications, a fact that reveals the importance of having a wide array of computer tools available (Parker et al., 2002).
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In summary, three basic concepts encompass the requirements of an IAM: transparency, structural flexibility and inter-institutional collaboration (Jaeger et al., 2002). Transparency is necessary to better understand, compare and learn from existing IAMs, as every model exhibits a methodological bias. Structural flexibility is suitable in order to reuse or replace parts of an IAM, since building models is a resource-intensive task and the capability of reusing legacy code within new IAMs is very desirable to respond to new questions raised by the decision maker. Inter-institutional collaboration is required because no single institution or scientific discipline alone has the expertise or computational resource to answer the complex socio-environmental problems addressed by integrated assessment.

Integrated assessment modeling is an approach that might be applied to a wide array of problems and environmental issues (Johnston et al., 2011). Environmental problems related to air pollution, water and land management, food production and economics have already been addressed successfully. For the particular case of this work, the current situation of air pollution in the Iberian Peninsula (Spain and Portugal) will be addressed under an integrated assessment modelling approach.

1.3 Air pollution: an IAM approach

The atmosphere is one of the five biogeochemical layers in which life develops. Its main component, air, is an important resource on which many living creatures rely. Its natural composition should not be altered; otherwise undesirable effects on life might take place. In general, the concept of pollution is that of degradation, of a loss of quality or a deviation from purity due to the introduction of external agents. Moreover, there is general consensus in affirming that in the absence of human activities at a given location, the environmental quality tends to be good enough or at least, the one determined by nature. Under this premise, the 2008/1/EC European Directive, related with the integrated pollution prevention and control defines the concept of pollution as the direct or indirect introduction, as a result of human activity, of substances, vibrations, heat or noise into the air, water or land which may be harmful to human health or the quality of the environment, result in damage to material property, or impair or interfere with amenities and other legitimate uses of the environment (Directive 2008/1/EC). To this respect, the state of air is often expressed as air quality (AQ), which is itself a measure of the concentration of pollutants at a given location (Monks et al., 2009).

Clean air is considered to be a basic requirement of human health and well-being (World Health Organization, 2005). The aforementioned highlights the need for reaching a full understanding of the air pollution processes, as well as assuring reasonable air quality standards. These needs have been recognised worldwide, and efforts have been carried out in the last decades to tackle air pollution by establishing stringent limits on emissions. It is therefore important to have enough information on the entire air pollution problem. This may include
1.3. Air pollution: an IAM approach

quantitative information about emissions, sources and temporal patterns in order to inform policy makers and citizens; a rational set of attainable air quality objectives; an assessment of potential impacts on health and welfare; an evaluation of the environmental costs and benefits of certain policies; a constant monitoring of the state of the environment; a proper assignation of liabilities and so on (EMEP - CORINAIR, 2007). To attain all these, public administrations shall conduct programs for the research, testing and development of methods for sampling, measuring, monitoring, analyzing and modeling air pollution processes (Clean Air Act, 2008).

For the specific case of air pollution, many models that describe parts of the problem exist already. For instance, atmospheric models simulate long-range transport, chemical reactions, atmospheric deposition rates, etc. Economic models provide information on the causes of emissions as well as the cost of reducing them through market-available techniques (Hordijk and Kroeze, 1997). Even further, there are models that assess the impact of air pollution on ecosystems such as forests or lakes. It is at this point that IAMs appear as relevant because they cover all the processes that link human activities to environmental effects which in most cases, have economic implications. In other words, they provide a thorough perspective on the entire air pollution problem, covering its causes, its effects and its consequences.

Any IA on air pollution needs to effectively link marginal changes in precursor emissions at the different sources to responses of impact-relevant air quality indicators at a receptor grid cell. Air pollution IAMs are essentially trans-disciplinary, encompassing different sciences that capture pollutant emissions (energy, agriculture, transport, household), complex atmospheric chemistry and dispersion, meteorology, responses of the natural environment to stimuli, abatement potentials, economics, politics, etc. This task has been traditionally carried out by comprehensive atmospheric chemistry and transport models which simulate a wide variety of complex reactions and physical interactions (Amann et al., 2011).

The application of such models under a multi-pollutant perspective obviously highlights the need of having information regarding the emission of such pollutants, as well as information about impacts and effects such as acidification, eutrophication and tropospheric ozone generation (Oxley and ApSimon, 2007). According to Hordijk and Kroeze (1997), IAMs must cover and explain substantially at least three of the following five components:

- Emission sources.
- Atmospheric transport and chemical transformations.
- Environmental effects.
- Abatement-mitigation strategies.
1.3.1 Emission sources

Several models are available for estimating the total amount of emissions that are generated by any activity at a given modeled domain. Such models might be as simple as guidelines for the estimation of emissions regarding the compilation of national emission inventories or much more complicated models that generate scenarios for future regional emissions based on a number of variables. The emissions and costs modules have as starting points two basic concepts, an activity (energy pathway, waste management, industrial production, solvent use) and a strategy resulting from abating the emissions for this energy use (a control strategy). The combination of both gives an emission scenario with is dependent on a set of emissions for each fuel mix and sector combination, particular to every country or modeled domain (Cocks et al., 1998; Cofala et al., 2007).

1.3.2 Atmospheric transport and chemical transformation

Models regarding the atmospheric transport and transformations usually consider chemical and physical processes with different detail degrees in 3-dimensions (longitude, latitude and altitude). Moreover, models can be classified in terms of their mathematical formulation. Lagrangian models consider a defined air parcel in which chemical reactions take place while being transported by the wind fields. Eulerian models, on the contrary, define a hypothetical box in the atmosphere through which material is transported and in which chemical reactions take place. In most cases, IAMs do not include a full long-range atmospheric transport model but a series of source-receptor matrices which are derived from results coming from more sophisticated models, usually 3-D models. A source-receptor matrix assumes a linear relationship between emitters of compounds (usually regions or sectors) and an air quality level at a given location (usually cells). To establish the source-receptor relationships of air pollutants, it is important to consider every atmospheric transport process as well as the chemical conversions and deposition processes that occur across all the spatial scales of the domain (Monks et al., 2009).

1.3.3 Environmental effects on ecosystems

Under an integrated assessment modeling approach, environmental effects are defined as a series of changes that are experienced directly caused by the occurrence or deposition of an airborne pollutant at a specific area. Examples of these might be the acidification of soils and surface waters or the distortion of the nitrogen cycle. The assessment of the produced environmental effects is quantified in two ways: (i) through a quantitative simulation of the environmental impact caused by a particular pollutant and (ii) the computation of the extent to which atmospheric concentrations or deposition rates exceed the pre-defined critical loads or levels. In general, the most common procedure for determining such effects is the calculation of the critical loads of exceedance.
To this respect, critical loads are specific for a given species and are quantified in terms of climate, geology, soil characteristics, vegetation type and land use. Other ways of calculating critical loads are based on the ability of ecosystems to buffer or neutralize pollutant charges. These critical loads are quantified based on steady-state models without considering dynamic aspects (Hordijk and Kroeze, 1997).

1.4 Current state of knowledge

The first efforts intended to develop an integrated assessment model date back to the 1970’s decade. These efforts intended to face the magnitude of the environmental threat caused by the rapid growth experienced in the post-war period (1950’s). The Earths System Model (ESM) was formulated by the International Institute for Applied Systems Analysis (IIASA) as to demonstrate the effect of continued growth, consumption and pollution on the planet. Models such as this one were driven by scientists using empirical data at the global and continental scale. Although they depicted aggregated patterns, they failed to provide tools to decision makers who operated at the local or national level. The first and second-generation IAMs were mostly developed within a single research group for addressing a single research question. Little attention was paid to methodological issues of general importance to IA modeling such as structural flexibility and transparency (Hinkel, 2009).

Changes in modeling approaches arose in part by changes in the financial support available. The funding priority and mechanisms of national governments changed to redirect funds to projects that were identified as important by end-users rather than supporting proposals by scientists in isolation. In this period, politicians and other decision makers decided to sponsor research that would eventually conduce to the availability of tools that would meet their particular needs. As a consequence, scientists found themselves giving answers to questions in terms of financial interest rather than of scientific nature to better understand the system. The question shifted from what are the consequences of this phenomenon? to how much would the consequences of this phenomenon cost? (Parker et al., 2002).

In 1977 the European Monitoring and Evaluation Programme (EMEP) was created as a technical and scientific backup organization for the United Nations Economic Commission for Europe (UNECE) and its negotiations on transboundary air pollution. Ever since, it has studied and determined European emissions in a domain with $150 \times 150$ km or $50 \times 50$ km grids as well as quantified concentrations and pollutant depositions through dispersion models. Furthermore, EMEP has been able to determine the impacts and benefits of an assumed abatement strategy under an IA approach (Fenger, 2009). In 1988 the abatement strategies were developed under the concept of critical load. By definition, a critical load is a load of pollutants where no unacceptable damage is likely to occur. The underlying idea was the negotiation of emission reductions based on the impacts rather than setting equal reduction
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percentages for all countries. Countries are ever since obliged to estimate their critical loads and levels for various areas, receptors and pollutants. At this point in time, a series of IAMs were formulated by different institutions in the world to provide answers to an additional problem often related to air pollution: global warming and greenhouse gases emissions. Their presence generated intense activity within the scientific community and the learned lessons during their modeling processes were applied to the actual IAMs used during negotiations (e.g. the National Emissions Ceilings Directive). In the following sections, the aims and main features of the most relevant IAM systems developed in this period are briefly discussed.

1.4.1 DICE (Dynamic Integrated model of Climate and the Economy)

DICE is an extended version of a traditional optimal growth model that includes the climate sector (Nordhaus, 1994). Its main objective is to maximize the discounted value of unity from consumption subject to a production function that includes a climate-damage factor. Emissions per unit of output are assumed to decline exogenously at a fixed rate and can be further reduced by costly emission-control measures.

1.4.2 RICE (Regional Integrated model of Climate and the Economy)

RICE is a regionalized version of the DICE model. It divides the world into a number of regions, endowed with an initial capital stock, population and technology. RICE is able to manage the possibility of different strategies undertaken by nations and three distinct approaches are worked out: market (uncontrolled), global cooperative and nationalistic policies.

1.4.3 MERGE (Model for Evaluation Regional and Global Effects of GHG reduction policies)

MERGE is an IAM that has as its core a revised version of the Global 2100 database and embodies a general equilibrium model with 5 world regions. In each of these regions the consumer makes both savings and consumption decisions. The simple climate model embedded represents the atmospheric lifetimes of $CO_2$, $CH_4$ and $N_2O$ which yield global changes in radiative forcing and global average temperature change. The key variable that it models is the willingness to pay in each region to avoid a specified temperature change that is a logistic function of regional income, in effect modeled as a world-wide public good.

1.4.4 IMAGE (Integrated Model to Assess the Greenhouse Effect)

IMAGE 1.0 is a model that links several other models from scientific areas with policies for controlling global climate change (Rotmans, 1990). It was designed to develop and evaluate long term climate strategies; it calculates on the basis of historical and future emissions of greenhouse gases, the global temperature and the sea rise. The model itself is a concatenation

The IMAGE 2 model (Alcamo, 1994; Alcamo and Kreileman, 1996) evolved from the earlier version by presenting a geographically-detailed global and dynamic overview of the lined society-biosphere-climate system. These are described by three fully linked subsystems: the energy-industry system, the terrestrial environment system and the atmosphere-ocean system. The model computes greenhouse gases emissions in 13 regions of the world as a function of energy consumption and industrial production. It also simulates the changes in global land cover and other factors that are taken into account to compute the flux of CO$_2$ and other greenhouse gases into the atmosphere.

1.4.5 ICAM (Integrated Climate Assessment Model)

The ICAM model in its three existing versions (ICAM 0, 1 and 2) were developed by the Carnegie Mellon University, at the Department of Engineering and Public Policy (Dowlatabadi and Morgan, 1993). This model incorporates a sophisticated and detailed description of the climate change problem, at each stage quantifying the uncertainties in the model components, following a stochastic modeling approach. It is able to simulate abatement strategies, adaptation to a changed climate and geo-engineering activities. Its development has involved the update of demographic data, fuel market, aerosols, terrestrial ecology and coastal impact modules. The spatial and temporal scales have also been refined to 5 years and 7 geo-political regions. It exhibits a differentiation between high and low latitudes, making it possible to examine the gross differences in the magnitude of climate change, as well as different economic circumstances.

1.4.6 ASAM (Abatement Strategies Assessment Model)

The ASAM model focuses on abating emissions within Europe in terms of establishing different emission ceilings. This model considered the following elements: (i) the emissions of each pollutant in each country; (ii) the transport of pollutants across Europe depending on the meteorology and the modeled time span; (iii) the deposition of pollutants and their sensitivity on the environment; and (iv) the differences in abatement costs and sensitivities for the different countries (ApSimon et al., 1994; ApSimon and Warren, 1996; Warren and ApSimon, 1999). ASAM relies on meteorological data which determine the long-range transport of pollutants which are provided as a series of country specific matrices. These matrices predict the deposition resulting in each of some 700 grid squares ($150 \times 150$ km) as a result of unit emission of pollution from every country. The source-receptor matrices used for this model have been provided by the European Monitoring and Evaluation Programme Meteorological Synthesizing Centre West (EMEP/MSC-W) in Oslo and calculated according to Barrett and Seland (1995). The critical loads were estimated by the Coordinating Centre for Effects (CCE).
in the Netherlands (Posch et al., 1997). Cost curves for this model have been calculated by IIASA (Amann et al., 1994) for each of the modeled pollutants (SO$_2$, NO$_x$, NH$_3$) which include a list of possible abatement techniques available for every country ordered in terms of their marginal cost (i.e. cost per ton of pollutant removed). This integrated assessment model compares the deposition at a determined time with a reference scenario with the critical or target loads at the same scale. It is also able to recalculate exceedances and selects new abatement steps based on the same cost-effectiveness criteria. Further information regarding emission ceilings, costs of abatement and levels of environmental protection can be obtained also from this model.

1.4.7 RAINS (Regional Air Pollution Information and Simulation)

The International Institute for Applied Systems Analysis (IIASA) formulated and designed the Regional Air Pollution Information and Simulation (RAINS) model as a decision-making tool in the light of the UNECE Sulfur Protocol. This model is aimed to the simulation of depositions coming from SO$_2$, NO$_x$ and NH$_3$ emissions, as well as their relationships with acidification and eutrophication targets on a country-by-country basis. This model is also able to calculate an optimal abatement or reduction that would guarantee ecosystem protection for every model grid. This model used to run over a $150 \times 150$ km$^2$ grid square established by EMEP, and has followed the resolution changes of the EMEP grid to $50 \times 50$ km in 1999 and to $0.1^\circ \times 0.1^\circ$ in 2013 (Cocks et al., 1998; Cofala and Syri, 1998). The integrated assessment model RAINS for acid deposition in Europe is also able to link energy scenarios with the further production of country-scaled emissions for sulfur, nitrogen and oxidant precursors (Alcamo et al., 1990; Amann et al., 1995). The RAINS model estimates the internationally (mainly Europe) cost-optimal allocation of emission reductions as well. In other words, it determines where and how much an emission should be decreased to have a minimal cost of removal and still meet pre-selected environmental targets (human health, vegetation and ecosystem protection levels) given by critical loads and levels and constraints such as maximum allowable costs (Ball et al., 2005).

The most important development in the RAINS model has been the integration of a multi-pollutant approach that includes the assessment of emissions of sulfur dioxide, nitrogen oxides, ammonia, non-methane volatile organic compounds (VOC), and primary emissions of fine ($PM_{2.5}$) and coarse ($PM_{10} - PM_{2.5}$) particles. It has been successfully applied on data regarding several European countries in terms of cost and environmental damage evaluation (Kaldellis et al., 2007). Its current structure is depicted in figure 1.1. Several finer-resolution adaptations of the RAINS model have been constructed to the specific cases of some European countries, such as the Netherlands with the model RAINS-NL (Aben et al., 2008) or Italy with RAINS-Italy (Vialetto et al., 2005). Other examples still in development include RAINS-Sweden (Sweden) (Sternhufvud and Åström, 2006) or the IMP model from Ireland (Kelly, 2006).
1.4. Current state of knowledge

1.4.8 UKIAM (United Kingdom Integrated Assessment Model)

The United Kingdom Integrated Assessment Model (UKIAM) (Oxley et al., 2003) encompasses information on emissions, atmospheric transport between sources and exposed areas, criteria for environmental protection, potential emission control measures and costs. The information provided by this model is relevant for any negotiations on the Gothenburg Protocol under the UNECE Convention on Long Range Transboundary Air Pollution (CLRTAP). It is a flexible model whose architecture facilitates the assessment of abatement strategies for a series of pollutants ($NH_3$, $SO_2$, $NO_x$ and $PM$) at different spatial scales. At the national scale, UKIAM is able to provide resolution down to 5 km to spatially optimize abatement strategies. It incorporates information coming from the Fine Resolution Atmospheric Multispecies Exchange model (FRAME) and the National Atmospheric Emissions Inventory for the United Kingdom (Oxley and ApSimon, 2007).

1.4.9 CIAS (Community Integrated Assessment System)

Warren et al., (2008) developed the Community Integrated Assessment System (CIAS), which is a modular and flexible integrated assessment system that addresses climate change and policy making. This model arose as a response for the integrated assessment of the economic and environmental aspects of the climate change problem. The main interest of this model was to simplify the complexity of the outputs from several sets of IAMs. It is also able to test the robustness of its outputs and it allows the user to combine many different individual,
integrated modeling approaches. This is interesting when comparing several modules of different levels of complexity and detail or to assess the goodness of a series of modeling assumptions.

1.4.10 GAINS (Greenhouse Gas and Air Pollution Interactions and Synergies)

The GAINS model brings together information on future economic, energy and agricultural developments as well as emission control potentials and costs (Amann et al., 2011). It also incorporates an atmospheric dispersion module and environmental sensitivities towards air pollution. It addresses threats to human health posed by fine particulate matter and tropospheric ozone, as well as risk of damage to ecosystems from acidification, excess nitrogen deposition (eutrophication) and high levels of ozone. It works under a multi-pollutant context, which quantifies the contributions of sulfur dioxide ($SO_2$), nitrogen oxides ($NO_x$), ammonia ($NH_3$), non-methane volatile organic compounds ($VOC$) and primary emissions of fine ($PM_{2.5}$) and coarse ($PM_{10}$ – $PM_{2.5}$) particles. It also includes information on six greenhouse gases such as carbon dioxide ($CO_2$), methane ($CH_4$), nitrous oxide ($N_2O$) and three F-gases. Additionally, GAINS has developed source-receptor relationships for changes in emissions of $SO_2$, $NO_x$, $NH_3$, $VOC$ and $PM_{2.5}$ for 43 European countries and four sea areas under a 50 km × 50 km grid resolution.

GAINS is able to examine 230 options for reducing $CO_2$ emissions from several category types through structural changes such as fuel substitution, energy efficiency improvements or end-of-pipe measures. GAINS quantifies for 43 countries and regions in Europe the application potentials of various options in the different sectors of the economy and the societal resource costs of these measures. Any mitigation potentials are estimated according to a baseline projection that is considered to reflect current planning. It is the successor IAM of RAINS and is widely available for online consultations ¹ (Klaassen et al., 2005).

1.4.11 Other European IAMs

The MINNI Project (Integrated National Model in support to the International Negotiation on Air Pollution) has been used as a decision-making tool by the Ministry of the Environment of Italy for the last 10 years, as well as in international negotiation processes. This integrated assessment model has been tested in terms of its sensitivity using results from 2005. It incorporates data coming from the Italian Emission Inventory and the GAINS-Italy emission estimates. It has been developed by the Italian National Agency for New Technologies (ENEA) and ARIANET (Zanini et al., 2005; Ciancarella et al., 2011).

¹http://gains.iiasa.ac.at/index.php/home-page
The Finnish IAM includes all the anthropogenic emission sources of multiple pollutants and several scenarios. A study using the Finnish IAM addressed population exposure caused by the emissions of primary fine particulate matter originated from road traffic and domestic wood combustion in 2000 and 2020. The evaluations were performed using source-receptor matrices (SRMs) based on the computations using a local and a regional scale atmospheric dispersion model, on two different grid resolutions: 1 and 10 km (Karvosenoja et al., 2011).

The SONOX model was developed by the Institute for the Environment Protection in Poland, replicating the sequence from emissions of sulfur and nitrogen species through their atmospheric transport and deposition, leading to the further examination of the exceedance of deposition tolerable by ecosystems. The model is of a modular structure combining sub-models representing the four basic processes: emission scenarios construction, development of atmospheric deposition patterns, calculating and mapping critical loads and identifying magnitude and geographical extent of critical loads exceedances. It departed from a modeling structure established at the University of Wrocław, being in some cases improved. Air quality simulations were carried out using FRAME (Oxley et al., 2003). The atmosphere was divided into 33 separate layers extending from the ground to an altitude of 2500 m. Layer thicknesses varied from 1 m at the surface to 100 m at the top of the domain. The model domain covered the entire area of Poland with a grid resolution of 5 km and grid dimensions of 160 x 160 km. Chemical schemes were drawn from FRAME and EMEP, where available (Nahorski and Juda-Rezler, 2011).

### 1.4.12 Integrated Assessment Modeling in Spain

The Technical University of Madrid (UPM) has been lately interested in the development and implementation of an IAM system for Spain. The main objective of this project is to provide the national and local administrations with a tool capable of supporting an efficient environmental policymaking process as to meet regulatory standards and international legislation agreements in the near future. It aims to integrate the research on air quality modeling and emission projections carried out in the last decade, using official data and statistics provided by the National ministries as well as European IAM activities. The system will be based on two major components, the Spain's Emission Projections Model (SEP) and the Integrated Assessment Modeling System for the Iberian Peninsula.

#### The Spain's Emission Projections Model (SEP)

This model is able to calculate emissions from the main atmospheric pollutants and greenhouse gases projected up to 2020. The quantified emissions are based on individual, highly-detailed projections for nearly 300 emission categories according to the SNAP activity classification. National values are obtained through an integrated methodology that assures a full consistency among individual projection in agreement with the National Atmospheric Emis-
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1.4.13 Integrated Assessment Modeling efforts in other areas

Integrated assessment modeling has been applied to a number of different environmental problems different from air pollution to global warming. Examples of these include water and river basins management, land use change modeling, environmental security and even disease management and population responses.

**Water management** has been addressed by several authors. Letcher et al., (2006) studied water allocation techniques through an IA approach for different zones in Thailand and South-east Asia. A similar study was conducted by Jia et al., (2007) for the Yellow River Basin in China, while Liu et al., (2008) and Johnston et al., (2011) have applied analogous approaches to different river basins in the United States. Further advances in IA concerning water have been carried out by Davies and Simonovic (2011) with their modeling and management practice for the global water resources under different scenarios (population changes, global warming, economic growth levels).

Integrated assessment modeling has been successfully applied to **agriculture** under the SEAMLESS (System for Environmental and Agricultural Modeling; Linking European Science and Society) framework. It was designed to compare policy alternatives interacting with agrotechnological options for a defined time horizon, established by a series of policy questions (Janssen et al., 2011).

IA has also been applied to **land use change** modeling in the case of the SIAT (Sustainability Impact Assessment Tools). It was created under the Sustainability Impact Assessment Tool for Environmental, Social and Economic Effects of Multifunctional Land Use in European Regions (SENSOR) fund of the European Union. This project describes and models changes and effects in the forestry, nature conservation, agriculture, energy, transport and tourism sectors (Verweij et al., 2010). Another modeling exercise has been proposed by Schaldach et al., (2011) through the LandSHIFT model, based on the concept of land use systems. It is built up from two main components: one that simulates land use changes and one that computes crop yields and net primary productivity.

**Environmental security** has been addressed by Alcamo et al., (2000) through the GLASS model (Global Assessment of Security System). This model has been designed to link severe environmental changes on a global scale, such as droughts, flooding and large-scale air pollution episodes, with risks and changes in society. Further integration of the GLASS model
1.5 IAM and air quality regulatory frameworks

1.5.1 International

In the international sphere, the Geneva Convention on Long-range Transboundary Air Pollution of 1979 (CLRTAP) is considered an essential framework for the control and reduction of pollution on a supra-national basis. This convention was signed by 34 governments and the European Union as the first international legally-binding instrument that dealt with air pollution under a broad regional scope. It came into force in 1983 and has been further extended by a number of protocols regarding specific pollutants; Helsinki (1985) and Oslo (1994) for sulfur; Sofia (1988) for nitrogen oxides; Geneva (1994) for volatile organic compounds; Århus (1998) for persistent organic pollutants and heavy metals (UNECE, 1979).

Three IAMs have been extensively used in the creation of environmental policies under the UNECE framework; the RAINS model of the International Institute for Applied Systems Analysis (IIASA) in Austria (Alcamo et al., 1990; Amann et al., 1998); the Abatement Strategies Assessment Model (ASAM) of Imperial College London (ApSimon et al., 1994; ApSimon and Warren, 1996); and the Coordinated Abatement Strategies Model (CASM) of the Stockholm Environment Institute (SEI, 1991).

1.5.2 European Union

Airborne pollution has been addressed in the European Union through a series of laws and legal instruments. The Directive 1996/62/CE of the European Council of September 27th, 1996, on ambient air quality assessment and management is the frame Directive from which many other directives and laws have originated. The general objective of this Directive was, among others, to define a common strategy in Europe to evaluate the ambient air quality of each of the member states through the use of common estimation methods and criteria (Directive 1996/62/EC). Directive 2008/50/EC of the European Parliament and of the Council of May 21st, 2008 on ambient air quality and cleaner air for Europe is the legal background of the “Clean Air for Europe” (CAFE) program. This Directive emphasises the need of protecting human health and the environment as a whole, to mitigate emissions at the source, as well as...
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identifying and implementing the most effective reduction strategies at local, national and community level (Directive 2008/50/EC). Directive 2008/50/EC also updates and unifies the regulatory frameworks of the former Directive 1996/62/CE and all the daughter Directives for particular pollutants.

1.5.3 Spain

The Royal Decree (Real Decreto) 102/2011 of January 28th is the transposition of Directive 1996/62/EC to the Spanish legal system, which along with Directive 1999/30/EC of the Council of April 22nd, 1999 regulates the limit emission values for airborne sulphur dioxide, nitrogen dioxide, particles and lead (modified by Decision 2001/744/EC of the Comission). Under Law 34/2007 on air quality and nature protection, the General State Administration is responsible for (i) defining any atmospheric polluting activity; (ii) compiling and updating periodically the national emission inventories; (iii) carrying out the evaluation, following and compilations of the technical information about pollution for complying with the obligations derived from international protocols and agreements; and (iv) integrating the information into the Spanish information system for pollution vigilance and control which would be further transmitted to the Autonomous Communities. These Communities will adopt control measurements and inspection procedures to guarantee the compliance with this Law and will eventually exert any sanctions as their ultimate prerogative (Real Decreto 102/2011).

1.5.4 Portugal

The Executive Decree (Decreto-Lei) No. 102/2010 of September 23rd has established air quality objectives taking into consideration the norms, orientations and programs of the World Health Organization destined to preserve the quality of the ambient air and to improve it. This decree also regulates the level of responsibility of each of the Portuguese public administrations according to their competences through definite execution programs (Decreto-Lei 102/2010).

1.6 Scope and objectives

1.6.1 Background

Research activities were initiated at the Environmental Modeling Laboratory of the Technical University of Madrid (UPM) in the year 2003, when the first atmospheric models were tested and implemented. Over the years, the computing infrastructure of the laboratory greatly increased, allowing a higher modeling complexity which resulted in several projects and scientific papers that have been published. The Environmental Modeling Laboratory has collaborated with institutions from different levels of the Spanish Government, either conducting research and development (R+D) projects or providing environmental consult-
1.6. Scope and objectives

ing. Nevertheless, AQMs are extremely complex and their skill depends on the accuracy of a large number of internal and external parameters (Seaman, 2000). The great amount of data they are fed with, as well as the different modeling hypotheses that are assumed in every case make the adaptation process of the model to a particular exercise a very difficult and time-consuming task. Moreover, the numeric algorithms that these models incorporate are to a great extent, computer intensive. Additionally, configuring, implementing and running an AQM requires a very high degree of technical and computing expertise, as well as the processing and interpretation of the obtained results. Altogether, these facts strongly suggest that running AQMs is not a simple activity, and that undergoing any tuning-up process is usually justified by the extent and importance of the project.

Experience over the years has dictated that policymakers and other stakeholders are frequently interested in having quick answers to sudden questions that are usually formulated out of intuition or curiosity. It would be obviously unfeasible to undergo a complete AQM set-up to answer these questions, especially during negotiation processes. Some other times, public administrations are interested in straightforward outcomes of specific scenarios that are a consequence of future policies. In every case, the limiting factors for the application of AQMs in policymaking and diagnosis are time, modeling skills and computational resources. In this line, the fact of having a fully-integrated AQM calls for the need of having a lighter version, that runs very quickly on a typical personal computer (PC) and whose results are fully processable with commonly-available tools and software.

1.6.2 General objectives

The creation and construction process of an integrated assessment modeling (IAM) system for the Iberian Peninsula has as principal objective the availability of a reliable tool for AQ scenario assessment which is able to provide real-time policy support needed by policymakers at local and national levels. According to Sternhufvud and Åström, (2006), stakeholders have expressed as important assets in IAM the description of alternative scenarios and the possibilities of evaluation the national quality objectives. In general, the created IAM should be able to estimate the impact of further emission reductions in Spain related to environmental policies and objectives. It should also provide an answer about whether the environmental objectives will be sufficiently met, as well as the economic and environmental consequences of the air pollution phenomena. The formulation and construction of this IAM will be based on the WRF, SMOKE and CMAQ models, which constitute the AQM that is commonly used in the Environmental Modeling Laboratory of the UPM. It includes an adaptation of the SMOKE model to the European reality and the integration of databases coming from SNAEI and SEP as inputs for the emission preparation process (Borge et al., 2008). The methodology used to assess health impacts, especially for secondary pollutants such as ozone and fine particles as well as other impacts has been considered. To this respect, it is worth noting that the WRF-SMOKE-CMAQ air quality model has been used for evaluating health and vegetation...
impacts in Spain, highlighting the fact that these impact assessments are probably the ultimate reason for any AQ modelling activities (Boldo et al., 2011; de Andrés et al., 2013).

1.6.3 Specific objectives

The objectives that are discussed in the section above were formulated with the aim of creating a conceptual framework that would justify the creation of the IAM system. However, these objectives might be too abstract and difficult to materialize, so a series of milestones have been established for this PhD thesis in terms of their feasability and their systematic consecution.

- To create a parametrization of the atmospheric dispersion and chemical processes. This parametrization will be applied to transform changes in the emissions of a given pollutant in the studied domain into the concentrations that result after these processes have occurred. This parameterization will be carried out for a number of activities or sectors that have a considerable impact in the AQ levels of the domain or, that are subject of being controled by environmental policy.

- To represent adequately the formation and dispersion processes of secondary pollutants, such as tropospheric ozone and particles as a response to changes in the emissions of their main precursors.

- To transform these atmospheric concentrations into policy-relevant indicators that hint on the possible impacts that air pollution has on the studied domain, related to human health, ecosystems, etc. Additionally, the temporal variations of these indicators need to be accurately represented.

- To understand the deviations that exist between the achieved parametrization and the complete AQM simulation in terms of the assumptions and simplifications that have been applied. Furthermore, it will be desirable to relate these deviations with the applicability potential of the IAM tool.

- To establish a comprehensive framework for the construction and modeling of IAM systems. The methodological aspects of this framework should be clear and robust enough to support the quality of the results yielded by the IAM tool.

- To create an easily - manageable and intuitive computational platform into which the IAM tool is embedded (i.e. a Graphical User Interface) in order to greatly increase the
1.6. Scope and objectives

applicability and use of the abovementioned indicators. In strict sense, full compatibility with traditional PC tools should be guaranteed.

- Finally, the extension of the IAM system to quantify impacts to ecosystems, vegetation, crops and forests as well as health should be described in order to fully complete it. Additionally, hints about the integration of an emission projection system could be considered at this point.
2 AERIS: a general description

In the past section it was stated that the main goal of this project was to design and apply an integrated assessment modeling (IAM) for the Iberian Peninsula. This section consists in a description of the specific model that was created to achieve the objectives presented in section 1.6. The following pages are devoted to the presentation of the model in terms of its structure and components as well as of its capabilities. This section intends to clearly describe the design basis and model limitations for a better understanding on the applicability of the system and the interpretation of its outputs.

2.1 Name

The designed integrated assessment modeling (IAM) for the Iberian Peninsula, as final product, was named AERIS which is an acronym of “Atmospheric Evaluation and Research Integrated model for Spain”. This name was purposely selected to match the latin word aer, aeris which stands for air, ether, atmosphere or even weather. Moreover, this name has a special significance because it is related to the Spanish word aire. The name AERIS will be used hereinafter when referring to the IAM for the Iberian Peninsula developed in this PhD thesis.

2.2 General approach

The AERIS model has been developed as a tool intended for the assessment of air pollution control strategies in Spain. It can also be used for evaluating the effect of policies carried out by Portugal with a lower degree of detail. AERIS is able to calculate ground-level concentration of sulfur dioxide (SO₂), nitrogen dioxide (NO₂), ammonia (NH₃) and two size-fractions of particulate matter (PM₁₀, PM₂.₅) as well as ground-level ozone (O₃). In particular, AERIS provides information about the policy-relevant air quality indicators specified by the Royal Decree 102/2011 of January 28th related to the improvement of air quality (Real Decreto 102/2011) which transposes the European Directive 2008/50/EC (Real Decreto 102/2011)…
2.3. Suitability and limitations

As most IAMs, AERIS was designed to be applied as a scenario analysis tool in the context of international negotiations as well as for the development of control strategies and policies of Spain and its administrative regions (Cofala and Syri, 1998). It provides a consistent framework for the analysis of emission reduction strategies and its convenience in terms of the air quality levels they produce. The current version of AERIS consists in a parameterization of the atmospheric dispersion and chemistry to estimate ambient concentration levels and atmospheric deposition, health impacts, crop losses and damage to ecosystems. The current version is not able to provide estimates of abatement costs under a cost-effective (optimal) perspective, yet the results of AERIS can be readily used for damage-cost estimations.

2.3 Suitability and limitations

AERIS has been designed as a simple, intuitive and user-friendly software tool to be run in any ordinary computer. Its configuration and execution as well as the post-processing of the results it yields do not require a high degree of technical skills. Despite this simplicity, it is the user’s duty to decide on the appropriateness of the results and to fully contextualize the interpretative value of AERIS. It should be clearly noted that AERIS has been built exclusively within an integrated assessment Modeling framework and is not intended to function outside it. In other words, AERIS cannot be used as a substitute of traditional AQMs for other scopes than the usual IAM-focus which is emminently consulting and policy making activities. In a general sense, IAMs are usually based upon uncertain or provisional knowledge and its construction inevitably involves subjective and value-laden assumptions (van der Sluijs, 2002). It is thus the user’s responsibility to judge the applicability and representativeness of the obtained results. This judgement must be based on the understanding of the fundamentals and limitations described in this chapter.

Essentially, AERIS consists in a parameterization of the AQM (described section 1.6). It has been configured to reproduce as accurately as possible the results produced by this conventional AQM through mathematic and statistical processes. This means that AERIS does not address directly any actual physical or chemical processes so any issues concerning the modeling of such processes cannot be explained to the IAM per se. This implies that AERIS would need to be reformulated to take into account future scientific improvements in modelling activities since it is a statistical representation of a particular version of a state-of-the-science chemical transport model. However, the chosen AQM and its specific configuration for the Iberian Peninsula have been fully evaluated and examined in terms of the appropriateness of the results it produces, as published in Boldo et al., (2011), Borge et al., (2007; 2008a,b; 2010; 2012), de Andrés et al., (2012) and de la Paz et al., (2013). The appropriateness of the statistical parameterization needed for a reasonable degree of confidence in the results provided by the IAM is fully evaluated in section 5.
Chapter 2. AERIS: a general description

2.4 Model applicability

The identification of the model applicability is a crucial step towards correctly directing the model to an interested audience. According to Alexandrov et al., (2011), delineating the applicability of a given model should be made using a four-tier approach: conceptual scheme, model formulation, computer code, and specific parameterization. To this respect, it is important to highlight that there must be a reconciliation between the extensiveness of the conceptual scheme and the specific conditions in which such a parameterization can be used (restrictive or not). In the same line, the model code should be characterized in terms of the range of model parameters and inputs it admits.

The four-tier description of model domain needs to be able to answer the following questions: (i) which environmental states may fall within the conceptual scope of the model?, (ii) which environmental states may be assessed (or explored) using the current version of a model in question or its computer code? and (iii) which environmental states may be assessed (or explored) using a specific parameterization of the model? For the specific case of AERIS, these questions can be answered by stating that the model is able to explore any environmental states similar to (or derived from) the established emission scenario reported by the Spanish and Portuguese emission inventories in year 2007 and its subsequent simulation with an air quality modeling system composed of the WRF-CMAQ models, configured as in Borge et al., (2007; 2008a,b; 2010; 2012), for the Iberian Peninsula and within a range of percentual emission variations from this emission scenario between -90% and 90%. Any environmental state that does not comply with these conditions needs to be consequently adapted. When a given environmental state complies with such established bounds, the model does not produce erroneous results and thus we can consider it an adequate performance region. It should be noted that outside this region, the performance level of the model and the credibility of its results will be obviously compromised (Mankin et al., 1975).

2.5 Credibility and reliability of the model

Any model should be endowed with a sufficient degree of credibility prior to its acceptance and use Alexandrov et al., (2011). Moreover, credibility should be supported by other issues such as the authenticity of problem ownership, skills and motivation of the developers, etcetera. Amann et al., (2011) state that credibility related to IAMs should refer to the perception of an actor on meeting the standards of scientific plausibility and technical adequacy of the model. It also highlights the fact that IAMs must incorporate sufficient detail and a comprehensive representation of reality to provide credibility. This credibility however, needs to be somehow modulated due to the inherent nature of integrated assessment, whose holistic perspective often blurs the traditional boundaries between scientific disciplines. There is a general agreement on the fact that model evaluation is the key starting point for establishing credibility. To this respect, sufficient efforts were made to evaluate and validate the model.
2.6. Novelty

under two different perspectives: (i) its statistical comparison in terms of its correspondence with the parent-AQM as well as with independent observations and (ii) the approval of the methodology and results through a scientific peer-review process (Vedrenne et al., 2014). The complete statistical evaluation process of the model (namely of its core formulation) has been presented in section 5, while the results of the peer-review processes can be found in the results dissemination section (chapter 12). Additionally, a call for transparency has been made in presenting in full-detail the complete modeling methodologies that allowed constructing AERIS by the means of this document.

2.6 Novelty

The purpose of designing and developing a new model is to make visible progress in the state-of-the-art (Jørgensen et al., 2006). It is important to highlight the novelty of AERIS in terms of its convenience to the state-of-the-art and to the completion of existing knowledge gaps. Usually, novelty is guaranteed by improving either the conceptual scheme or computer code of a prior model (Alexandrov et al., 2011). In this case, the novelty of AERIS can be made evident in two ways: (i) its complementary status of the WRF-CMAQ modeling system as a screening tool for air-quality evaluation in the Iberian Peninsula and (ii) its extended capabilities and finer resolution than European-level IAMs such as IIASA’s GAINS (Amann et al., 2011). Moreover, the main motivation for developing AERIS was to create a reliable tool for support needed by policy makers at local, regional and national levels, trying to be useful to as many stakeholders as possible. This is especially relevant for Spain, whose institutional division in autonomous communities makes necessary the elaboration of different regional air quality management plans. Furthermore, it should provide answers about whether the environmental objectives will be sufficiently met, as well as the associated economic and environmental consequences. An additional reason for creating AERIS is the fact that continental IAMs are unable to deliver spatially-resolved results suitable for national or regional policies and are usually restricted to Europe-wide common features, being national particularities out of reach (D’Elia et al., 2009). Furthermore, the ancillary information used for the compilation of emission inventories (i.e. bottom-up approaches) or the description of the meteorological conditions is usually of a better quality (Moussiopoulos et al., 2012).

2.7 Structure of the model

The structure of the current version of the AERIS model is modular, following the current trends in integrated assessment. This means that different processes are modeled and described by different modules, with independent programming structures. Since IAMs should consider all the interacting processes involved, the segmentation of AERIS in modules is advantageous when bringing together expertise from various disciplines (i.e. describing impacts to human health, ecosystems or monetary evaluations) (Hinkel, 2009). The flowchart of the general structure of the IAM is shown in figure 2.1.
Figure 2.1: Schematic flowchart of the AERIS modeling system. $p_i$ is the emissions variation percentage of sector $i$ with respect to baseline scenario.
2.7. Structure of the model

2.7.1 Description of the modules

As it has already been stated, the modeling system of AERIS consists in a series of interconnected modules that describe and calculate different variables according to the purpose of the evaluation. Each of these modules has specific characteristics and different dependencies with either internal or external datasets. In this section, a brief description on the basic aspects of each of these modules is given. The detailed presentation of the same modules can be found in the following sections of this work.

- **Emission module.** The emission module of AERIS has been built considering emissions taken from the National Emission Inventories of Spain (SNEI) and Portugal (PNEI) \((\text{MARM, 2009; APA, 2010})\) as well as EMEP gridded-emissions for the rest of the countries in the modeling domain (Andorra, France, Morocco and Algeria) for a baseline scenario (year 2007). The emissions of this baseline scenario refer to this year because they correspond to a representative year of high economic growth and intense polluting activity in Spain, being the last year before the onset of the most recent economic crisis in southern Europe and because it was a year of average meteorological conditions in the Iberian Peninsula (MAGRAMA, 2013). Ideally, any abatement applied or agreed under new protocols will produce reductions in this baseline scenario. The baseline scenario encompasses a set of policy-relevant activities that are described under the SNAP nomenclature, according to the EMEP/CORINAIR methodology used in SNEI and PNEI (EEA, 2007).

- **Spain's emission projections model.** Although not strictly a module developed under the framework of AERIS, the Spain's emission projections model (SEP) allows computing a future emission scenario that will be compared to the baseline scenario to derive the necessary emission variation percentages \((p_i)\) for the correct running of AERIS. The description of the SEP model is not being addressed in this work and for any further documentation the reader must refer to Lumbreras et al., (2008; 2009a,b). As with the module before, the SEP model requires a wide range of external data such as population estimates, vehicle fleets, economic growth previsions, and so on.

- **Air quality system.** The air quality system is the core of AERIS. It is based in a set of source-receptor matrices (SRMs) that have been derived from a statistical parameterization of a consistent number of air quality simulations. The air quality system of AERIS describes the complex meteorological and chemical processes that influence air quality through the use of three sequential modules: atmospheric dispersion, secondary pollutants module and indicator calculation. Although differentiated, these three modules have been gathered to constitute the air quality system under a global idea of “atmospheric transport and transformation module”. The constructed SRMs are sector and pollutant specific across the studied domain which means that there is one individual SRM for every sector and pollutant that is considered by AERIS. In total, AERIS has 51 individual SRMs of which 14 describe the emission-concentration...
Chapter 2. AERIS: a general description

link for NOx, 8 describe SO2, 12 describe PM10 and PM2.5 respectively and 5 describe NH3. In conclusion, AERIS mimics air quality simulations based on the WRF model for the description of meteorology and the CMAQ model for the atmospheric chemistry and dispersion. Although simply described in this paragraph, the construction of the air quality system is the central issue of this work, with several sections devoted to its formulation and validation. Further details on this module can be found in section 4.

• Deposition module. The objective of this module is to provide atmospheric deposition estimates of nitrogen and sulfur species (precursor gases) as a function of the air quality concentration levels estimated by the air quality system and built-in land-use information and properties. The module has been programmed to quantify yearly accumulated depositions per unit of area. In order to correctly determine deposition, this module requires internal datasets only, namely the concentration profiles of nitrogen and sulfur species. Further details on this module can be found in section 6.

• Health impacts module. The health impact module has as main goal the determination of damages to human health in the middle to long term as a function of concentration estimates of particulate matter (PM2.5) and tropospheric ozone (O3). The internal dependencies of the model are the respective air quality levels of the before mentioned pollutants, while the external dependencies are related with population counts at domain-cell level as well as epidemiologic and statistical parameters, where applicable. Further details on this module can be found in section 9.

• Environmental impacts module. In the current version of AERIS, the environmental impacts module is able to quantify damages to ecosystems and soils, expressed as absolute or average accumulated exceedances of critical loads caused by the deposition of nitrogen and sulfur species. Additionally, this module is able to estimate absolute crop losses for several plant species of commercial interest as a consequence of tropospheric ozone levels. This module is external data-intensive and relies on a series of critical loads database for ecosystems as well as on land covers for the assessed crops. The internal data that are used by this module are the profiles of accumulated deposition per unit of area and air quality levels. Further details on this module can be found in section 8 and 7.

2.8 AERIS software implementation

One of the most important motivations of this project was to actually materialize the undertaken modeling approaches in a distributable model, subject of being used as tool by actors and stakeholders. To this respect, it is important to keep in mind that the final users of AERIS might not necessarily be high-skilled computer users and could be unfamiliar to air quality modelling. As a consequence, AERIS is (currently) being delivered embedded in a MATLAB®-based graphic user interface (GUI) as final product. MATLAB® is a programming language that supports cell arrays to the definition of classes in object-oriented programming. It is
2.9. Availability and licensing

The current version of the AERIS model is available only under agreement between the Environmental Modeling Laboratory of the Technical University of Madrid (UPM) and stakeholders and actors. Additionally, the AERIS model is not currently being distributed to end-users under any licence agreements. Interested parties and potential users are requested to address any enquiries to the developers for further information.

2.10 Processing tools and ancillary software

2.10.1 MATLAB

MATLAB® is the core software upon which the IAM is based. The modeling system has been created in MATLAB® and written for its use within its platforms. The vast majority of the calculations, data processing, statistical analysis and visualization routines were carried out by the application of different programs ran into this software. MATLAB® is a numerical and mathematical computation tool that is available commercially, which is basically used for...
Chapter 2. AERIS: a general description

simulation purposes. It relies in a series of matrix-manipulation techniques and a strong numerical calculator; it also has algebra functionalities that run under a symbolic toolbox (Sen and Shaykhian, 2009). Additionally, MATLAB® is a programming language which supports a similar data structure than that of C++, or from the so-called cell arrays for the definition of classes in object oriented programming. In other words, it is equipped with all the essential constructs of a higher programming language at a moderate cost. Its use and learning involves little programming skills, while providing quickness in simulations and results retrieval (Ibrahim, 2011).

MATLAB® provides an open environment equipped with sophisticated visualization capabilities that allow creating maps and plots with a high quality and interpretative value (Bekas et al., 2005). Additionally, MATLAB® was used to build a Graphic User Interface (GUI), through the implementation of the Guide Package. This package groups a set of tools designed to build GUIs easier and faster and has made this process as easy as program development, using a Rapid Application Development package (Azemi and Yaz, 1999). The final purpose of the GUI is to allow an easy interaction of the user with the MATLAB® codes (mainly input file preparation and output file display) (Sokos and Zahradnik, 2008).

2.10.2 ArcGIS

The construction of an IAM system frequently involves the use of a Geographic Information System (GIS). A GIS is an effective management tool used for the processing of geographical information resources, with a wide application in the fields of environmental impact assessment (Zhong et al., 2011). The GIS used for the construction of the IAM was ArcGIS®, which is a collection of GIS components and developer resources with great mapping capability. Moreover, it is one of the most robust and widespread GIS software with great compatibility with common PC-tools such as Microsoft Office® (Ormsby et al., 2010). The use of a GIS allowed georeferencing meteorological fields, emissions, concentrations and outputs from the IAM to their corresponding location in the studied domain.

2.10.3 VERDI

The Visualization Environment for Rich Data Interpretation (VERDI) was extensively used for the conversion of I/O API files into GIS-compatible files, such as shapefiles or ASCII grids. Moreover, its use was very helpful for the quantification of policy-relevant indicators (such as maxima or 8-h means). VERDI is a flexible and modular Java-based visualization tool that has been specifically designed for the visualization of multivariate gridded datasets, such as the outputs obtained from CMAQ and other environmental models (Adams and He, 2011). VERDI is an easily-installable tool that runs in Windows®, allowing an efficient import process of AQM outputs to more usually-available processing tools. It is also able to provide pictures and maps, as well as temporal series.
2.11 Facts on the construction of AERIS

In this section, some facts about the general construction process of the IAM are presented. This information is provided in order to demonstrate the complexity of an AQM in its general usage and to highlight the suitability of AERIS for quick evaluations and screening exercises. Regarding time, we can identify the following stages: (i) emission inventory preparation time, (ii) air quality simulation time, (iii) data extraction and processing time, (iv) construction of the SRMs time and (v) construction and update of the GUI time. The average times involved in each of these phases for one experimental run of the AQM are presented below.

1. Emission inventory preparation time: 20 minutes.
2. Air quality simulation time: 840 minutes.
3. Data extraction and processing time: 35 minutes.
4. Construction of the SRMs time: 10 minutes.
5. Construction and update of the GUI time: 20 minutes.

For every experimental run, a total time of 925 minutes was needed. Since the complete construction process of AERIS involved carrying out 190 runs of the AQM, the total needed time was 2899 hours or 120 days. Approximately 91% of the total time was spent running the AQM. The first run of the AQM was carried out on March 3rd, 2012 and the last one was completed on September 6th, 2013. This period of time includes weekends, vacations and interruptions due to maintenance. An analogous quantification can be carried out for the amount of data that had to be managed. The average data amount produced in each of the before mentioned phases for one experimental run of the AQM is the following for a proficient user.
Chapter 2. AERIS: a general description

1. Emission inventory preparation data: 4774 MB.
2. Air quality simulation data: 37005 MB.
3. Data extraction and processing data: 532 MB.
4. Construction of the SRMs data: 125 MB.
5. Construction and update of the GUI data: 24 MB.

In total, for every run the volume of data that is generated equals 42460 MB. The complete number of runs needed for the construction of AERIS generated a total volume of 7.69 TB that had to be correctly managed and stored in disks.

2.12 Final remarks on the description of AERIS

The main objective of this chapter was to introduce AERIS as a model in terms of its most important features. This description should be sufficient to understand in general terms the relevance and novelty of the IAM, as well as its general formulation. More specific details on model implementation and basic execution techniques can be found in appendix A.1. In-depth description on the different model components is given in the following chapters, which contain a full description on the general production process of AERIS. is devoted to the description of the air quality modeling system on whose results the parameterizations that conform AERIS were made. The fourth chapter is dedicated to a detailed and rigorous description of the modeling practices that allowed describing in a simple and operative way the complex processes that participate in the air pollution phenomenon. The fifth chapter is dedicated to the validation of the parameterizations that originated our model, as well as evaluating the validity of the underlying modeling hypotheses. The sixth chapter describes the construction and design of a module that quantifies atmospheric deposition processes, while the seventh chapter relates such deposition processes with damages or impacts on ecosystems and soils. The eighth chapter is devoted to describing the impacts of gaseous air pollutants on crops and vegetation, while the ninth chapter is dedicated to the description of impacts on human health as a consequence of the exposure to particulate matter and ozone. The final chapter consists in an in-depth analysis of the credibility and reliability of AERIS in terms of its comparative performance with “reference” air pollution IAMs such as GAINS. At the end, the reader should be completely familiar with the basic methodology of AERIS and its relevance for the successful description of the air pollution problem in the regional context of the Iberian Peninsula.
Air quality model & processing tools

As it has been stated in chapter 1, the construction of an Integrated Assessment Modeling system (IAM) has to be carried from the results of an Air Quality Modeling system (AQM) from a state-of-the-science, full chemical-transport model with a particular configuration or set up. This configuration is intimately related with the geographic domain of interest (in this case, the Iberian Peninsula) and should reflect it as accurately as possible. In the forecoming sections, a complete description of the AQM, its configuration and adaptation to the Iberian Peninsula is presented. Additionally, a detailed description of the software, hardware and other tools used for the construction of AERIS is shown. The combination of the methodological aspects in chapter 4 with the configuration options presented in this chapter provide the IAM system with a robust scientific basis.

3.1 Air quality modeling system

The air quality modeling system (AQM) used is based on the Community Multiscale Air Quality (CMAQ) model (Byun and Ching, 1999; Byun and Schere, 2006). Emissions were processed by the Sparse Matrix Operator Kernel Emissions (SMOKE) modelling system (Institute for the Environment, 2009) as described in Borge et al., (2008). The meteorological fields needed to simulate air pollution processes have been generated with the Weather Research and Forecasting (WRF) modelling system (Skamarock and Klemp, 2008). A schematic representation of the AQM is shown in figure 3.1. This AQM has been fully operative at the Environmental Modeling Laboratory of the Technical University of Madrid since year 2007. It has been used to conduct several air pollution studies and its results have been fully contrasted by the scientific community (Boldo et al., 2011; Borge et al., 2007; 2008a,b; 2010; 2012; de Andrés et al., 2012; de la Paz et al., 2013).

The Community Multiscale Air Quality (CMAQ) model is a multi-pollutant, multiscale air quality model that incorporates a series of state-of-science techniques for the simulation of both primary and secondary atmospheric pollutant. It is also able to describe the processes
that are involved in its transport, transformation and deposition, on both regional and urban scales. CMAQ is a reliable tool for assessing air quality through the simulation of ambient air concentrations and deposition processes (wet or dry) of most pollutants. Its algorithms can handle all the major issues concerning photochemical oxidants, particulate matter, and acid and nutrient deposition under a holistic approach.

The simulation system is also able to address tropospheric ozone, visibility and fine particles under a one atmosphere perspective, where the utmost complex interactions between regional and urban scales are confronted. It is thus quite versatile too for representing several spatial and temporal scales (Borge et al., 2009). CMAQ has been formulated to address regulatory assessments as well as scientific studies conducted by both, government and research institutions. CMAQ is also a valuable tool for simulating concentrations over a wide range of meteorological conditions and a variety of geographical areas (Byun and Ching, 1999).

The Meteorology-Chemistry Interface Processor (MCIP) was used for linking the outputs from a meteorological model (in this case, WRF) and the Chemical Transport Model (CTM) of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. The linking process results in a complete set of meteorological data needed for AQ simulations. This processing tool was created due to the fact that most meteorological models are not designed for air quality modeling purposes. It produces two types of files (time-dependent and time-independent) in I/O API format which are fully compatible with the SMOKE and CMAQ models, allowing complete information flow and exchange processes (Wang and Tonnesen, 2002). This tool processing routine is licensed as free software and is fully available at the Community Modeling and Analysis System (CMAS) Center.
3.1. Air quality modeling system

One of the most interesting features it includes is an advection and diffusion module that addresses horizontal diffusion through an eddy diffusion approach (Pleim, 2007). Through this module, the formation of aerosols and reactions between pollutants in aqueous phase is also described. A plume-in-grid module, which is also incorporated, includes a number of algorithms that deal with subgrid scale physical and chemical processes that have an impact in plumes released at given point sources. Within the modelling system, a particle modeling and visibility routine is included which is in fact one of the major advancements of CMAQ; it intends to address issues concerning fine and coarse particles, such as those related to sulfate, nitrate, ammonium, organic fractions of particles and aerosol water. This module might also be able to describe the deposition of semi-volatile organic compounds (SVOC) through the use of parametrisations (Byun and Ching, 1999; Eder and Yu, 2006).

Emissions have been modelled and processed with the Sparse Matrix Operator Kernel Emissions (SMOKE) Modelling System. It allows data processing through a high performance computing sparse-matrix algorithms and is based on a parallel approach to emissions processing and was redesigned and improved with the support of the United States Environmental Protection Agency (USEPA). This tool is quite useful in decision making regarding controls for regional and urban applications. It also includes a mechanism for preparing inputs for air quality research, having a prognostic function as well. To this respect, it is worth pointing out that SMOKE has been oriented to applications in the United States, so a further adaptation stage had to be implemented in order to deal with Spanish conditions.

SMOKE is able to deal with most gaseous pollutants such as carbon monoxide (CO), nitrogen oxides (NOx), volatile organic compounds (VOC), ammonia (NH3), sulphur dioxide (SO2), particulate matter (either PM2.5 or PM10) and a large number of toxic pollutants such as heavy metals, benzene or formaldehyde. An emissions processor such as SMOKE has as baseline function the transformation of resolution of emission inventory data to the input resolution of an air quality model. It transforms thus, the emission inventory through temporal allocation, chemical speciation and spatial allocation according to the specific AQM requirements (Institute for the Environment, 2009).

The meteorological fields have been generated through the Weather Research and Forecasting (WRF) model, also known as Advanced Research WRF (ARW). This model includes the latest developments for modeling under a fully comprehensible nonhydrostatic approach (Skamarock and Klemp, 2008). The ARW modeling system is a flexible, state-of-science simulation system that is suitable for a huge range of applications to describe mostly any scale size and specifically tested and evaluated for air quality modelling applications in the Iberian Peninsula (Borge et al., 2008b).
Chapter 3. Air quality model & processing tools

Figure 3.2: The Iberian Peninsula seen from the space.

The three models that compose the AQM used in the construction of AERIS are **free access** open-source models, that can be easily downloaded from the Internet. They admit any changes in the code and are supported by an active community of users through online fora\(^2\).

### 3.2 Model configuration

In every case the **model configuration** was carried out by incorporating the details that are presented as follows. The meteorology was simulated with the WRF model whose inputs (terrain elevation, land use and land-water masks, soil humidity and temperatures) from the United States Geological Survey (USGS) and the European Centre for Medium-Range Weather Forecasts (ECMWF). The main input to drive WRF simulations is the meteorological contained in the global reanalyses, combined with observations. These datasets are available from NCEP (Global Tropospheric Analyses Final Analysis). The dynamic options and parameterisations for the meteorology simulations are the following, according to what has been already tested and published in *Borge et al.*, (2008a).\(^2\)

- **Boundary layer scheme.** Yonsei University (YU) Planetary Boundary Layer scheme (Hong et al., 2006).\(^2\)

- **Microphysics.** WRF Single - Moment 6 - class (WSM6) microphysics scheme (Hong and Lim, 2006).\(^2\)

- **Surface model.** Noah Land - Surface model (Chen and Dudhia, 2001).\(^2\)

- **Radiation.** Longwave: Eta Geophysical Fluid Dynamics Laboratory (GFDL) longwave radiation scheme (Schwarzkopf and Fels, 1991).\(^2\) Shortwave: MM5 shortwave radiation scheme (Dudhia, 1989).\(^2\)

Emission datasets have been prepared entirely according to the modeling hypotheses stated in Borge et al., (2008a), which is a full adaptation of the SMOKE model to the particular conditions of Spain. Further comments regarding the origin and nature of the emission inventories, as well as the considerations carried out for keeping consistency with the integrated assessment modeling system are found elsewhere in this work. The coupling of the emissions with the related chemistry and transport model (CMAQ) was accomplished through the Meteorology-Chemistry Interface Processor (MCIP). The basic configuration of the chemistry and transport model is the following:

- **Advection.** Yamartino global mass-conserving scheme (Yamartino, 1993).
- **Vertical diffusion.** Asymmetric Convective Model version 2 (ACM2) (Pleim, 2007).
- **Chemical mechanism.** CB-05 gas-phase mechanism (Yarwood et al., 2005).
- **Numerical integrator.** Euler Backward Iterative (EBI) solver (Hertel et al., 1993).
- **Aerosols.** $4^{th}$ generation model CMAQ aerosol mechanism with extensions for sea salt emissions (Bhave et al., 2005) and thermodynamics (Nenes et al., 1999).

### 3.3 Modelling domain

#### 3.3.1 General description

The **Iberian Peninsula** is located in south-western Europe and occupied by **Spain** and **Portugal**. It extends over approximately 581,000 km$^2$ (figure 3.2). The Spanish territory in the modelling domain is (498,541 km$^2$) and includes the Balearic Islands (4,992 km$^2$) and the autonomous cities of Ceuta and Melilla in the coast of North Africa (32 km$^2$) (Ministerio de la Presidencia, 2012). Portugal has a total extension of 92,090 km$^2$ and is located in the western section of the Iberian Peninsula, bordered exclusively by Spain. A very small fraction of the north-eastern peninsula's territory is occupied by **Andorra** (468 km$^2$) (CIA, 2012).

The peninsula is crossed by a number of **mountain ranges**, many of their divides exceeding 2000 m above sea level. Enclosed by these mountain ranges, two large central plateaus and some tectonic basins define the main drainage network, which includes several rivers of more than 500 km long (Tagus, Douro, Ebro, Guadalquivir) (del Barrio et al., 2010).

Synoptic air masses create a NW to SE precipitation gradient, ranging from Atlantic humid climate zones on the north and west coasts, to pure Mediterranean on the eastern coast, the SE corner becoming the most arid zone of Europe. Indicative total annual precipitation in those extremes is 1600 and 140 mm/yr, respectively (figure 3.2). In addition, altitudinal temperature and precipitation gradients are associated with the main mountain ranges, creating a genuinely...
alpine climate in the Pyrenees, and well distributed extra-zonal belts of humidity elsewhere (Ministerio de la Presidencia, 2012)... The Iberian Peninsula is home to over than 55 million people, being one of the most populated regions in the European Union. Spain is the country with the largest population in the area (45 million), while Portugal hosts an amount of only 10 million (CIA, 2012)... The Iberian Peninsula has several densely populated urban centers such as Madrid, Barcelona, Lisbon, Valencia and Porto.

### 3.3.2 Modeled Domain

The modeled domain consisted in a grid of 16 km spatial resolution, centred at 40° N, 3° W. It has 75 cells in the east-west direction and 60 in the north-south direction (4,500 cells), covering the entire Iberian Peninsula (Spain, Portugal and Andorra). Extended areas of France, Morocco and Algeria are also included on this domain. The geographic representation of the gridded domain is shown in figure 3.3.

### 3.4 Emission Inventory

In order to increase accuracy and consistency, the modeled domain (D2) took boundary conditions from a larger domain at European-scale (D1) into which is nested (figure 3.4). It has been widely accepted that emission-related inputs must be as detailed and specific as possible for the different domains involved in the simulation, and simultaneously they must be consistent across the scales (Borge et al., 2007)... In addition, they have to be flexible and detailed enough to reflect the outcome of relevant measures and meet the modeling system requirements (Borge et al., 2012)... Consequently, a specific emission inventory has been developed and adapted for each of the four modeling domains in this application. Emission processing was performed with SMOKE in every case.
3.4. Emission Inventory

3.4.1 Domain 1 - Europe (D1)

Anthropogenic emissions were taken from the EMEP inventory, which consists of a gridded inventory ($50 \times 50 \ km^2$) that covers Europe completely and which was compiled from national submissions to the Convention on Long-range Transboundary Air Pollution (LRTAP) (Vestreng, 2003). The temporal profiles and vertical distribution needed to resolve the emissions were those used in the EuroDelta experiment (van Loon et al., 2007). Biogenic VOCs (isoprene, monoterpenes and other biogenic volatile organic compounds) have been computed off-line (the Global Emission Inventory Activity, GEIA) and processed into SMOKE by implementing the algorithms proposed by Guenther et al. (1996). Both inventories were consistent with the EMEP/CORINAIR methodology used to compute emissions in the Spain’s National Emission Inventory (SNAEI) (EEA, 2009). This domain provides boundary conditions for the smaller domain (Domain 2 - D2).

3.4.2 Domain 2 - Iberian Peninsula (D2)

The emissions used for this domain were taken from the National Emission Inventories of Spain (SNEI) and Portugal (PNEI) and processed with SMOKE. Hourly, 16-\textit{km} resolved emissions from 184 area-source categories were used along with detailed information regarding temporal patterns and release conditions of 1720 stacks belonging to 62 point-source categories. The inventory was chemically speciated according to the Carbon Bond CB-05 mechanism, a lumped structure chemical mechanism including 156 reactions and 69 species including aerosols (Yarwood et al., 2005). The chemical composition of VOCs, $PM_{2.5}$ and $NO_x$ emissions in the inventory was specified through 221 chemical speciation profiles built from the relevant information contained in the EMEP-CORINAIR guidebook and the USEPA SPECIATE database (EEA, 2009; Hsu et al., 2006).
Chapter 3. Air quality model & processing tools

Figure 3.5: NUTS-3 regions of Spain within the considered modeling domain.

Figure 3.6: NUTS-3 regions of Portugal within the considered modeling domain.
The Spain's National Emission Inventory (SNEI) is compiled every year by the Spanish Ministry for the Environment (Ministerio de Agricultura, Alimentación y Medio Ambiente - MAGRAMA) (MAGRAMA, 2009). It constitutes the most reliable and comprehensive information regarding past emissions of atmospheric pollutants at a national level, according to what will be discussed in section 4.2. The National Emission Inventory follows a SNAP nomenclature and the general methodology specified by the CORINAIR framework (EMEP-CORINAIR, 2007). The maximum spatial resolution of the database is the fourth level (NUTS-3) of the NUTS territorial classification for statistical purposes, proposed by Eurostat and which corresponds to the provincial level (apart from point-sources) (Eurostat, 2011). It is worth noting that the emissions reported at a NUTS-3 level underwent a process of spatial allocation through the use of surrogate data. This process was carried out following a classical approach of activity ratios computation in each grid cell (Boulton et al., 2002; UNC, 2006), supported by a GIS. The geographical allocation was driven by land use information coming from the CORINE Land Cover 2000 (EEA, 2000).

### 3.4.3 Layer assignment

The emissions reported in the abovementioned inventories have been allocated into a series of vertical layers within the 3-D modeling domain. Up to 8 layers were included in the first kilometer above ground level to allow a high resolution inside the boundary layer. It has been assumed that area sources emit into the lower vertical layer of the modeling domain, while the emissions coming from point sources are processed with SMOKE to accurately reproduce its initial buoyancy and momentum (Borge et al., 2008).

Figure 3.7 shows an example of the distribution of the vertical layers considered in the modeling domain. Since the vertical coordinate system depends on the local topography (terrain-following sigma-coordinates), the layer definition is specific to each point. The example illustrate the near-surface levels in the Madrid region. The allocation processes are highly
dependent on the type of source that is being modelled (stack height, gas flow, exit velocity and temperature) and meteorological conditions. Figure 3.8 represents the spatial allocation within vertical layers of the emissions of \( \text{SO}_2 \) generated by all the considered sectors that emit this pollutant in AERIS (section 4.2). It can be seen that area sources, such as cities or international shipping limit their emissions to the lowest pressure level (ground level), while sources such as coal-fired power plants distribute their emissions within several pressure layers, depending on their operative conditions.

### 3.5 Exchange data formats

One of the main issues in data management is that data are structured for simulation on grid arrays. For example, species concentrations and emission rates are stored in four dimensional (4-D) arrays that contain the concentration of each species in each cell grid for each time step. Meteorological data such as temperature and pressure are one scalar per grid point and can be stored in 3-D arrays, while boundary conditions and domain top layer heights are usually represented in 2-D arrays (Miehe et al., 2002). The generic structure of these files is shown in figure 3.9, for a typical 4-D array file.

To this respect, the construction of the AERIS system based on the AQM required using input data in very different formats. Addressing the format-compatibility issue is paramount when dealing with multi-model systems, since these typically produce large four-dimensional datasets that range from tens of megabytes to several gigabytes. A fundamental component for effective collaboration is to save model results in a form that is machine-independent, binary
and self-describing. Therefore, it is very important to rely on standardization and conventions (Brandmayer and Karimi, 2000).

### 3.5.1 NetCDF - I/O API

The NetCDF (Network Common Data Form) format is probably the most popular and common in the earth sciences community. It meets the before mentioned criteria and is relatively simple (less than 30 function calls). Moreover, it is freely available and is supported by Unidata, having interfaces for many languages such as Fortran, C, C++, Java, Perl, MATLAB® and IDL (Signell et al., 2008). A typical NetCDF model represents data as a set of multi-dimensional arrays that have sharable dimensions. They also have a series of metadata attached to individual arrays to the file. In NetCDF terminology, the arrays are considered as variables that may have attached attributes (Hartnett and Rew, 2008). Particularly, information flows across SMOKE and CMAQ require the use of the I/O API (Input/Output Applications Programming Interface) variation of the NetCDF libraries, which has been specifically designed for environmental modeling. I/O API is an easy-to-learn, easy-to-use programming library for data storage and access, available from both Fortran and C (Coats, 1995).

### 3.5.2 Comma-separated value (CSV) files

The use of comma-separated value files (CSV) was crucial for the construction of AERIS, due to the fact that complex array files such as NetCDF can be simplified into these files through the use of several available conversion tools. CSV files are common interchange formats that are useful for storing tabular data, since they have one line for each feature in the table (layer) where at least two fields per line must be present. In the concrete case of AERIS, CSV files did not need any headers or special naming conventions. In a way, it can be said that CSV files are the simplest array-files that exist and that are compatible through a numerous set.
of distributions, they are easy to produce manually and managed through typical desktop programs such as text or script editors. This format was chosen for AERIS’s SRMs, input files, intermediate files and output files (chapter 2). Its compatibility with the software used for processing was also a reason for this choice.

3.6 Hardware and equipment

As it has been somehow implied in the past sections, AQMs (and more generally, numerical models) require considerable computational efforts to run their simulations. The time and efficiency of these simulations is determined by the available hardware infrastructure and its quality (Jiménez-Hornero et al., 2006). As a consequence, the construction of the SRMs of AERIS involved the extensive use of a custom-made parallel computer cluster running Linux, due to its low cost, flexibility and accessibility. The computer cluster consists of 16 nodes, one master and fifteen slaves using the Message Passing Interface paradigm (MPI) library for parallel implementation which has been developed for C++ and Fortran applications (Karniadakis and Kirby, 2003). Each of these computers has an Intel Core 2 Duo microprocessor (3.33 GHz) and the master has a 1 TB hard disk in which the operating system has been installed (Debian GNU/Linux 6.0 squeeze) and the output files are written. The nodes are connected through a local network where the master node acts as the main console (figure 2.2). Necessary calculations other than those inherent to air quality simulations, programming and data processing routines for the construction of AERIS as an independent application were carried out in a typical desktop PC equipped with an AMD Athlon™64 X2 Dual Core Processor (1 GB RAM). This PC ran Windows®XP and OpenSUSE 10.2 as operative systems.

3.7 Credits

It is worth noting that the configuration of the AQM that was needed for the construction of AERIS was not developed by the author of this thesis. Although the methodology has been fully explained in this section, for further details readers should be referred to the following publication which are strictly devoted to the description of the AQM that has been fully exploited by the author for the production of the IAM.

Advanced air quality models (AQMs) are essential tools to understanding atmospheric processes so that the influence of emissions on air quality can be described. Therefore, they have been extensively used as tools for assessing the result of the implementation of pollutant emissions abatement strategies in recent years (Karvosenoja and Johansson, 2003; Schöpp et al., 2005).

It has been discussed in the introduction that the main goal of AERIS is to forecast atmospheric concentration values as a result of changes in the emissions produced by a given sector. The integrated assessment modelling approach that is developed and explained in this section is eminently based on a series of results provided by the deterministic AQM discuss in chapter 3 and their parameterization. The main aim is to obtain similar results in almost real-time. To this respect, a parameterization methodology of this AQM was needed in order to accurately imitate its results. The assumptions regarding the links between emissions and resulting air quality as well as the general procedure are explained in this section.

4.1 Studied pollutants

The pollutants that were considered as subject of study in this work are the most relevant in terms of their legal regulations and the health impacts they are usually associated with. These pollutants are subject of policy and control strategies, since they are regulated by a number of international agreements and standards, most notably the Geneva Convention (CLRTAP). As a consequence, AERIS has been modeled to describe their emissions and atmospheric fate through the before mentioned SRMs for a number of activity sectors that are described later. The following gaseous pollutants are currently considered by AERIS: nitrogen oxides ($NO_x$), sulfur dioxide ($SO_2$), tropospheric ozone ($O_3$) and ammonia ($NH_3$). Additionally, two size-fractions of particulate matter have been selected: particles with an aerodynamic diameter of less than 10 micrometers ($PM_{10}$) and particles with a diameter of less than 2.5 micrometers ($PM_{2.5}$).
4.1.1 Nitrogen oxides - $NO_x$

Nitrogen oxides are basically emitted during the combustion of carburant and fossil fuels. The main emission sources are transport (persons, freight, air-traffic), non-transport engines, heating installations, industry and agriculture. Nitrogen oxides are emitted as gaseous species - either nitrogen monoxide ($NO$) or dioxide ($NO_2$). Nitrogen monoxide and dioxide are highly reactive in the atmosphere, being the reason of indicating emissions as a sum of $NO$ and $NO_2$ (figure 4.1). After a short stay in the atmosphere, nitrogen returns to the biosphere as dry nitrate deposits along with rain or snow, introducing supplementary nitrogen into the ecosystems. Nitrogen also compounds play an important role in the formation of ozone at ground level and other photo-oxidants, especially during summer smog periods. Such induced pollutants have adverse effects on vegetation and human health. Nitrogen compounds contribute also to the formation of secondary aerosols, having a direct impact on fine particles (Kelly et al., 2010). Gaseous $NO_2$ is particularly dangerous for human health, since it entrains inflammatory manifestations at a respiratory tract level. It intensifies also the irritant effects of allergenic substances. When nitrogen dioxide augments suddenly, a higher level of deceases and hospitalizations are registered caused by respiratory diseases as well as heart diseases and infections (CFHA, 2005; Kampa and Castanas, 2008).

4.1.2 Sulfur dioxide - $SO_2$

Sulfur dioxide ($SO_2$) comes from both, anthropogenic and natural sources. The main anthropogenic source of such emissions is the combustion of fossil fuels that contain sulfur, such as coal or petroleum (figure 4.2). Another source of sulfur is petroleum refining, smelting processes of sulfidic ores, sulfuric acid production and paper industry (EEA, 2010). Sulfur may be emitted naturally at volcanoes and through various biological processes in the oceans. Some other emissions have been registered for forest fires and sulfur springs (Vestreng et al., 2007). Some of the most important effects of deposited sulfur compounds include the loss of neutralization capacity in soil and water, the loss of nutrients (e.g. potassium and magnesium) in soils and the consequent liberation of toxic aluminium to the soil solution.
and waters. Whether sulfur is stored in soils or slowly released will depend directly on the biogeochemical conditions at the given place; therefore, it is to be expected that their negative effects may last for decades (Smith et al., 2001). Sulfur compounds are also deemed of having negative impacts on human health and are related to some extent with climate change too (Georgoulias et al., 2009). Although acid rain has been traditionally the most studied issue concerning sulfur compounds emissions, it is now the formation of particulate matter that draws attention. Sulfur dioxide is an aerosol precursor that is likely to be transformed into sulfate aerosols (Vestreng et al., 2007).

4.1.3 Particulate matter - \( PM_{10}, PM_{2.5} \)

Particles come from very different sources, which are generally classified into three categories: anthropogenic and natural sources of primary particles. In the anthropogenic source of primary particles, mobile sources like road traffic - cars, trucks and vans - are widely found, although construction engines and machines are also important (figure 4.3). In this category, it is also evident the presence of heating and combustion installations, industrial processes, construction zones, agricultural surfaces and livestock facilities and to a lesser extent, incineration of agricultural and forestry waste. Particles are almost entirely originated by combustion processes (fine particles included in \( PM_{2.5} \)) as well as abrasion and resuspension phenomena (coarse particles, included in \( PM_{10} \)). Other sources such as fungi and bacteria generation during waste storage processes might also be included (CFHA, 2007).

Secondary particles are produced via diverse and complex chemical reactions in the atmosphere and are further transformed into secondary particles. Such gases are sulfur oxides (\( SO_2 \)), nitrogen oxides (\( NO, NO_2 \)), ammonia (\( NH_3 \)) and diverse volatile organic compounds (\( VOC \)) (Mihalopoulos et al., 2007). Among the main sources for this category, road traffic (\( NO_x, NMVOC \)), non-traffic motors (\( NO_x, NMVOC \)), solvent and fuel activities (\( NMVOC \)), agriculture (\( NH_3 \)), industrial and domestic heating installations (\( NO_x, SO_2 \)), cement and construction sectors (\( NO_x, SO_2 \)), as well as waste incineration (\( NO_x, SO_2 \) and \( VOC \)) are counted.
Among the natural particle sources, volcanoes (particles and gases), oceans (marine aerosols in coastal zones), soil erosion in dry locations (mineral dust formed by the disaggregation of rocks and sand under the wind effects) are present. Forest and prairie fires, pollens, spores and microorganisms (virus, bacteria, and fungi) as well as plants (NMVOC) are other important particle sources (CFHA, 2007).

Studies conducted in Europe have shown that exposure levels to particles are associated with an increased mortality. Particles, especially particles with diameters smaller than 2.5 μm have been shown to carry the most adverse health effects into people, manifesting basically as lung cancer and other types of cardiopulmonary mortality. Coarse particles (PM_{10} – PM_{2.5}) affect principally the lungs and the respiratory airways. The fine fraction of particles (PM_{2.5}) has a special health concern in many countries since it can penetrate deeply into the respiratory system and get into the bloodstream through a rapid absorption or worse, remain embedded in lung tissue for prolonged periods. Short term effects to high particle episodes include eye irritation, respiratory inflammation, infections, bronchitis, pneumonia, headaches and allergic reactions. Short term effects include respiratory disease, lung cancer and damage to organs like the brain or nerves (Boldo et al., 2011).

4.1.4 Tropospheric ozone - O₃

Tropospheric ozone (O₃) is formed predominantly through a series of photochemical reactions that involve precursors like nitrogen oxides (NOₓ) and volatile organic compounds (VOC). The atmospheric photochemical processes involve hundreds of species and include a series of complex phenomena that occur at different temporal and spatial scales (Varotsos, 1994; Atkinson, 2000). Tropospheric ozone accumulates especially during favourable meteorological conditions, reaching hazardous levels. The formation of tropospheric ozone has deep implications on atmospheric chemistry, since it plays a significant role in controlling the chemical lifetimes and reaction products of many atmospheric species and also influence organic
4.1. Studied pollutants

![Manure spreading over fields in Palencia (Castilla - León).](image)

4.1.5 Ammonia - NH$_3$

Ammonia is the most important alkaline constituent in the atmospheric boundary layer. Along with sulfur dioxide (SO$_2$) and nitrogen oxides (NO$_x$), it has a significant effect on aerosol formation and deposition processes. For example, the presence of NH$_3$ can increase the oxidation rate of SO$_2$ in the clouds by more than one order of magnitude, inducing high precipitation rates of sulfur as sulfate. Additionally, ammonia enhances the formation of secondary aerosols by producing ammonium nitrate (NH$_4$NO$_3$) and ammonium sulphate ((NH$_4$)$_2$SO$_4$), which are responsible for a high proportion of the deterioration of visibility and health effects (Sotiropoulou et al., 2004).

It is well established that the major source of NH$_3$ emissions to the atmosphere is the volatilization from decomposing livestock waste as well as waste storage (figure 4.4), with the second
major source being losses from agricultural plant canopies, particularly following the application of N fertilizers (Sutton et al., 2000). NH$_3$ emissions cause serious negative environmental effects such as acidification and eutrophication of natural ecosystems and contribute substantially to the formation of secondary atmospheric particulates (Erisman and Schaap, 2004).

4.2 Studied sectors and activities

According to what has been presented in section 4.4.1, the modeling approach followed for the construction of AERIS involves describing the emission of a certain pollutant by a given sector through the creation of one source-receptor matrix (SRM). However, in any geographic domain there are usually hundreds of sectors and activities that release pollutants to the atmosphere with some of them contributing more importantly to the total emissions of a given pollutant. Since the parameterization and modeling process needs to be kept as simple as possible, it is obvious that SRMs will be constructed only for those sectors.

Table 4.1: Description of the SNAP sectors.

<table>
<thead>
<tr>
<th>SNAP group</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SNAP 01</td>
<td>Combustion in energy and transformation industries</td>
</tr>
<tr>
<td>SNAP 02</td>
<td>Non-industrial combustion plants</td>
</tr>
<tr>
<td>SNAP 03</td>
<td>Combustion in manufacturing industry</td>
</tr>
<tr>
<td>SNAP 04</td>
<td>Production processes</td>
</tr>
<tr>
<td>SNAP 05</td>
<td>Extraction and distribution of fossil fuels and geothermal energy</td>
</tr>
<tr>
<td>SNAP 06</td>
<td>Solvent and other product use</td>
</tr>
<tr>
<td>SNAP 07</td>
<td>Road transport</td>
</tr>
<tr>
<td>SNAP 08</td>
<td>Other mobile sources and machinery</td>
</tr>
<tr>
<td>SNAP 09</td>
<td>Waste treatment and disposal</td>
</tr>
<tr>
<td>SNAP 10</td>
<td>Agriculture</td>
</tr>
<tr>
<td>SNAP 11</td>
<td>Other sources and sinks</td>
</tr>
</tbody>
</table>

The election of the emission sectors that were modeled through SRMs was accomplished by an analysis of their emissions and their overall contribution. In every case, this judgment needs to be carried out with data coming from a reliable emission inventory which in this case was the National Emission Inventory of Spain (SNEI) for year 2007. Additionally, the emission sectors were chosen according to whether they are or may be subject of emission abatements and policy control.

The SNEI has been compiled according to the CORINAIR methodology and is consistent with the Selected Nomenclature for Air Pollution (SNAP)$^3$ (EMEP - CORINAIR, 2007).$^3$ An example of this code is presented for domestic heating activities in section 4.4.1 as SNAP 020202

$^3$
4.2. Studied sectors and activities

Table 4.2: Studied emission activities and relevant pollutants for Spain.

<table>
<thead>
<tr>
<th>SNAP code</th>
<th>Description</th>
<th>( NO_2 )</th>
<th>( SO_2 )</th>
<th>( PM_{10} )</th>
<th>( PM_{2.5} )</th>
<th>( NH_3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>010000</td>
<td>Coal-fired power plants ( \geq 300 ) MW</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
</tr>
<tr>
<td>020202</td>
<td>Residential plants ( &lt; 500 ) MW</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
</tr>
<tr>
<td>030000</td>
<td>Combustion in manufacturing</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>040000</td>
<td>Production processes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>070101</td>
<td>Passenger cars - highway driving</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
</tr>
<tr>
<td>070103</td>
<td>Passenger cars - urban driving</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
</tr>
<tr>
<td>070201</td>
<td>Light - duty vehicles - highway driving</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
</tr>
<tr>
<td>070203</td>
<td>Light - duty vehicles - urban driving</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
</tr>
<tr>
<td>070301</td>
<td>Heavy - duty vehicles - highway driving</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>070303</td>
<td>Heavy - duty vehicles - urban driving</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0707/08</td>
<td>Break, tire and road abrasion</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>080500</td>
<td>Airports (air traffic)</td>
<td>·</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>080600</td>
<td>Agriculture (machinery)</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td></td>
<td></td>
</tr>
<tr>
<td>080800</td>
<td>Industry (machinery)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100101</td>
<td>Culture w/ fertilizers - permanent crops</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>·</td>
</tr>
<tr>
<td>100201</td>
<td>Culture w/ fertilizers - arable land crops</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>·</td>
</tr>
<tr>
<td>100500</td>
<td>Other agricultural activities</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>·</td>
</tr>
<tr>
<td>110000</td>
<td>Other sources and sinks</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Methodology hierarchically classifies emissions in 11 groups according to the nature of the sectors that produce them (Table 4.1) and assigns a unique 6-number code to each sector for identification purposes. Table 4.2 shows the individual emission activities that have been selected for the development of SRMs and that are included in the current version of AERIS along with their respective SNAP codes and the pollutants for which they are relevant.

In addition to the sectors mentioned in Table 4.2, SRMs were developed for the total pollutants emitted by Portugal. To characterize its emissions, information from the National Emission Inventory of Portugal (PNEI) for year 2007 was used. Details on the emission compilation, harmonization and processing for modelling can be found somewhere else (Borge et al., 2008a; Lumbreras et al., 2012). Although the emissions reported in the PNEI are detailed enough to distinguish between sectors, this detail degree is unnecessary because Portuguese emissions cannot be controled by Spanish stakeholders. This means that Spanish environmental decisions are not likely to be equally reproduced in Portugal. However, Portuguese emissions are up to a certain extent considerable and should be taken into consideration because of their influence on the Iberian air quality levels.

In the same line, the strategic geographic location of the Iberian Peninsula whose coasts stretch in the Mediterranean Basin and the Atlantic Ocean make it a zone with a high influence
Chapter 4. Emissions & air quality module

Table 4.3: Sectorial contribution to the total emissions in Spain (2007).

<table>
<thead>
<tr>
<th>SNAP code</th>
<th>NO₂</th>
<th>SO₂</th>
<th>PM₁₀</th>
<th>PM₂.₅</th>
<th>NH₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>010000</td>
<td>14.5</td>
<td>67.8%</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>020202</td>
<td>1.4%</td>
<td>1.1%</td>
<td>6.2%</td>
<td>16.7%</td>
<td>–</td>
</tr>
<tr>
<td>030000</td>
<td>13.9%</td>
<td>5.8%</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>040000</td>
<td>–</td>
<td>3.1%</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>070101</td>
<td>8.9%</td>
<td>–</td>
<td>1.3%</td>
<td>3.8%</td>
<td>–</td>
</tr>
<tr>
<td>070103</td>
<td>4.7%</td>
<td>–</td>
<td>2.0%</td>
<td>5.6%</td>
<td>–</td>
</tr>
<tr>
<td>070201</td>
<td>1.4%</td>
<td>–</td>
<td>0.5%</td>
<td>1.5%</td>
<td>–</td>
</tr>
<tr>
<td>070203</td>
<td>2.8%</td>
<td>–</td>
<td>0.8%</td>
<td>2.3%</td>
<td>–</td>
</tr>
<tr>
<td>070301</td>
<td>7.2%</td>
<td>–</td>
<td>1.0%</td>
<td>2.9%</td>
<td>–</td>
</tr>
<tr>
<td>070303</td>
<td>4.0%</td>
<td>–</td>
<td>0.7%</td>
<td>2.1%</td>
<td>–</td>
</tr>
<tr>
<td>0707/08</td>
<td>–</td>
<td>–</td>
<td>3.1%</td>
<td>4.8%</td>
<td>–</td>
</tr>
<tr>
<td>080500</td>
<td>0.5%</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>080600</td>
<td>7.8%</td>
<td>0.8%</td>
<td>16.9%</td>
<td>21.9%</td>
<td>–</td>
</tr>
<tr>
<td>080800</td>
<td>4.6%</td>
<td>0.0%</td>
<td>8.1%</td>
<td>10.5%</td>
<td>–</td>
</tr>
<tr>
<td>100101</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>8.7%</td>
</tr>
<tr>
<td>100201</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>22.5%</td>
</tr>
<tr>
<td>100500</td>
<td>–</td>
<td>–</td>
<td>8.7%</td>
<td>1.9%</td>
<td>29.6%</td>
</tr>
<tr>
<td>110000</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>24.7%</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>72.2%</td>
<td>78.7%</td>
<td>27.2%</td>
<td>72.5%</td>
<td>85.6%</td>
</tr>
</tbody>
</table>

of shipping-related emissions. To this respect, international ship transit was also modeled with its own SRM for SO₂ and NOₓ. In order to confirm the preponderance of the before mentioned sectors as to limit analysis only to them, the contributions of each of them to the total were calculated. Table 4.3 presents these contributions in terms of a percentage of the emissions of the respective sector to the total emissions of a given pollutant. The following sections contain a detailed explanation of each of the considered sectors for the construction of AERIS. In these sections, information regarding the composition of the sector, its inventory compilation process and its spatial allocation will be given as well as the relevance of each of these sectors to the air quality levels in Spain for policy purposes.

4.2.1 010000 - Coal-fired power plants ≥ 300 MW

This sector is a variation of SNAP sector 010101 (Combustion plants ≥ 300 MW), since it only includes those facilities that currently consume coal in all of its varieties as main fuel. The included varieties are hard coal, lignite, coke, bituminous and sub-bituminous coals. Moreover, this sector does not make a distinction between the different technologies used for the transformation of these fuels, including various types such as dry bottom (DBB) and wet bottom boilers (WBB) as well as fluidized bed combustion (FBC) technologies. According to the SNEI, most of the power plants already have implemented different technologies to
minimize the emission of pollutants to the atmosphere such as desulfurization processes for \( \text{SO}_2 \) or special burners for \( \text{NO}_x \). Nevertheless, emissions have been computed for these facilities as a function of the consumed fuel (MARM, 2009). To this respect, the only coal-fired power plants that exist in Spain are 15 facilities that belong to five different electric companies and are located throughout the territory, as listed in table 4.4. The geographic locations of the considered coal-fired power plants is depicted in figure 4.5.

### 4.2.2 Residential plants < 50 MW

The emissions of this sector are related to any boilers with a nominal power of less than 50 MW and which are mainly installed in the residential sector. This concrete sector was chosen as representative of the SNAP 02 group basically because the vast majority of the boilers used for heat generation in Spain have a nominal power of less than 50 MW (MARM, 2009). The considered activity variable is, as with the previous sector, the consumption of fuels and is also dependent on a series of emission factors that have been taken from the CORINAIR methodology. In this case, the SNEI specifies that emissions come from the consumption of various fuels such as natural gas, LPG, diesel fuel, wood and coals of vegetal origin. Residential heating plants are modeled as area sources and are present throughout the Spanish territory. The emissions quantified by the SNEI have been spatially allocated paying attention to the population density data coming from the CORINE Land Cover 2000 database (EEA, 2000). For modeling purposes, this surrogate was named surrogate 01 and as it can bee seen in figure 4.6.

<table>
<thead>
<tr>
<th>Power Plant</th>
<th>Auton. Comm.</th>
<th>Electrical company</th>
<th>Lat</th>
<th>Lon</th>
</tr>
</thead>
<tbody>
<tr>
<td>C.T. Aboño</td>
<td>Princip. de Asturias</td>
<td>HC Energía</td>
<td>43.55°N</td>
<td>5.72°W</td>
</tr>
<tr>
<td>C.T. Alcudia</td>
<td>Islas Baleares</td>
<td>Endesa Generación</td>
<td>39.81°N</td>
<td>3.08°E</td>
</tr>
<tr>
<td>C.T. Anillas</td>
<td>Castilla y León</td>
<td>Unión Fenosa</td>
<td>42.83°N</td>
<td>6.51°W</td>
</tr>
<tr>
<td>C.T. As Pontes de García Rdz.</td>
<td>Galicia</td>
<td>Endesa Generación</td>
<td>43.45°N</td>
<td>7.83°W</td>
</tr>
<tr>
<td>C.T. Compostilla</td>
<td>Castilla y León</td>
<td>Endesa Generación</td>
<td>42.83°N</td>
<td>6.51°W</td>
</tr>
<tr>
<td>C.T. La Robla</td>
<td>Castilla y León</td>
<td>Unión Fenosa</td>
<td>42.78°N</td>
<td>5.61°W</td>
</tr>
<tr>
<td>C.T. Lada</td>
<td>Princip. de Asturias</td>
<td>Iberdrola Generación</td>
<td>43.31°N</td>
<td>5.69°W</td>
</tr>
<tr>
<td>C.T. Litoral</td>
<td>Región de Murcia</td>
<td>Endesa Generación</td>
<td>36.98°N</td>
<td>1.91°W</td>
</tr>
<tr>
<td>C.T. Los Barrios</td>
<td>Andalucia</td>
<td>Endesa Generación</td>
<td>36.18°N</td>
<td>5.41°W</td>
</tr>
<tr>
<td>C.T. Meirama</td>
<td>Galicia</td>
<td>Unión Fenosa</td>
<td>43.22°N</td>
<td>8.41°W</td>
</tr>
<tr>
<td>C.T. Narceca</td>
<td>Princip. de Asturias</td>
<td>Unión Fenosa</td>
<td>43.28°N</td>
<td>6.38°W</td>
</tr>
<tr>
<td>C.T. Pasajes de S. Juan de Lezo</td>
<td>País Vasco</td>
<td>Iberdrola Generación</td>
<td>43.32°N</td>
<td>1.91°W</td>
</tr>
<tr>
<td>C.T. Puertollano</td>
<td>Castilla-La Mancha</td>
<td>Viesgo Generación</td>
<td>38.64°N</td>
<td>4.12°W</td>
</tr>
<tr>
<td>C.T. Teruel</td>
<td>Aragón</td>
<td>Endesa Generación</td>
<td>40.99°N</td>
<td>0.38°W</td>
</tr>
<tr>
<td>C.T. Velilla del Río Carrión</td>
<td>Castilla y León</td>
<td>Iberdrola Generación</td>
<td>42.81°N</td>
<td>4.84°W</td>
</tr>
</tbody>
</table>

Table 4.4: Coal-fired power plants ≥ 300 MW in Spain.
4.2.3 030000 - Combustion in manufacturing

For the purposes of the SNEI and of AERIS, the term **combustion in manufacturing** defines any combustion process that takes place within any industrial centers but that is not specific of any particular manufacturing industry. Regardless of the type of activity, they are grouped as specified in the 2007 version of SNEI in three subgroups: (i) Unspecific industrial combustion (030100), Combustion processes without contact (030200) and Combustion processes with contact (030300). Moreover, according to the SNEI, the following industrial activities that reported having combustion devices within their processes.

- Iron and steel industries.
- Nonferrous materials.
- Transportation equipments.
- Non-energetic mining.
- Pulp and paper industries.
- Wood and lumber activities.
- Fabric and leather industries.
- Chemical and petrochemical industries.
- Non-metallic minerals.
- General machining.
- Food and tobacco industries.
- Printing and offset activities.
- Construction activities.
- Other sectors.

The description of the combustion in manufacturing sector through a SRM includes **only** those sources that could be modeled as **area sources**. The fact of excluding the point sources
4.2. Studied sectors and activities

Figure 4.6: Implemented surrogates for spatial allocation - (Nos. 01, 02, 08 and 10).

from this SRM as well as not elaborating specific matrices for them is a result of the great variety of industries that exist which cannot apply abatement options in the same way. This is a consequence of the different emission abatement technologies that each of these point sources incorporates.

According to the SNEI, area sources were described in terms of their emissions through the use of emission factors which are dependent of the concrete technology that each of the before mentioned activities implements within its facilities, as well as fuel consumptions as the main activity variable. To this respect, fuel consumption of the following fuels were considered: bituminous coals, coke, black lignite, wood, woodchips, agricultural waste, fuel oil, diesel fuel, kerosene, natural gas, LPG and biogas (MARM, 2009). The total contribution of area sources to the SNAP 03 emissions of NO\textsubscript{x} in 2007 was of 71.6\%, while the contribution to the emissions of SO\textsubscript{2} equalled 56.2 \%. These contributions suggest that most of the combustion activities in manufacturing are being carried out at installations that are not easily identifiable. As a result, the allocation procedure for the emissions of this sector followed a surrogate (surrogate 02) elaborated from industrial and commercial land uses specified by the the CORINE Land Cover 2000 database (EEA, 2000). Figure 4.6 shows the spatial distribution of surrogate 02 throughout the Iberian Peninsula.
4.2.4 040000 - Production processes

The processes that this sector intends to describe are those manufacturing and production processes that are not related to combustion activities. However, these processes usually have an important energetic demand, basically through heat transfer operations. Unlike sector SNAP 03, the description of SNAP 04 has been carried out according to the specific industrial activities that actually generate the emissions of interest. In general, it can be said that the industrial activities that are being described by this sector are very different in nature and it is clear that the available abatement options may greatly vary between them. The considered activities by this sector are the following.

- Petroleum industries.
- Iron and steel industries.
- Organic chemical industries.
- Halocarbons and sulfur hexafluoride.
- Non-ferrous metal industries.
- Inorganic chemical industries.
- Wood, paper pulp, food and other industries.
- Minor industries.

The description of this sector in the SNEI is very complex, since most of the industrial processes generate atmospheric emissions differently. Chemical conversions as well as unit operations (distillation, mixing, pre-treatments, etc.) are consistently described through a detailed methodology that can be directly consulted at the SNEI 2007 document (MARM,
2009) ... The variety and complexity of the industrial activities led to limit the elaboration of a SRM referred only to area sources. It should be noted that area sources contribute only to 10% of the total SO₂ emissions in 2007, the rest being emitted exclusively by point sources. Due to the fact that these point sources are of very different type, it is an ultimately complex task to independently develop SRM for each industry or source cluster so analysis was limited only to area sources. Additionally this decision was made as a compromise of number of simulations and the share of emissions due to this sector as well as the reduced significance of common potential measures or evolution hypothesis for such heterogeneous group of activities.

Table 4.5: Vehicle classification criteria.

<table>
<thead>
<tr>
<th>Fuel Type</th>
<th>Vehicle Technology</th>
<th>Pass. Cars</th>
<th>LDV</th>
<th>HDV</th>
<th>Buses</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gasoline</td>
<td>Conventional</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gasoline</td>
<td>Pre - ECE</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gasoline</td>
<td>ECE 15/01 - 04</td>
<td>•</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gasoline</td>
<td>Euro I - 91/542/CEE I</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Gasoline</td>
<td>Euro II - 91/542/CEE II</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Gasoline</td>
<td>Euro III - 99/96/CE I</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Gasoline</td>
<td>Euro IV - 99/96/CE II</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Gasoline</td>
<td>Euro V - 99/96/CE III</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Diesel</td>
<td>Conventional</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diesel</td>
<td>Euro I - 91/542/CEE I</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Diesel</td>
<td>Euro II - 91/542/CEE II</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Diesel</td>
<td>Euro III - 99/96/CE I</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Diesel</td>
<td>Euro IV - 99/96/CE II</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Diesel</td>
<td>Euro V - 99/96/CE III</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Hybrid</td>
<td>Euro IV - 99/96/CE II</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>LPG - Natural gas</td>
<td>Euro I - 91/542/CEE I</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>LPG - Natural gas</td>
<td>Euro II - 91/542/CEE II</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>LPG - Natural gas</td>
<td>Euro III - 99/96/CE I</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>LPG - Natural gas</td>
<td>Euro IV - 99/96/CE II</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
</tbody>
</table>

4.2.5 070000 - Road traffic

In this section, the description of the seven SRMs that were developed for the characterization of the SNAP 07 category is presented. Road traffic is an especially sensitive and important sector to be characterized within an European control and policy framework due to the fact that several cities in the continent face serious problems when meeting air quality regulations due to road traffic emissions (Fontaras et al., 2014). As a consequence, the creation of separate SRMs for the most important traffic-related sectors was necessary in order to conduct detailed consultations to AERIS on these matters. As with the previous sectors, the complete description of the road traffic sector was carried out according to the information coming from
the 2007 version of the SNEI. The basic methodology that was followed for the estimation of the emissions related to traffic activity was the CORINAIR methodology, which implies using emission factors coming from the Computer Programme to Calculate Emissions from Road Transport (COPERT III) (Ntziachristos and Samaras, 2000).

In general lines, the difference between passenger cars, light-duty vehicles (LDV) and heavy-duty vehicles was made according to their weight, fuel and engine size, using as information source a complete vehicle database. **Passenger cars** were defined as vehicles destined mainly to the private transportation of individuals with different motor capacities. **LDV** were defined as those vehicles with a weight of \( \leq 3.5 \text{ t} \), used fundamentally for the transportation of goods and materials. Finally, the category of **HDV** was established for those vehicles used for transportation of persons, goods, and materials with a weight of \( \geq 3.5 \text{ t} \), divided in four categories: (i) \( \leq 7.5 \text{ t} \), (ii) \( \leq 16 \text{ t} \), (iii) \( \leq 32 \text{ t} \) and (iv) \( \geq 32 \text{ t} \) (MARM, 2009). For the purposes of the construction of AERIS, no distinction is being made between the before mentioned categories of vehicles in terms of the fuels that they consume. This approach is simple but it allows to reflect any policy of measure even fuel-specific ones, since the problem can be easily reduced to a prescribed reduction in emissions for each particular vehicle segment. For example, the **passenger cars**' category includes passenger cars that use either gasoline, diesel or LPG. The main distinction that is made is derived from the SNAP classification, which disaggregates road traffic in terms of the **driving patterns**. To this respect, the characterization of the driving patterns for the Spanish case was made through the use of surrogates. These surrogates were defined through the use of road lengths weighted by average traffic data as a function of road types and only two of them were elaborated: surrogate 08 (highway driving) and surrogate 10 (urban driving) (figure 4.6).

Additionally, the **road abrasion** and **tire and break wear** processes were properly characterized by a general SRM. These sectors are especially relevant sources of \( PM \), accounting in European countries for about 40% of the total particle emissions related to road traffic (Winiwarter et al., 2010). In terms of its description, the SNEI relies on the ordinary CORINAIR methodology which considers the emissions being a function of tire type, vehicle-induced turbulence, road conditions, weather and meteorology, use of studded tires, wetness of roads, temperature, sanding, salting and presence of side-strips (Gustafsson et al., 2005). Further information on the processing and generation of the road traffic related emissions, the assumed hypotheses for modeling this sector as well as other general considerations can be found in Lumbreras et al., (2009). Comments on the process of elaboration of the road traffic surrogates are published in Borge et al., (2008).
4.2. Studied sectors and activities

4.2.6 080000 - Other mobile sources and machinery

This sector is a very diverse one, basically because it includes all the other transportation modes that cannot be classified as “on-road”. Although this sector is dealt with aggregately, two specific sets of SRMs were developed for agricultural (080600) and industrial (080800) machinery. It is worth noting that no point sources were considered other than airports, as explained in (section 4.2.7). In a broader sense, according to the 2007 version of the SNEI the following activities are present in the national territory belonging to SNAP 08.

- 080201 - Railways (shunting locs).
- 080501 - Domestic airport traffic.
- 080600 - Agriculture.
- 080800 - Industry.
- 080203 - Railways (locomotives).
- 080502 - International airport traffic.
- 080700 - Forestry.

Agricultural machinery (080600) includes the emissions imputable to tractors and harvesters that incorporate internal combustion engines. The emissions have been estimated taking into consideration a census of agricultural machinery published by the Spanish Ministry of Agriculture in 2007. The activity variable is, as usual, the diesel consumption per unit of installed power, corrected by usage intensity. Emission factors were taken from the CORINAIR manual as explained in Samaras and Zierock, (1994). Finally concerning industrial machinery (080800), information for the correct description of this activity was obtained also from expert judgments, as well as from information coming from the Spanish Ministry of Infrastructures, with emission factors coming from the usual references used throughout the compilation of the SNEI.

Table 4.6: Airports with LTO ≥ 10,000 per year in Spain.

<table>
<thead>
<tr>
<th>Airport Name</th>
<th>Lat</th>
<th>Lon</th>
<th>Nat. LTO</th>
<th>Int. LTO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aepo. de Madrid - Barajas</td>
<td>40.47°N</td>
<td>3.55°W</td>
<td>111,295</td>
<td>110,534</td>
</tr>
<tr>
<td>Aepo. de Barcelona - El Prat</td>
<td>41.29°N</td>
<td>2.07°E</td>
<td>82,317</td>
<td>81,960</td>
</tr>
<tr>
<td>Aepo. de Palma de Mallorca</td>
<td>39.55°N</td>
<td>2.73°E</td>
<td>38,011</td>
<td>54,026</td>
</tr>
<tr>
<td>Aepo. de Málaga - Costa del Sol</td>
<td>36.67°N</td>
<td>4.49°W</td>
<td>22,249</td>
<td>37,733</td>
</tr>
<tr>
<td>Aepo. de Alicante</td>
<td>38.28°N</td>
<td>0.56°W</td>
<td>11,758</td>
<td>25,356</td>
</tr>
<tr>
<td>Aepo. de Valencia</td>
<td>39.48°N</td>
<td>0.48°W</td>
<td>23,686</td>
<td>12,392</td>
</tr>
<tr>
<td>Aepo. de Bilbao</td>
<td>43.30°N</td>
<td>2.91°W</td>
<td>18,340</td>
<td>7,992</td>
</tr>
<tr>
<td>Aepo. de Ibiza</td>
<td>38.87°N</td>
<td>1.37°E</td>
<td>14,694</td>
<td>9,413</td>
</tr>
<tr>
<td>Aepo. de Sevilla</td>
<td>37.41°N</td>
<td>5.89°W</td>
<td>18,111</td>
<td>5,019</td>
</tr>
<tr>
<td>Aepo. de Girona - Costa Brava</td>
<td>41.91°N</td>
<td>2.76°E</td>
<td>1,475</td>
<td>11,994</td>
</tr>
<tr>
<td>Aepo. de Menorca</td>
<td>39.86°N</td>
<td>4.21°E</td>
<td>10,952</td>
<td>4,566</td>
</tr>
</tbody>
</table>
Chapter 4. Emissions & air quality module

Figure 4.8: Geographic location of the considered airports.

4.2.7 080500 - Airports

As it has already been stated in the preceding section, airports that exceed a number of 10,000 yearly landing-take off cycles (LTO) (either of domestic or international nature) have been considered as point sources and therefore, modeled separately from the rest of SNAP 08. The airports that have been modeled as described in this section are located in cities that concentrate an important part of the national population, and are especially relevant in terms of the airplane fleets they house. It is worth noting that the airports with more than 10,000 yearly LTO located in the Canary Islands were not considered because they lie outside the modeled domain (section 3.3.2).

Due to the fact that these airports were considered as point sources, they were placed directly over the modeling domain without any surrogation process. The LTO cycle is considered as the activity variable without making any distinction on the aircraft type that carried it out. Information on these LTO cycles were obtained from the Spanish Ministry of Infrastructures, while the emission factors were elaborated directly during the inventory compilation process according to the airplane fleet present in every airport and the characteristics of the engines. These emission factors were determined from information provided by the Spanish Airport Authority (AENA) and IATA.
4.2.8 100100 - Cultures with fertilizers

This sector describes the emissions associated to agricultural activities that use nitrogenized fertilizers, either of mineral type (basically chimio-synthetic) or animal manures, waste or wastewater sludge composts. AERIS incorporates descriptions of two sub-sectors that differentiate between permanent crops (SNAP 100101) and arable land crops (SNAP 100102). **Permanent crops** are those produced from plants which last for many seasons, rather than being replanted after each harvest. On the contrary **arable land crops** refer to those plants that in order to be grown, need to be seeded in ploughed land that is properly conditioned for these purposes. In general terms, the only relevant pollutant that these sectors quantify is **ammonia**. To accomplish this, ammonia emissions are quantified from the contributions of mineral nitrogenized fertilizers (especially of synthetic origin) as a function of the soil type and weather.

The basic approach is that (for a given amount of fertilizer used) emissions should be higher wherever there are warmer weathers and high soil-\(pH\) values. In the case of organic fertilizers, an analysis of the composition of the most common fertilizers has been carried out and applied with a similar methodology to soils. Information about the climatic conditions that exist at a given location was provided by the National Spanish Meteorology Agency (AEMET) and the soil type information from geological surveys available at national scale (MARM, 2009). The spatial allocation procedure for the emissions related to these two sectors has been carried out through the use of spatial surrogates (figure 4.7). These surrogates were elaborated with data obtained from the National Agricultural Atlas of Spain, a publication that is available from the Spanish Ministry of Agriculture. To this respect, surrogates 14 and 15 distinguish between the different crop types.

4.2.9 100500 - Other agricultural activities

It should be noted that despite the fact that sector 100500 is coded in the SNAP nomenclature as **manure management**, for the modeling purposes of AERIS other agricultural activities were included in this category, basically those related to **farming activities**, namely SNAP 100500 and 100900. The most relevant subgroups these activities include are manure management practices for dairy cows, fattening pigs, sows, sheep, horses, laying hens and broilers. The manure **management activities** that are described by this group include anaerobic lagoons, liquid systems, solid storage and dry piling, herding, daily spreading and use as fuels. For the correct quantification of the emissions of ammonia, the SNEI considers main manure composition values, varying between animals and ages. **Activity variables** are taken directly from the number of cattle heads available in Spain in 2007 according to the SNEI, while the **emission factors** are obtained from the CORINAIR manual (MARM, 2009). Spatial allocation techniques relied, as usual, on surrogation through the use of information about the location of farms and agricultural soils throughout the Spanish territory (surrogate 08 - figure 4.7).
4.2.10 110000 - Other sources and sinks

Although this sector is named as "other sources and sinks", it is essentially related to sources and sinks of natural type according to a definition given by Winiwarter et al., (1999). For the purposes of AERIS, a SRM was developed only to describe changes related to emissions of ammonia being produced by natural sources, which are basically wetlands (swamps and marshes).

4.2.11 Portugal

As it was already stated, SRMs were elaborated for Portugal, modeled as an independent "macrosector". This prevents simulating sector-specific abatement measures that may be adopted in Portugal but allows AERIS to reflect the influence of Portuguese emissions to Spanish air quality levels, specifically for regions along the border. For the characterization of the emissions of Portugal, the Portuguese National Emission Inventory of 2007 was extensively used (PNEI). As with the Spanish version, this inventory is fully consistent with the CORINAIR methodology and the Selected Nomenclature for Air Pollution (SNAP) (EMEP - CORINAIR, 2007).

It should be noted that SRMs for Portugal were developed for each of the before mentioned pollutants and without any distinction of the sectors that produced them. Although the PNEI obviously provides emissions for each of the SNAP activities, considering them is certainly not useful under an IAM perspective (i.e. Portuguese policy cannot be elaborated by Spanish stakeholders). The fact, however, of Portugal being included in AERIS follows the need of quantifying, at least superficially, its influence on Spanish (or Iberian) air quality levels. As a
matter of fact, considering Portugal as a “macrosector” means returning to the most traditional methodology for obtaining the SRMs, widely used for the construction of IIASA RAINS/GAINS with the EMEP model (Simpson et al., 1997). Figure 4.9 is an example of the atmospheric dispersion and chemistry outputs of tropospheric ozone \( \text{O}_3 \) attributed to Portugal at the EMEP domain.

4.2.12 International shipping

Similar to Portugal, the international shipping around the Iberian Peninsula has been modeled as an independent “sector”. Considering the international ship transit as a sector is very useful due to the fact that the emissions produced by ships and boats, for both, international transport, cargo or fishing activities are very relevant in the Atlantic and Mediterranean contexts, particularly in the strait of Gibraltar. Ship transit across the strait represent up to 12.5% of the international shipping activities by sea (Tzannatos, 2010). According to Borge, (2006), ship transit accounted for around 49% and 28% of the emissions of \( \text{SO}_2 \) and \( \text{NO}_x \) respectively in the Iberian Peninsula modelling domain. In order to model this sector, the EMEP grid was used with data coming from the CORINAIR methodology and from specific studies of The Lloyd’s Register of Shipping in 1995 and MARINTEK (Jonson, 2000). The spatial aggregation of this sector has been carried out through a surrogate variable which is an adaptation of the EMEP grid to that of AERIS, namely surrogate 25 (figure 4.7).

4.3 Modeling Hypotheses

Let there be a modeling domain, which consists of a rectangular grid of \( n \) rows and \( m \) columns. For this domain, we have a matrix of emissions of an \( i \) pollutant produced by a given \( j \) sector - \( [E_{i,j}]_{n \times m}^0 \). The emissions represented by this set (zero superscript) will be referred as the baseline scenario. Let this baseline scenario vary by multiplying each of the emissions of pollutant \( i \) produced by sector \( j \) by a given \( k \) coefficient, creating an altered scenario - \( [E_{i,j}]_{n \times m} \). When this \( k \) coefficient represents relative values of future emissions, the result is referred to as future scenario.

\[
[E_{i,j}]_{n \times m} = k \cdot [E_{i,j}]_{n \times m}^0
\]

Assuming that both emission scenarios are processed accordingly with an AQM, each of them will produce the corresponding concentration dataset. Thus, the concentrations obtained after simulation with the AQM are a function of the emissions of each sector that produced them, being sector-dependent.

\[
[C_i]_{n \times m} = f ([E_{i,j}]_{n \times m})
\]

\[
[C_i]^0_{n \times m} = f ([E_{i,j}]^0_{n \times m})
\]
The difference produced in both, emissions and concentrations after applying the variation coefficient \((k)\) can be then computed as a "delta" or a net change.

\[
[C_i]_{n×m} = [C_i]_{n×m}^0
\]

\[
[ΔE_{i,j}]_{n×m} = [E_{i,j}]_{n×m} - [E_{i,j}]_{n×m}^0
\]

\[
[ΔE_{i,j}]_{n×m} = (k - 1) \cdot [E_{i,j}]_{n×m}^0
\]

Since concentrations are conditioned by emissions in, it is reasonable to assume that the net change in concentrations is equal to the net change in emissions, multiplied by a proportionality constant, \(R\).

\[
[C_i]_{n×m} = R \cdot [ΔE_{i,j}]_{n×m}
\] (4.1)

According to this approach, the emissions that correspond to the baseline scenario must be known and kept constant every time a future scenario is to be modelled. Being this so, the proportionality constant \((R)\) can be substituted by a matrix of proportionality coefficients \([G]_{n×m}\). In order to reflect this substitution, Equation 4.1 can be reorganized and rewritten as follows:

\[
[C_i]_{n×m} = R \cdot (k - 1) \cdot [E_{i,j}]_{n×m}^0
\]

\[
[C_i]_{n×m} = [G_{i,j}]_{n×m} \cdot k
\]

Moreover, the variation coefficient \((k)\) can be transformed to express percentual variation of the emissions of sector \(j\) for pollutant \(i\) \((p_{i,j})\) rather than arbitrary values. It should be noted that \(p_{i,j} < 0\) for abatement measures, since they imply a decrease in emissions. The \(k\) variation coefficient is related with the variation percentage as in the expression \(k = 1 + \frac{p_{i,j}}{100}\).

The application of the before mentioned considerations allows reaching an expression which is the conceptual core of the approach followed by the integrated assessment modeling system developed in this PhD Thesis. This expression is described by equation 4.2:

\[
[C_i]_{n×m} = [G_{i,j}]_{n×m} \cdot p_{i,j}
\] (4.2)

Where the term \([G_{i,j}]_{n×m}\) is referred to as source-receptor matrix and consists of a set of coefficients that relates the percentual variation in the emissions of a certain pollutant by a
4.4 Computation of the Source - Receptor Matrices

Given a sector to the concentration changes of such pollutant caused by this emission shift. In the light of the above, the resulting concentrations of an altered emission scenario can be estimated by adding the concentration change ($\Delta C$) to the concentrations corresponding to the baseline scenario ($C_0$), according to equation 4.3.

$$[C_i]_{n \times m} = [G_{i,j}]_{n \times m} \cdot p_{i,j} + [C_i]^0_{n \times m}$$ (4.3)

In practice, global concentration changes are caused by variation in emissions produced by several sectors. Therefore, the concentration of pollutant $i$ is the sum of the concentration changes produced by the variation of a total $J$ emission sectors, as described in equation 4.4. The additivity hypothesis is tested in chapter 5.

$$[C_i]_{n \times m} = [C_i]^0_{n \times m} + \sum_{j=1}^{J} [G_{i,j}]_{n \times m} \cdot p_{i,j}$$ (4.4)

The present work was focused eminently in the obtention of the transfer matrices for the main pollutants and for a wide array of emission sectors. To achieve this, an AQM was selected, properly configured and adapted to the modeled domain of interest (the Iberian Peninsula). Then, a great number of simulations was carried out in order to obtain a significant amount of data to carry out polynomial regressions and statistical analysis needed to define the $[G_{i,j}]$ factors or source-receptor matrices. Once running properly, a great number of simulations was carried out in order to obtain a significant amount of data to carry out polynomial regressions and statistical analysis. The characteristics of the chosen AQM, as well as its particular configuration and application to the Iberian Peninsula were discussed in the previous sections.

4.4 Computation of the Source - Receptor Matrices

The modeling hypotheses explained in section 4.3 as a particular adaptation and application of the well-known methodology based in source-receptor matrices. A source-receptor matrix (SRM) is a relationship that describes the sensitivity of a receptor element to a given source (changes in concentrations due to changes in emissions). The receptor could be, for example, the average concentration of a certain atmospheric pollutant in a given grid cell during a given time interval (Seibert and Frank, 2004). The construction of the AERIS system by the use of SRMs is relevant because they represent the atmospheric conditions (i.e. transport phenomena) that explain the concentration and deposition of a given pollutant at the receptor locations. The elements of a SRM can be considered as fate factors. Its main advantage is simplicity: for a given source, the resulting receptor values can be obtained by a simple...
matrix-vector multiplication, avoiding the evaluation of the entire numerical model of the transport and dispersion processes (Seibert and Frank, 2004; Roy et al., 2012). In conclusion, a SRM provides the important connection between emissions and concentrations over different time and spatial scales (Bartincki, 1999).

The use of an AQM is an important part of AERIS since it allows calculating ambient air concentrations and deposition levels that are related to environmental quality objectives. The changes in emission levels, due to implementation of abatement measures, result in changes in air concentration and deposition levels. Since these parameters are dependent on emission levels as well as the meteorological and geographical conditions, atmospheric models are required to be able to describe the dispersion, highlighting the complexity inherent to the process of computing a SRM (Sternhufvud and Åström, 2006).

SRMs are especially useful if a parameterization of an Eulerian AQM is to be carried out (section 3.1). Basically, SRM are generated for a concrete spatial domain by reducing or increasing emissions of one or more pollutants by a given percentage, re-running the AQM and comparing the results with the base-case or reference scenario (Tarrasón et al., 2004). The nonlinearities due to model chemistry or numerical methods used to solve atmospheric transport can be easily adapted to simpler linear cases through the use of these matrices.
4.4. Computation of the Source - Receptor Matrices

Bartincki (1999) proposes four methodologies for obtaining these SRM through the use of Eulerian AQMs. Figure 4.10 describes the above mentioned methods for the estimation of SRM; for the concrete case of a complex AQM, method 4 has proven to be more adequate for the advection algorithms. Additionally, this method was selected because of its reasonable degree of linearity and the absence of zeros in emissions which are usually deemed of making air quality simulations less stable (Bott 1989).

In the case of the IAM system that has been constructed in this work, and according to what has been already explained in section 4.3, the SRMs will not be computed for countries but for emission activities and sectors. This hypothesis has been formulated in the understanding that the emission sectors have a specific geographic location which does not change. Examples of these locations are particular factories, airports, highways, urban areas, etc. Another difference with the methodology proposed by Bartincki (1999) is that AERIS is not limited to deposition processes. The constructed IAM focuses on atmospheric concentrations (AQ levels) and policy-relevant indicators.

After the simulations have been carried out, the results are treated according to the modeling hypotheses discussed in section 4.3. In other words, the results are fitted according to a polynomial model by the means of a statistical regression which is responsible for yielding a complete array of transformation coefficients. The election of the optimal polynomial model is based on the minimum error criterion which is assessed through the corresponding correlation coefficients. A particular example on how the transfer matrices for a single emission sector is given in the following sections in order to illustrate this process.

4.4.1 Computation of the Source Receptor Matrices: an example

This section is devoted to the explanation of the process for modeling and obtaining the SRM for a given emission sector under a given meteorological scenario. This explanation implies that the modeler relies on a robust and functional AQM, which draws information from comprehensive data sources (i.e. emission inventories). The description of the AQM that was used to construct the SRMs of AERIS as well as its configuration was presented in detail in chapter 3. It is important to note that the basic objective of this process is to conduct a series of experiments in order to provide enough data to carry out a statistical regression, whose coefficients will conform the SRM. The statistical regression process will aim to correlate percentual variations in the emissions of a sector with air quality data (outputs from the AQM) for every greed in the modeling domain.

To illustrate this case, the SRM of sulfur dioxide ($SO_2$) for domestic heating activities related to combustion plants with a $< 50$ MW power (SNAP 020202) is presented. The selected activity sector is relatively easy to model since it behaves as an area source and the chosen pollutant
Chapter 4. Emissions & air quality module

Figure 4.11: Mean $SO_2$ concentrations from the baseline scenario of emissions ($\mu g/m^3$).

is very characteristic of the combustion processes. Figure 4.12 shows the mean annual $SO_2$ emission rate ($g_{mol}/s$) for SNAP 020202 in year 2007. This emission field is the $SO_2$ baseline scenario, noted in section 4.3 as $[E_{i,j}]_{n \times m}$. With the emissions of the baseline scenario, a number of arbitrary perturbations will be applied in the form of a percentual variations, referred to as $p_{i,j}$ in section 4.3.

It is worth noting that these discretionary variations need to be limited in terms of the technological feasibilities of the technologies that reduce (or increase, where applicable) the emissions of a given pollutant. The correct selection of the magnitude and number of these variations is crucial for having a significant variation range to correlate with polynomial models. Let a set of four discretionary perturbations of the baseline scenario be considered:

$$p_{SO_2,020202} = \{ -90\%, -50\%, 50\%, 90\% \}$$

This vector of variations will be selectively applied only to the $SO_2$ emissions of the modeled sector (SNAP 020202). These variations are applied to every grid cell where emissions from SNAP 020202 are located (Figure 4.12). The generated emission datasets are then fed to the deterministic AQM. The model run outputs will create a set of five $SO_2$ concentration fields, which are a function of its respective emissions. If these outputs are intersected with the cells of the chosen modeling grid with dimensions $n \times m$, then we obtain the respective matrices of air quality data with the same dimensions. In this case, the dimensions of the domain
are 75 $\times$ 60 which correspond to a total of 4500 cells. In other words, every output will be composed by 4500 $SO_2$ concentration values. Additionally, the concentrations resulting from the emissions of the baseline scenario are also obtained (figure 4.11), denominated $[C_i]_{n\times m}^0$ in section 4.3. However, according to the modeling hypotheses that have been already discussed in the past sections, it is necessary to calculate absolute variations between the concentrations obtained from the model runs based on the baseline scenario and altered emissions scenario emissions. These variations are computed as a simple subtraction or “delta”, noted as $[\Delta C_i]_{n\times m}$ in section 4.3.

The spatial representation of these concentration differences is shown in figure 4.13. For the purposes of constructing a SRM, these spatial representations are not as useful as inspecting the variation in concentration that occurs at the cell level. Taking the above mentioned in consideration, for any cell we have a set of five air quality outputs as well as five emission variation percentages:

$$C_{SO2, 2002} = \{C_{-90\%}, C_{-50\%}, C_{0\%}, C_{50\%}, C_{90\%}\}$$

$$p_{SO2, 2002} = \{-90\%, -50\%, 0\%, 50\%, 90\%\}$$

In order to verify that the relationship illustrated by equation 4.2 is valid, an inspection of the air quality outputs has to be carried out. To this respect, a plot of these outputs against the variation percentages was carried out for every cell; this procedure allowed assuming an
adequate regression model for the obtention of the grid cell-specific coefficients of the SRMs. Figure 4.14 illustrates the inspection process carried out at four random cells of the domain. Each of the points of the plots corresponds to the mean concentration of SO$_2$ in the given cell after a full simulation of the complete domain. It can be seen that the relationship between variations in emissions and concentrations that these cells exhibit is eminently linear, so it is obvious that a linear regression model can be successfully applied.

\[
[\Delta C_i]_{n \times m} = [G_{i,j}]_{n \times m} \cdot p_{i,j} + [\gamma_{i,j}]_{n \times m}
\]

For this model, an additional term is included \([\gamma_{i,j}]_{n \times m}\). This term corresponds to the intercept of a common linear regression model and for the purposes of the construction of the SRMs will act as a “background factor” that represents the relative importance of other sources (any other than the one being perturbed). The smaller the intercept, the larger the influence of the sector being perturbed in that grid cell for that pollutant. For this concrete case, we have 4500 results for each of the five simulations, which yields a total 22500 data points that need to be correctly processed. This calls for having a simple, efficient and dynamic statistic tool which in this case was MATLAB®.

The fitting process carried out in MATLAB® allowed obtaining the regression coefficients with a statistical confidence of $\alpha = 0.95$ (95%). Once the regression has been conducted, the evaluation of its goodness has to be carried out. The most common performance indicator of
4.4. Computation of the Source - Receptor Matrices

the goodness of a polynomial regression is the **Pearson’s correlation coefficient** \( r \). Intrinsically, this coefficient is a statistic that measures the degree to which two variables correlate linearly and is limited between 0 and 1. Coefficients of 1 indicate a perfect linear relationship between data, while coefficients close to 0 suggest that no such relationship exists (USEPA, 2007). For the concrete case of SNAP 020202, the correlation coefficient for the 4500 \( \times \) 5 pairs of data polled together was \( r = 0.9994 \), which indicates that the selected regression model is adequate for the obtention of the SRM coefficients. Once that the quality of the regression has been correctly assessed, the regression coefficients can be arranged to conform the **source-receptor matrix** (SRM). This arrangement can be made according to the most adequate needs that the computation architecture of AERIS might demand. Perhaps the most illustrative way to present a SRM is through its deployment over the modeling domain in order to identify regions or zones that are highly affected by emission changes.

Figure 4.15 represents the obtained SRM which describes the proportionality that exists between percentual variations in the emissions of \( \text{SO}_2 \) from SNAP 020202 and changes in the mean monthly concentration of this pollutant in the selected domain. As expected, the zones that are susceptible of being affected by the emissions of this sector exhibit the highest numbers of the matrix while zones that are unaffected present zeros. It is important to note that the obtained SRM by itself does not allow to quantify **absolute** mean monthly concentrations, because it has been modeled according to **equation** 4.2 to yield **changes** or “deltas”. To obtain the absolute values, the concentrations of the **baseline scenario** must be
Figure 4.15: SO\textsubscript{2} mean monthly concentration SRM from SNAP 020202 emissions - $[G_{i,j}]_{n \times m}$.
4.4. Computation of the Source - Receptor Matrices

Table 4.7: Total emissions of the SNAP groups at the BS - [$t$/yr].

<table>
<thead>
<tr>
<th>SNAP code</th>
<th>$NO_x$</th>
<th>$SO_2$</th>
<th>$PM_{10}$</th>
<th>$PM_{2.5}$</th>
<th>$NH_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SNAP 01</td>
<td>376,994</td>
<td>997,812</td>
<td>24,829</td>
<td>15,220</td>
<td>109</td>
</tr>
<tr>
<td>SNAP 02</td>
<td>60,024</td>
<td>25,697</td>
<td>26,960</td>
<td>25,406</td>
<td>0</td>
</tr>
<tr>
<td>SNAP 03</td>
<td>305,499</td>
<td>124,873</td>
<td>15,717</td>
<td>11,871</td>
<td>0</td>
</tr>
<tr>
<td>SNAP 04</td>
<td>13,445</td>
<td>37,479</td>
<td>10,754</td>
<td>5,606</td>
<td>16,163</td>
</tr>
<tr>
<td>SNAP 05</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>146</td>
<td>0</td>
</tr>
<tr>
<td>SNAP 06</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>771</td>
</tr>
<tr>
<td>SNAP 07</td>
<td>530,634</td>
<td>2,738</td>
<td>47,806</td>
<td>36,710</td>
<td>8,539</td>
</tr>
<tr>
<td>SNAP 08</td>
<td>210,163</td>
<td>10,884</td>
<td>47,806</td>
<td>47,786</td>
<td>28</td>
</tr>
<tr>
<td>SNAP 09</td>
<td>5,338</td>
<td>8,038</td>
<td>82</td>
<td>78</td>
<td>8,504</td>
</tr>
<tr>
<td>SNAP 10</td>
<td>22,819</td>
<td>4,235</td>
<td>19,260</td>
<td>3,139</td>
<td>316,253</td>
</tr>
<tr>
<td>SNAP 11</td>
<td>41,215</td>
<td>432</td>
<td>104</td>
<td>0</td>
<td>121,733</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>1,566,134</td>
<td>1,212,190</td>
<td>415,646</td>
<td>145,985</td>
<td>452,103</td>
</tr>
</tbody>
</table>

added according to equation 4.3. Finally, it is necessary to evaluate the quality of the results yielded by the parameterization against the predictions of the full AQM. To carry out this, the SRM was multiplied by the five variation percentages and then the concentrations of the baseline scenario were added. The goodness of this correspondence has been quantified according to the before mentioned statistical correlation coefficient.

4.4.2 Scenario modeling

Modeling through the use of scenarios is very useful when trying to describe the future evolution of the environment. In the context of AERIS a scenario is a description of what could possibly happen in terms of emissions from the sectors and pollutants considered. Alcamo (2008) clearly outlined the convenience of modeling environmental problems by setting scenarios, due to the fact that they can provide an interdisciplinary framework for analyzing complex environmental problems and envisioning their solutions.

As it has been already discussed in section 4.3, the establishment of a baseline scenario is necessary for building the SRM that ultimately lead to the creation of the IAM. The objective of the baseline scenario is twofold. It is essential to quantify the magnitude of the emissions, their location and nature as well as the social, economic and technical conditions that exist at the studied domain as a reference case. Furthermore, this characterization needs to be referred to a certain year, whose relevance might be either determined by the relevance of the historic circumstances at this time or by the availability of information. And second, the availability of an adequate reference point to assess the goodness of policies and environmental actions. In
Chapter 4. Emissions & air quality module

the case of AERIS, the chosen baseline scenario can be defined as “the air quality levels of NO\textsubscript{2}, SO\textsubscript{2}, O\textsubscript{3}, PM\textsubscript{10}, PM\textsubscript{2.5} and NH\textsubscript{3} in relation with the emissions quantified by the SNEI and the PNEI versions of 2007 under the meteorological conditions of that same year.”

Table 4.8: Emissions of the studied sectors at the BS - [t/yr].

<table>
<thead>
<tr>
<th>SNAP group</th>
<th>NO\textsubscript{x}</th>
<th>SO\textsubscript{2}</th>
<th>PM\textsubscript{10}</th>
<th>PM\textsubscript{2.5}</th>
<th>NH\textsubscript{3}</th>
</tr>
</thead>
<tbody>
<tr>
<td>010000</td>
<td>235,331</td>
<td>805,700</td>
<td>17,632</td>
<td>14,899</td>
<td>98</td>
</tr>
<tr>
<td>020202</td>
<td>19,215</td>
<td>12,426</td>
<td>23,280</td>
<td>24,420</td>
<td>0</td>
</tr>
<tr>
<td>030000</td>
<td>197,064</td>
<td>63,686</td>
<td>8,609</td>
<td>6,270</td>
<td>0</td>
</tr>
<tr>
<td>040000</td>
<td>3,958</td>
<td>33,731</td>
<td>7,203</td>
<td>3,801</td>
<td>14,264</td>
</tr>
<tr>
<td>070101</td>
<td>124,764</td>
<td>558</td>
<td>4,955</td>
<td>4,955</td>
<td>5,010</td>
</tr>
<tr>
<td>070103</td>
<td>65,926</td>
<td>506</td>
<td>7,393</td>
<td>7,393</td>
<td>246</td>
</tr>
<tr>
<td>070201</td>
<td>19,626</td>
<td>145</td>
<td>1,910</td>
<td>1,910</td>
<td>107</td>
</tr>
<tr>
<td>070203</td>
<td>39,633</td>
<td>224</td>
<td>3,048</td>
<td>3,048</td>
<td>37</td>
</tr>
<tr>
<td>070301</td>
<td>100,968</td>
<td>500</td>
<td>3,867</td>
<td>3,867</td>
<td>76</td>
</tr>
<tr>
<td>070303</td>
<td>56,689</td>
<td>226</td>
<td>2,781</td>
<td>2,781</td>
<td>28</td>
</tr>
<tr>
<td>0707/08</td>
<td>0</td>
<td>0</td>
<td>11,532</td>
<td>6,350</td>
<td>0</td>
</tr>
<tr>
<td>080500</td>
<td>7,310</td>
<td>343</td>
<td>9</td>
<td>9</td>
<td>0</td>
</tr>
<tr>
<td>080600</td>
<td>109,898</td>
<td>7,865</td>
<td>28,727</td>
<td>28,727</td>
<td>13</td>
</tr>
<tr>
<td>080800</td>
<td>64,913</td>
<td>132</td>
<td>13,761</td>
<td>13,761</td>
<td>8</td>
</tr>
<tr>
<td>100101</td>
<td>3,155</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>91,748</td>
</tr>
<tr>
<td>100201</td>
<td>8,297</td>
<td>0</td>
<td>730</td>
<td>0</td>
<td>35,218</td>
</tr>
<tr>
<td>100500</td>
<td>0</td>
<td>0</td>
<td>16,553</td>
<td>2,825</td>
<td>120,639</td>
</tr>
<tr>
<td>110000</td>
<td>37,093</td>
<td>388</td>
<td>93</td>
<td>0</td>
<td>100,559</td>
</tr>
<tr>
<td>Portugal</td>
<td>145,250</td>
<td>22,918</td>
<td>80,563</td>
<td>64,762</td>
<td>48,970</td>
</tr>
<tr>
<td>Int. shipping</td>
<td>642,166</td>
<td>444,069</td>
<td>53,989</td>
<td>48,590</td>
<td>36</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>1,566,134</strong></td>
<td><strong>1,212,190</strong></td>
<td><strong>415,646</strong></td>
<td><strong>145,985</strong></td>
<td><strong>452,103</strong></td>
</tr>
</tbody>
</table>

As it has already been discussed in section 4.2, the reason of referring the baseline scenario to year 2007 obeys to the availability of the emission inventories that were used for creating the SRMs. Additionally, year 2007 is considered as characteristic of an activity peak in emissions, so it is appropriate for illustrating any reductions as a consequence of policy making. Furthermore, the 2007 versions of the emission inventories have already been processed with the conventional AQM, and the results have been extensively compared and published (section 2.3).

The characterization of the baseline scenario (BS hereinafter) in terms of its emissions of pollutants is presented in two formats. First, as gross totals for the complete SNAP categories and for each of the pollutants managed by AERIS. And then, as totals for each of the studied emission sectors (section 4.2). These values are presented in tables 4.7 and 4.8.
4.5 General model equations

A general overview of the modeling framework that was used for the construction of the SRMs is given in section 4.4. In this section, the form of the equations that allow quantifying mean monthly concentrations from these SRMs will be presented for every pollutant described in section 4.1. It should be noted that some pollutants are either of a completely secondary (i.e. not emitted) nature or have an important proportion of secondary components, an issue that is also addressed by AERIS and explained in this part. The general model equations presented here have been adapted from those published in Amann et al., (2011)

4.5.1 Primary gaseous pollutants

$NO_2$, $SO_2$ and $NH_3$ airborne concentrations are described through a primary pollutant equation approach. Although most of ambient $NO_2$ is of secondary nature it can be conveniently described only through $NO_x$ emissions, since $NO$ and $NO_2$ are dealt with aggregately in the inventory. Dependencies of other precursors and oxidants such as $O_3$ can be embedded in the coefficients of the transfer matrices without the need of explicitly consider them in the formulation. This set of pollutants constitutes the easiest modeling case in AERIS and the general equation for each of them can be written as in equation 4.5 for a total number of $J$ considered sectors. Despite the fact that equation 4.5 is only referred to $NO_2$, it is equivalent for the other two modeled primary gaseous pollutants. The nomenclature implemented for these equations has already been introduced in section 4.3.

\[
[C_{NO_2}]_{n \times m} = \sum_{j=1}^{J} [G_{NOx,j}]_{n \times m} \cdot p_{NOx,j} + [C_{NO_2}]^0_{n \times m} \tag{4.5}
\]

4.5.2 Particulate matter

Modeling particulate matter implies adapting the basic expression shown in equation 4.5 as a consequence of the important contribution of secondary particles to the total particulate matter concentration. As it has been already explained in section 4.1, the concentration of particulate matter not only depends on the emissions of primary particles, but also on the emissions of $NO_x$, $SO_2$ and $NH_3$. These secondary contributions where modelled as a function of the resulting concentrations of the primary gaseous pollutants as in equation 4.6.

\[
[C_{PM}] = \sum_{j=1}^{J} [G_{PM,j}] \cdot p_{PM,j} + [G_{PM}^{NOx}] \cdot p_{NOx} + [G_{PM}^{SO2}] \cdot p_{SO2} + [G_{PM}^{NH3}] \cdot p_{NH3} + [G_{PM}]^0 \tag{4.6}
\]

\footnote{For space purposes, the subindex $n \times m$ might be omitted}
At this point, we have introduced two new types of terms: $p_i$ and $[G_{PM_{SO2}}]$. The first term is the total variation percentage in the emissions of a given primary gaseous pollutant and the second term is the SRM that correlates this variation with its contribution to the total particle mass. It should be emphasized that different SRMs have been developed according to the fraction of particulate matter that is being studied, namely $PM_{10}$ or $PM_{2.5}$.

4.5.3 Tropospheric ozone

Creating a parameterization for tropospheric ozone is somewhat complex due to the fact that this pollutant is not emitted directly and its formation depends strongly on the available concentrations of nitrogen oxides ($NO_x$) and volatile organic compounds ($VOC$). To this respect, a multivariable dependency was considered (equation 4.7). For the development of the equation of tropospheric ozone, we modeled it as a typical two-variable response surface problem whose experimental inputs were AQM outputs for the two pollutants mentioned before. The two independent variables that determined our mean monthly concentration of ozone were the mean monthly concentration of nitrogen dioxide - $[C_{NO2}]$ - and the total variation percentage of volatile organic compounds - $p_{VOC}$. Additionally, the terms $[G_{O3u,v}]$ are the matrices that module the interaction between variables that yield a final concentration of $O_3$ once the parameters mentioned before have been determined. This approach is based on the model proposed by Guariso et al., (2004).

$$[C_{O3}] = [G^{O3}_{00}] + [G^{O3}_{10}] \cdot [C_{NO2}] + [G^{O3}_{01}] \cdot p_{VOC} + [G^{O3}_{11}] \cdot [C_{NO2}] \cdot p_{VOC} + [G^{O3}_{10}] \cdot [C_{NO2}]$$  \hspace{1cm} (4.7)

4.6 Policy-relevant indicators

As it has been already mentioned, the concentrations that AERIS provides are presented as indicators that are meaningful for the policy making process. Due to the fact that the use of AERIS is a parameterization of a traditional AQM, it cannot produce arbitrary average concentrations from hourly values since it would require an equivalent number of specific transfer matrices. Instead, IAMs are rather interested in representing policy-relevant indicators that are useful to assess the compliance of air quality standards. To this respect, AERIS was configured to produce via the use of SRMs the mean monthly concentrations of January and August of 2007 and through a further adaptation, the mean annual concentration. By an additional process using observations, the indicators derived from the Air Quality Directive (2008/50/EC) and the Royal Decree 102/2011 could be estimated.

4.6.1 Annual mean concentration

The annual mean concentration is usually representative of an average behavior in the dispersion and atmospheric chemistry of pollutants during a given calendar year. However,
4.6. Policy-relevant indicators

Calculating an annual mean concentration from hourly data (which can be easily achieved with typical AQM outputs) requires 8760 values for a single pollutant. It is obviously unfeasible to carry out the same number of SRMs for the above mentioned pollutants and sectors, so a different approach was followed.

According to what was already explained in section 4.4, SRMs were obtained for monthly runs. January and August were the monthly periods selected for the construction of SRMs since they are representative of winter and summer conditions in the Iberian Peninsula. In order to estimate the annual mean concentration from these two mean monthly concentrations, we assumed a adjustment coefficient \( q \) which will act as a proportionality constant between both concentrations (equations 4.8, 4.9).

\[
[C_{i,\text{annual}}]_{n \times m} = q_{01,\text{annual}} \cdot [C_{i,01}]_{n \times m}
\]  

\[
[C_{i,\text{annual}}]_{n \times m} = q_{08,\text{annual}} \cdot [C_{i,08}]_{n \times m}
\]

With \([C_{i,01}]_{n \times m}\) and \([C_{i,08}]_{n \times m}\) being the mean monthly concentrations of January and August, and \(q_{01,\text{annual}}, q_{08,\text{annual}}\) the respective adjustment coefficients. In order to calculate the numeric value of the adjustment coefficients, a complete annual run of the baseline scenario was carried out with the AQM. Assuming that the mathematical relationship between the mean monthly and mean annual concentrations for this annual run is also described by equations 4.8 and 4.9, adjustment coefficients were calculated accordingly.

\[
q_{01,\text{annual}} = [C_{i,\text{annual,2007}}]_{n \times m} / [C_{i,01,2007}]_{n \times m}
\]

\[
q_{08,\text{annual}} = [C_{i,\text{annual,2007}}]_{n \times m} / [C_{i,08,2007}]_{n \times m}
\]

Since both adjustment coefficients produce annual mean concentration values, the estimate’s representativeness can be increased by calculating the mean of the annual means produced by the January and August equations (equations 4.10):

\[
[C_{i,\text{annual}}]_{n \times m} = 0.5 \cdot (q_{01,\text{annual}} \cdot [C_{i,01}]_{n \times m} + q_{08,\text{annual}} \cdot [C_{i,08}]_{n \times m})
\]

Due to the fact that these adjustment coefficients have been calculated using the baseline scenario of AERIS with the same AQM, they can be considered valid for any future scenarios.
provided that these are modeled as deviations from this baseline scenario. The appropriateness of this approach will be discussed in the following chapters of this work.

4.6.2 Indicator estimation method

As it has been stated at the beginning of this section, the estimation method for calculating the indicators derived from Royal Decree 102/2011 consisted basically in a correlation between annual mean concentrations and the respective indicators reported by a number of monitoring stations located throughout the Iberian Peninsula (Spain and Portugal).

In order to have a sufficiently big and consistent statistical sample, we used data from 331 stations background stations located in the Iberian Peninsula, out of which 280 were located in Spain and 51 in Portugal. These stations have been classified according to their emplacement in urban background (133 stations), suburban background (92 stations) and rural background (106 stations). The reason for choosing only background monitoring locations was the fact that observations from this kind of stations are more representative of the spatial scale that is described by AERIS. In other words, the measurements of these stations are unlikely to be conditioned by local concentration gradients that cannot be reproduced by a mesoscale modelling system. Figure 4.16 shows the geographic location of the selected monitoring locations. The observations of each of these sites were obtained from the European air quality database (AirBase) of the European Topic Centre on Air Pollution and Climate Change Mitigation (EIONET).\(^5\) The list of stations can be found in the appendix A.3. It should be noted that observations from different years were used for a given monitoring location. Some stations had, in the most optimistic case, observations from 1987 to 2011, so a wide and comprehensive range of meteorological conditions could be reflected when this approach is applied.

The basic approach for this estimation method consists in finding a mathematical expression that correlates the mean annual concentration with the respective indicator. A priori we cannot know the best model that could correctly fit both datasets, so different best fits were chosen for each of the indicators attending, as usual, to the correlation coefficient (equation 5.1). In every case, a deep screening process on data correspondence was carried out in order to assure consistent data pairs. This process implied eliminating outliers and no-data values. Due to the fact that the measurements from the selected monitoring locations are representative of different area types (urban, suburban and rural), the cells of the AERIS domain have been differentiated according to these classes. This classification procedure will allow applying the most adequate regression equation to each cell according to their emplacement areas. To accomplish this, the geographic location of cities, urban population data and urban covers (as GIS-files) were obtained from the 2011 Revision of the United Nations World Urbanization

\(^5\)Data available at: http://acm.eionet.europa.eu/databases/airbase
Figure 4.16: Geographic location of the considered AirBase monitoring locations.
Table 4.9: Urban agglomerations in the domain with more than 400,000 inhabitants.

<table>
<thead>
<tr>
<th>City</th>
<th>Country</th>
<th>Population</th>
</tr>
</thead>
<tbody>
<tr>
<td>Madrid</td>
<td>Spain</td>
<td>5,263,000</td>
</tr>
<tr>
<td>Barcelona</td>
<td>Spain</td>
<td>4,251,000</td>
</tr>
<tr>
<td>Grande Lisboa</td>
<td>Portugal</td>
<td>2,821,697</td>
</tr>
<tr>
<td>Algiers</td>
<td>Algeria</td>
<td>2,086,212</td>
</tr>
<tr>
<td>Porto - Vila Nova de Gaia</td>
<td>Portugal</td>
<td>1,816,045</td>
</tr>
<tr>
<td>Valencia</td>
<td>Spain</td>
<td>1,499,000</td>
</tr>
<tr>
<td>Sevilla</td>
<td>Spain</td>
<td>1,262,000</td>
</tr>
<tr>
<td>Porto - Vila Nova de Gaia</td>
<td>Portugal</td>
<td>1,816,045</td>
</tr>
<tr>
<td>Valencia</td>
<td>Spain</td>
<td>1,499,000</td>
</tr>
<tr>
<td>Sevilla</td>
<td>Spain</td>
<td>1,262,000</td>
</tr>
<tr>
<td>Bilbao</td>
<td>Spain</td>
<td>947,000</td>
</tr>
<tr>
<td>Málaga</td>
<td>Spain</td>
<td>844,000</td>
</tr>
<tr>
<td>Oviedo - Gijón - Avilés</td>
<td>Spain</td>
<td>863,050</td>
</tr>
<tr>
<td>Alicante - Elche</td>
<td>Spain</td>
<td>793,000</td>
</tr>
<tr>
<td>Oran</td>
<td>Algeria</td>
<td>735,166</td>
</tr>
<tr>
<td>Tanger - Tetouan</td>
<td>Morocco</td>
<td>669,685</td>
</tr>
<tr>
<td>Zaragoza</td>
<td>Spain</td>
<td>639,000</td>
</tr>
<tr>
<td>Palma de Mallorca</td>
<td>Spain</td>
<td>593,000</td>
</tr>
<tr>
<td>Granada</td>
<td>Spain</td>
<td>498,000</td>
</tr>
<tr>
<td>Toulouse</td>
<td>France</td>
<td>441,802</td>
</tr>
<tr>
<td>Vigo</td>
<td>Spain</td>
<td>413,000</td>
</tr>
</tbody>
</table>

Prospects (UN, 2012). The classifying process of the domain cells was carried out according to the following criteria:

- **Urban cells.** For a cell to be considered as urban, its intersection with the urban cover GIS-file should indicate the presence of an urban agglomeration and the population of the intersected city should be higher than 400,000 inhabitants (2011) according to the definition of a consolidated urban nucleus by the United Nations World Urbanization Prospects (UN, 2012). Considering the spatial resolution used, this implies an average population density of 1,562 hab/km².

- **Suburban cells.** A cell was considered as suburban when its intersection with the urban cover GIS-file indicated the presence of an urban agglomeration other than those contained in table 4.9. To this respect, any cells with urban areas where the population is less than 400,000 inhabitants were considered as suburban. Figure 4.17 presents the urban agglomerations of the Iberian Peninsula and adjacent countries under the modeling domain of AERIS.

- **Rural cells.** All other cells that do not comply with any of the before mentioned criteria have been labeled as rural and shown transparent in figure 4.17.
4.6. Policy-relevant indicators

Figure 4.17: Urban agglomerations present in the modeling domain.

The selected indicators derived from Royal Decree 102/2011 that can be calculated by the current version of AERIS are listed below. For every indicator, AERIS has three regression models that differentiate between urban, suburban and rural cells. In the forthcoming sections, some references to the fitted models will be made:

- 19\textsuperscript{th} highest hourly concentration of $NO_2$ - $\mu g/m^3$.
- 25\textsuperscript{th} highest daily concentration of $SO_2$ - $\mu g/m^3$.
- 4\textsuperscript{th} highest hourly concentration of $SO_2$ - $\mu g/m^3$.
- 36\textsuperscript{th} highest daily concentration of $PM_{10}$ - $\mu g/m^3$.
- 26\textsuperscript{th} highest maximum 8-hour daily concentration of $O_3$ - $\mu g/m^3$.
- Sum of means over 35 ppb (SOMO\textsubscript{35}) of $O_3$ - $\mu g/m^3h$.\footnote{SOMO\textsubscript{35} is not used in the air quality legislation. It is the new indicator for health impact assessment recommended by WHO and is complementary to the 26\textsuperscript{th} highest maximum 8-hour concentration of $O_3$.}
- Daylight accumulated dose over a threshold of 40 ppb (AOT\textsubscript{40}) of $O_3$ - $\mu g/m^3h$.\footnote{SOMO\textsubscript{35} is not used in the air quality legislation. It is the new indicator for health impact assessment recommended by WHO and is complementary to the 26\textsuperscript{th} highest maximum 8-hour concentration of $O_3$.}
4.6.3 19th highest hourly concentration of NO₂

The 19th highest hourly concentration of NO₂ is a complementary policy-indicator to the annual mean (also known as the 99.8th percentile) and used for the protection of human health (Amann et al., 2014). To this respect, legislation implies that hourly concentrations for this pollutant should not be exceed 200 µg/m³ more than 18 times a year (Denby et al., 2012). A linear regression model has proved to be the most appropriate alternative due to the trends observed in the distribution of the data pairs (equation 4.11). The statistical regression plots for each of these points can be found in the Appendix A.3, separated according to the type of monitoring location. In these same plots, the regression curves are also presented with their correlation coefficients.

\[
[Max_{19,NO₂}] = a_{Max_{19,NO₂}} \cdot [C_{NO₂,annual}] + b_{Max_{19,NO₂}} \quad (4.11)
\]

4.6.4 25th highest daily concentration of SO₂

The 25th highest daily concentration of SO₂ is one of the two considered policy-indicators in Royal Decree 102/2011 and in European legislation. Legislation was set the limit value of daily concentrations for this pollutant in 350 µg/m³ which cannot be exceeded more than 24 times a year. In other words, this indicator corresponds to the 93rd percentile. A linear regression model was adopted for this indicator due to the distribution of points, which can be found in the Appendix A.3. Equation 4.12 is the chosen regression model.

\[
[Max_{25,SO₂}] = a_{Max_{25,SO₂}} \cdot [C_{SO₂,annual}] + b_{Max_{25,SO₂}} \quad (4.12)
\]

4.6.5 4th highest hourly concentration of SO₂

The 4th highest hourly concentration of SO₂ is the second policy-relevant indicator that is contained in Royal Decree 102/2011 and corresponds to the 99.9th percentile. This indicator has been derived attending to the limit value of 125 µg/m³ which cannot be exceeded more than 3 times a year. As with the two preceding indicators, the most adequate model for the regression was a linear model as written in equation 4.13. The corresponding regression plots for this indicator can be found in the appendix A.3.

\[
[Max_{4,SO₂}] = a_{Max_{4,SO₂}} \cdot [C_{SO₂,annual}] + b_{Max_{4,SO₂}} \quad (4.13)
\]
4.6.6 36th highest daily concentration of $PM_{10}$

The 36th highest daily concentration of $PM_{10}$ is an indicator derived from a legal limit of 50 $\mu g/m^3$ that cannot be surpassed more than 35 times a year and it corresponds to the 90.4th percentile (Dimitriou and Kassomenos, 2014). Equation 4.14 illustrates the model that was chosen for calculating this indicator.

$$[Max_{36, PM10}] = a_{Max36, PM10} \cdot \{C_{PM10, annual}\} + b_{Max36, PM10} \quad (4.14)$$

4.6.7 26th highest maximum 8-hour daily concentration of $O_3$

The 26th highest maximum 8-hour daily concentration of $O_3$ has been derived from a limit of 120 $\mu g/m^3$ which cannot be exceeded more than 25 times every year. Due to the fact that tropospheric ozone exhibits an eminently non-linear nature in its concentrations, the chosen regression model was a three-coefficient power equation, according to what is shown in equation 4.15. The regression procedure for this indicator, as with the following ozone-related indicators, was carried out in MATLAB®, which allows assuming highly non-linear models for fitting.

$$[Max_{26, O3}] = a_{Max26, O3} \cdot \{C_{O3, annual}\}^{b_{Max26, O3}} + c_{Max26, O3} \quad (4.15)$$

4.6.8 Sum of means over 35 ppb (SOMO$_{35}$) of $O_3$

This indicator corresponds to the sum of means over 35 ppb of ozone and is an indicator that is strongly related to human health impacts. The threshold of 35 ppb as cut-off was chosen practically because it is equivalent to the current background ozone level in Europe. Moreover, it has a more linear response to NO$_x$ emissions and is therefore more interesting under an IAM point of view (Amann et al., 2008). The chosen model for representing this indicator, as with the previous one, is a non-linear power model of two coefficients (Eq. 4.16).

$$[SOMO_{35, O3}] = a_{SOMO35, O3} \cdot \{C_{O3, annual}\}^{b_{SOMO35, O3}} \quad (4.16)$$

4.6.9 Daylight accumulated dose over a threshold of 40 ppb (AOT$_{40}$) of $O_3$

The daylight accumulated dose over a threshold of 40 ppb of ozone has been developed as an indicator that is closely related to the cumulative impacts of this pollutant on vegetal organisms. It is of particular relevance when addressing impacts related to the loss of crops
Chapter 4. Emissions & air quality module

and damage to forests (De Marco et al., 2014). It is calculated as the sum of the difference between hourly concentrations above 80 μg/m³, from May to July, using only concentrations measured between 8:00 and 20:00 hrs, European Central Time (ECT). For this indicator, Royal Decree 102/2011 has established two limits for the protection of vegetation. Namely, 18000 μg/m³ h in a five-year period and 6000 μg/m³ h (de Andres et al., 2012). The chosen model for regression is a non-linear power model of two coefficients shown in equation 4.17. The regression plots and correlation coefficients can be found in the appendix A.3.

\[
AOT_{40,O3} = a_{AOT_{40,O3}} \cdot \left[C_{O3,\text{annual}}\right]^{b_{AOT_{40,O3}}} (4.17)
\]

4.7 Source regionalizing

As it has been explained in the sections before, the geographic scale of AERIS eminently focuses on Spain and Portugal under a “national” perspective. However for the concrete case of Spain, air pollution prevention, improvement and preservation tasks have been transferred to the 19 autonomous communities while the implementation of the European Directive remains at a national level. The institutional division of Spain requires the elaboration of different regional air quality management plans, which highlights the importance of having an integrated assessment tool which can provide answers on the outcomes of the adoption of these regional policies (D’Elia et al., 2009).

To this respect, evaluating the effect of limiting policies (in the understanding that these will be reflected as changes in emissions) to a number of autonomous communities of Spain is possible with AERIS. To achieve this, emission sources have been “regionalized” according to their geographic location and run separately in the AQM. Each of this runs provides a regional baseline scenario which is strictly, a mathematical subset of the national baseline scenario since the same emission inventories and baseline years have been used for their configuration. As a consequence, the sum of the 19 regional baseline scenarios would approximately correspond to the national baseline scenario. Furthermore, since the construction of the SRMs involved altering the emissions of the relevant sectors on a nationwide scale, the application of variation percentages (\( p_i \)) is also consistent on the regional scale. This hypothesis is essential for guaranteeing the “fitness-for-purpose” of the outcomes of these regional evaluations. It should be noted that the indirect effects of abatement policies in a given region may have in the emissions of others are not considered. The autonomous communities that have been modeled in AERIS correspond to the 16 territorial units within the Iberian Peninsula (the Canary Islands lie outside the modeling domain) as well as the 2 autonomous cities under Spanish suzerainty in North Africa (Ceuta and Melilla). The autonomous communities included in AERIS are listed in table 4.10 and shown within the modelling domain in figure 4.18.
4.7. Source regionalizing

Table 4.10: Autonomous Communities of Spain.

<table>
<thead>
<tr>
<th>AERIS Name</th>
<th>Official Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>Andalucía</td>
<td>Andalucía</td>
</tr>
<tr>
<td>Aragón</td>
<td>Aragón</td>
</tr>
<tr>
<td>Asturias</td>
<td>Principado de Asturias</td>
</tr>
<tr>
<td>Cantabria</td>
<td>Cantabria</td>
</tr>
<tr>
<td>Castilla y León</td>
<td>Castilla y León</td>
</tr>
<tr>
<td>Castilla-La Mancha</td>
<td>Castilla-La Mancha</td>
</tr>
<tr>
<td>Cataluña</td>
<td>Cataluña/Cataluña</td>
</tr>
<tr>
<td>Ceuta</td>
<td>Ciudad Autónoma de Ceuta</td>
</tr>
<tr>
<td>Comunidad de Madrid</td>
<td>Comunidad de Madrid</td>
</tr>
<tr>
<td>Comunidad Valenciana</td>
<td>Comunitat Valenciana/Comunidad Valenciana</td>
</tr>
<tr>
<td>Extremadura</td>
<td>Extremadura</td>
</tr>
<tr>
<td>Galicia</td>
<td>Galicia</td>
</tr>
<tr>
<td>Islas Baleares</td>
<td>Illes Balears/Islas Baleares</td>
</tr>
<tr>
<td>La Rioja</td>
<td>La Rioja</td>
</tr>
<tr>
<td>Navarra</td>
<td>Comunidad Foral de Navarra/Nafarroako Foru Komunitatea</td>
</tr>
<tr>
<td>Melilla</td>
<td>Ciudad Autónoma de Melilla</td>
</tr>
<tr>
<td>Murcia</td>
<td>Región de Murcia</td>
</tr>
<tr>
<td>País Vasco</td>
<td>Euskadi/Pais Vasco</td>
</tr>
</tbody>
</table>

In general, regionalizing the approach means adapting the baseline scenario to a reduced subset in which only the emissions of those sectors present in the territorial unit (autonomous community) are simulated. Following the methodology explained in section 4.3, the modified equation that describes the concentrations of a given pollutant \(i\) as a function of changes in the emissions of a sector \(j\) in a given autonomous community \(k\) can be written as in equation 4.18:

\[
[C_{i,k}]_{n \times m} = \sum_{j=1}^{J} [G_{i,j}]_{n \times m} \cdot p_{i,j,k} + [C_{i,k}]_0^{0} \quad (4.18)
\]

Where \([C_{i,k}]_0^{0}\) is the so-called adapted baseline scenario or regional baseline scenario which results from a separate simulation of the \(k\) autonomous community. The correspondence of the regional baseline scenarios with the national baseline scenario as the sum of the contributions of the analyzed territorial units \((K)\) and is assured by equation 4.19:

\[
[C_{i}]_0^{0} = \sum_{k=1}^{K} [C_{i,k}]_0^{0} \quad (4.19)
\]
An example of the **regional baseline scenarios** is shown in figure 4.19. When the outcome of policies wants to be analyzed only for concrete regions such as Aragón or Ceuta and Melilla, AERIS is able to compute **concentrations** as a function of emission changes that occur in the respective administrative units. Contrasting these concentration profiles with the "nationwide" baseline scenario can also be carried out with AERIS in order to contextualize the evaluation in a national perspective. An additional advantage of having a series of regional baseline scenarios available is the assessment of **regional contributions** to the general air quality problem in Spain. Analyzing the contribution of the Spanish autonomous communities may be helpful for conducting source-apportionment studies at a finer spatially-resolved scale, aiming to provide relevant hints for a description of local or urban scales processes relevant for policy-making (Douros et al., 2012; Pirovano et al., 2015).

### 4.8 Extensions to other modules

The **modeling framework** presented in this section completely describes the procedures that were followed to obtain the **source-receptor matrices** (SRMs) that are used for predicting concentration changes due to changes in emissions, referred to a baseline scenario. Further adaptations of the results provided by these SRMs allow calculating **indicators** that are relevant under a **policy-making** point of view, most of which are contained in European and Spanish-level laws on air quality. In summary, the modeling framework that was applied for
4.8. Extensions to other modules

Constructing AERIS combines the outputs of an air quality model (AQM) along with observations and measurements from all over the Iberian Peninsula. For the purposes of this section, the estimation of air quality levels can be considered as fully-described. However, other modules have also been developed for AERIS in order to describe pollutant deposition or impacts on other aspects such as ecosystems, vegetation, crops, human health, etcetera, regardless of legal considerations. The description of these modules is addressed in the following sections. Yet, it is important to highlight that this impact description is a continuation of the presented methodology and is certainly subject to its uncertainties and hypotheses.

Figure 4.19: Resulting concentrations from the exclusive emissions of a) $PM_{2.5}$ in Aragón, b) $NO_\chi$ in Ceuta/Melilla, c) $PM_{10}$ in Comunidad de Madrid and d) $SO_2$ in Navarra.
5 Air quality system validation

The past sections of this work have been dedicated to the detailed explanation of the emissions and air quality system\footnote{In this section the term "model" refers to the AERIS coupled emission module - air quality system.} of AERIS in terms of the underlying modeling hypotheses, its construction process and the methods that have been used for this purpose. This section is devoted to the validation of the modules in order to see if the SRMs and the general parameterization works, aiming to use it in future policy support activities. The main objective of this section is to demonstrate that AERIS is capable of sufficiently reproducing the performance of the complex AQM and its related extensions.

5.1 Validation rationale

A model validation process is defined as the quantification of the degree to which a model is accurate in its representation of a real phenomenon from the perspective of the intended use of the model (Ling and Mahadevan, 2013). However, any model evaluation is a complex procedure that involves numerous steps such as scientific evaluation, code verification, and sensitivity analysis, which are ultimately aimed to build good model practices in terms of development as well as critical review (Thunis et al., 2012).

In general, model validation procedures are carried out qualitatively and quantitatively. Qualitative validation is very common in engineering and usually involve procedures such as graphical comparisons between predictions and reference datasets. However, quantitative methods are the most reliable options and they usually rely on statistics and provide supplement on subjective judgements and systematically account for errors and uncertainties (Ling and Mahadevan, 2013). Moreover, conducting a model validation process is necessary due to the fact that models intended for practical use entail the risk of misuse whenever their limitations are not completely understood or misinterpreted (Jakeman et al., 2009).
5.1. Validation rationale

It is crucial that the model is validated in terms of its purpose ("fit for purpose"), which involves gaining as much understanding as possible of the final use of the produced estimates (Alexandrov et al., 2011). An important issue that needs to be kept in mind at every stage of the validation process is that model results should be **credible**. To this respect, **credibility** refers to whether an actor perceives information as meeting standards of scientific plausibility and technical adequacy (Cash et al., 2003). To provide credibility, computer models must incorporate sufficient detail and complexities to accurately represent reality (Amann et al., 2011). As a consequence, model credibility is increased by modeler-manager dialogues and especially, by **rigorous** validation tests against **references** or **independent data**, uncertainty assessments and peer reviews (Jakeman et al., 2006; Eder et al., 2014).

The above paragraphs outline a generic validation framework that is not always possible to carry out. For the concrete purpose of AERIS, the model's objective is the **reproduction** of the estimates produced by the conventional AQM sufficiently well so that AERIS can be used instead for a given scenario, thus avoiding long computing times. More importantly, AERIS is still a model under development and is constantly being improved, so its diffusion and use are still going to be **limited** for a period of time.
Chapter 5. Air quality system validation

For the time being the validation framework of AERIS, which consists of a simple and comprehensive procedure, comprises the analysis of the correspondence between SRM estimates and the full AQM. This basically involves examining whether the parameterization of the AQM by the means of a SRM provides results that are somehow equivalent to those provided by the AQM alone. The evaluation should not be focused on the performance of the AQM itself, but rather on the ability of the SRM to produce comparable results. More concretely, the analysis procedure is composed of the following phases, as illustrated in Figure 5.1.

- **Stage 1(a): Evaluation of the source-receptor matrices (SRMs).** This phase involves the evaluation of the SRMs in terms of its statistic correspondence with the estimates produced by the AQM.

- **Stage 1(b): Evaluation of the congruence of the modeling approach - additivity test.** The additivity test is used for analyzing if the sum of the respective variation percentages applied to different SRMs performs similarly than the AQM under a simple, controlled emission scenario.

- **Stage 1(c): Evaluation of the secondary parameterizations.** The evaluation of the secondary parameterizations allows validating the assumed modeling approaches that complement the estimates given by SRMs (contributions, indicators, etc.).

- **Stage 2: Evaluation of the performance to a fully-controlled emission scenario.** This phase implies analyzing the performance of the complete set of SRMs against a fully controlled emission scenario simulated by the AQM.

- **Stage 3: Evaluation of the performance to a real-policy emission scenario.** The final stage of the proposed evaluation involves studying the correspondence between the estimates produced by the complete set of SRMs against an AQM simulation from a complex emission scenario with more sectors than those considered by the IAM.

5.2 Validation parameters and criteria

In order to rely on objective criteria for assessing the credibility of the model, a set of statistics have been chosen as validation parameters. The use of statistic parameters is intended to have a better overview of the IAM performance in the spirit of finding a compromise between the complexity of the evaluation and the need of providing simple and straightforward indicators for diagnosis. This fact is especially important for the analysis of the modeling results due to the fact that the number of cells in the studied domain equals 4500. The proposed indicators are statistical quantities typically used for benchmarking purposes and seek to characterize the quality of the correspondence under different perspectives (Thunis et al., 2011; Thunis and Clappier, 2014). For the concrete case of integrated assessment, these parameters have been thoroughly assessed in Vedrenne et al., (2013) and are the following.
5.2. Validation parameters and criteria

- **Pearson’s correlation coefficient** \( (r) \), which is a measure of the spatiotemporal agreement of predictions and the reference dataset.

- **Mean Bias** \((MB)\) and **Normalized Mean Bias** \((NMB)\), which measure the net ability of the modeled prediction to over or under estimate the reference dataset.

- **Mean Error** \((ME)\) and **Normalized Mean Error** \((NME)\), which quantify the total amount of error between comparison datasets, without compensation of deviations of opposite signs.

### 5.2.1 Pearson’s correlation coefficient

\[
r = \frac{\sum_{i=1}^{N} (M_i - \overline{M})}{\sqrt{\left(\sum_{i=1}^{N} (M_i - \overline{M})^2\right) \cdot \left(\sum_{i=1}^{N} (P_i - \overline{P})^2\right)}}
\]

(5.1)

Where:

- \( M_i \rightarrow \) Modeled data obtained from AERIS - [\( \mu g / m^3 \)].

- \( \overline{M} \rightarrow \) Mean of the modeled data obtained from AERIS - [\( \mu g / m^3 \)].

- \( P_i \rightarrow \) Predictions obtained from the full AQM - [\( \mu g / m^3 \)].

- \( \overline{P} \rightarrow \) Mean of the predictions obtained from the full AQM - [\( \mu g / m^3 \)].

The **Pearson’s correlation coefficient** \( (r) \) is a widely used performance statistic that measures the degree to which two variables correlate linearly (section 4.4.1). Correlation coefficients of 1 indicate perfect linear relationship between datasets, while coefficients equalling zero indicate that no such relationship between variables exists (USEPA, 2007).

Although it is generally accepted that the Pearson’s correlation coefficient is a standard measure of the correspondence between variables, it is an indicator that should be used carefully. In some cases, when datasets present outliers or extreme pairs, the value of this coefficient might be affected by a compensation effect between high and low values (Wilmott, 1982).
Chapter 5. Air quality system validation

5.2.2 Mean Bias

\[
MB = \frac{1}{N} \sum_{i=1}^{N} (M_i - P_i)
\]  
(5.2)

The mean bias (MB) is a performance indicator that averages the difference between two datasets over each pair in which the values of the reference datasets are greater than zero. If the mean bias equals zero, this indicates that the model over predictions exactly cancel the model under predictions or that there is an exact correspondence between datasets. The model bias has been defined in such a way that positive values indicate that the model prediction exceeds the observation, while negative values indicate likewise, underestimations (USEPA, 2007).

5.2.3 Mean Error

\[
ME = \frac{1}{N} \sum_{i=1}^{N} |M_i - P_i|
\]  
(5.3)

The mean error (ME) is defined as the average difference between all model-reference pairs and is very similar to the mean bias, with the exception that the error includes only absolute deviation between the two (Boylan and Russell, 2006).

5.2.4 Normalized Mean Bias - Normalized Mean Error

\[
NMB = \frac{\sum_{i=1}^{N} M_i - P_i}{\sum_{i=1}^{N} P_i} \cdot 100
\]

\[
NME = \frac{\sum_{i=1}^{N} |M_i - P_i|}{\sum_{i=1}^{N} P_i} \cdot 100
\]  
(5.4)

The normalized mean bias (NMB) and normalized mean error (NME) are recommended as indicators because they facilitate the range of concentration magnitudes. These indicators average the difference between the datasets (model predictions and references) over the sum of reference values. Moreover, they typically give a better sense of model performance due to the fact that they do not require a reference minimum threshold, while they assume that the reference datasets are the absolute truth (Boylan and Russell, 2006). It is also a useful performance indicator because it avoids overinflating the range of values of the reference dataset (USEPA, 2007).
5.2. Validation parameters and criteria

5.2.5 Reference dataset

In the above sections the concept of a reference dataset has been introduced along with the concepts of the statistic validation. The reference dataset is the group of data or model outputs that will be used as comparison standard for the validation of the outputs of AERIS, namely the predictions obtained from the full air quality model under different analysis circumstances. These datasets have been chosen as reference since the objective of AERIS is to reproduce the predictions of the AQM reasonably well. The evaluation does not focus on the appropriateness or goodness of the AQM results, which have already been evaluated in several studies and publications (Boldo et al., 2011; Borge et al., 2006; 2008; 2010; 2012; 2014).

5.2.6 Evaluation criteria

The criteria that were followed in order to validate the outputs of AERIS were different depending on the phase of the evaluation (figure 5.1). In general, datasets were analyzed in term of their agreement with at least one of the before mentioned statistic indicators, according to the validation stage in every case. It should be noted that no universal consensus has been reached so far on criteria and thresholds for model performance evaluation (Chemel et al., 2010).

The general criteria that were used for considering a given performance as adequate can be formulated as follows:

- **Evaluation of linearity.** The evaluation of linearity is perhaps the simplest and most important analysis that is applied to the datasets because it gives information on two essential modeling issues of the IAM. First, the correctness of the assumption of the existing linearity between emissions and concentrations used for the construction of SRMs (section 4.4) and second, the correspondence between the predictions of the IAM and the AQM. This analysis criterion is very common in modeling for integrated assessment purposes, such as in Amann et al., (2008) for the analysis of the linear approach for SRMs and in Amann et al., (2011) for the correspondence between the IAM and the AQM. The evaluation of linearity is carried out by the assessment of the Pearson’s correlation coefficient \( r \), priming the highest possible values of this indicator.

- **Error quantification.** The definition of error for the purposes of the validation of AERIS, can be expressed as the absolute deviation (in any relevant units) between the predictions of the IAM and those of the AQM. Therefore, the quantification of the total deviation between datasets is necessary in order to know the reliability of the outputs and ultimately, of the modeling framework. This evaluation will be carried out by analyzing the values of the mean error \( ME \) and the normalized mean error \( NME \).

- **Evaluation of accuracy.** In order to estimate if the predictions produced by AERIS are in order of magnitude with those of the AQM and if they correctly catch the most important phenomena at the given scale, an accuracy criterion needs to be established. To this respect, the definition of accuracy can be made as the ability of the model to reproduce
the magnitude of the estimates of the AQM. In other words, this analysis will focus on the over or underpredictions of AERIS when compared to the AQM. As a result, the mean bias ($MB$) and the normalized mean bias ($NMB$) will be used as relevant indicators for assessing the tendency of the IAM towards over or underprediction. In case of perfect agreement between IAM and AQM; MNE would equal 0%, meaning that there is no additional loss of accuracy by using IAM instead of AQM (Russell and Dennis, 2000; Chemel et al., 2010).

### 5.2.7 Graphic validation resources

In order to validate the model, the evaluation relied on the use of graphical tools along with the quantification of the statistic indicators mentioned above. To this respect, the use of scatterplots was common in order to graphically interpret linear patterns between datasets, to support the value of the Pearson's correlation coefficient and to examine data spreads (Appel et al., 2007). More generally, a scatterplot is a mathematical diagram that displays values for two variables for a set of data in Cartesian coordinates ($x, y$) as a collection of points. The disposition of these points along a central diagonal line ($y = x$) indicates a perfect linear correspondence between datasets and thus, a value of $r = 1$ (Utts, 2005). Although there are many other graphics that are constantly used for the evaluation of AQMs, for the purposes of the validation of AERIS only the scatterplots make sense because datasets are not temporally-resolved.

### 5.3 Limitations of the validation rationale

In general lines, the validation rationale that has been explained above can be considered a typical operational evaluation of an AQM. As a consequence, it should be kept in mind that this type of evaluations do not provide information on the adequacy of models for the representation of concentrations and its complex underlying processes (Dennis et al., 2010). Moreover, one must not forget that Eulerian AQM are non-linear systems whose results may considerably deviate from the linear approach addressed by AERIS.

The examination of modeling practices by the means of statistic indicators or mathematical analyses is not enough to validate models in a formal sense. However, the validation procedure may have a diagnostic value that can provide enough understanding on the abilities and skills of the model. It should also be noted that the selected evaluation criteria are not absolute truth and that, according to the application, the compliance of the model is context-relative (Steyn and Galmarini, 2008).
5.4 Evaluation of primary pollutants

The first validation stage consists in the evaluation of the source-receptor matrices (SRMs). This procedure has already been introduced in (section 4.4.1) and involves reproducing with the SRM and the respective variation percentages, the original AQM outputs that were used for the construction of the given SRM. The evaluation at this stage allows investigating whether the applied linear regression model is an adequate parameterization for a given sector or pollutant. The analysis procedure is carried out by statistically comparing the outputs of the AQM and AERIS for the arbitrary emission variations that were used to build the SRM, namely $-90\%$, $-50\%$, $0\%$, $50\%$ and $90\%$. The Pearson's correlation coefficient ($r$) is calculated for the five pairs of datasets simultaneously, as a measure of the overall statistic correspondence produced by the SRM. It should be noted that according to (section 4.4.1), a visual inspection of the linearity of the AQM results was needed at different cells of the domain. This inspection would a priori identify the adequateness of choosing a linear model for the construction of the SRM for the selected cells. However, conducting this inspection for every cell of the domain is unfeasible, so a general evaluation relying on statistics is better suited. The evaluation of the SRMs has been made for the two sets of months that were chosen as representative of the winter and summer conditions in the Iberian Peninsula, namely January and August, for every studied pollutant and its respective sectors (section 4.2). Additionally, the concept of the gamma matrix, $[\gamma_{i,j}]_{n \times m}$, was introduced as a measure of the parameterization's deviation for nil variation percentages ($p_i = 0\%$). This gamma matrix is intimately related with the intercept parameter when the applied regression model is of the form $y = a \cdot x + b$. By examining the mean of the gamma matrix, one can get an idea about the overall deviation in the reproduction of the baseline emissions of the given sector.

Table 5.1: Pearson's correlation coefficients and mean gamma values for $NO_2$ SRMs.
Figure 5.2: IAM vs. AQM scatterplot for NO₂ mean concentration of SNAP 070101 (August).

5.4.1 Evaluation of the NO₂ source-receptor matrices.

Table 5.1 presents the correlation coefficients⁸ and the means of the gamma matrix, which are the necessary indicators for the evaluation of the NO₂ SRMs. According to the evaluation criteria stated in section 5.2.6, the NO₂ SRMs reproduce through a linear relationship the concentrations of pollutant as a consequence of the percentual changes in emissions since each of the correlation coefficients is $r \geq 0.65$. It should be noted that the means of the gamma matrices in each case indicate that the deviation in the reproduction of the baseline scenarios by AERIS and the AQM is small in every case. Although no criterion was previously established for the gamma means, for the case with the highest deviation (SNAP 010000) the value of the mean corresponds to a 2% of the average of the mean annual concentrations of NO₂ in 2007 for the modeled domain. An example of the linear behavior exhibited between the AQM outputs and the estimates of AERIS can be seen in the scatterplot of SNAP 070101 (August), as depicted in figure 5.2. In this scatterplot, the data points for the five emission variations distribute uniformly along the $y = x$ line, reflecting an excellent statistic correspondence according to the above mentioned criteria and supported by its respective correlation coefficient from table 5.1 ($r = 0.9995$). Moreover, figure 5.2 does not exhibit any point outside the factor of two (FAC2) region (shaded). Examining the number of points within the FAC2 region is useful because it gives an idea about the bias of the data distribution (Carslaw, 2011).

---

⁸Unless otherwise stated, the term “correlation coefficient” refers to the Pearson's correlation coefficient.
5.4. Evaluation of primary pollutants

5.4.2 Evaluation of the SO\textsubscript{2} source-receptor matrices.

Following the same analysis line than in the section before, the values of the correlation coefficients and the means of the gamma matrices are shown in table 5.2. In this case, assuming a linear relationship between the concentrations of SO\textsubscript{2} and the variations in emissions seems to be an adequate approach since the correlation coefficients are above $r \geq 0.65$ (Thunis et al., 2011). The values of the gamma means ($\bar{\gamma}$) for this pollutant also hint on the relatively low deviations in the reproduction of the baseline emissions of their respective sectors.

Table 5.2: Pearson’s correlation coefficients and mean gamma values for SO\textsubscript{2} SRMs.

<table>
<thead>
<tr>
<th>SNAP group</th>
<th>$r_{01}$</th>
<th>$r_{08}$</th>
<th>$\bar{\gamma}_{01}$ [ppm]</th>
<th>$\bar{\gamma}_{08}$ [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>010000</td>
<td>0.9992</td>
<td>0.9998</td>
<td>$4.67 \times 10^{-5}$</td>
<td>$5.16 \times 10^{-6}$</td>
</tr>
<tr>
<td>020202</td>
<td>0.9999</td>
<td>0.9999</td>
<td>$7.81 \times 10^{-7}$</td>
<td>$1.63 \times 10^{-6}$</td>
</tr>
<tr>
<td>030000</td>
<td>0.9991</td>
<td>0.9999</td>
<td>$1.09 \times 10^{-5}$</td>
<td>$1.60 \times 10^{-6}$</td>
</tr>
<tr>
<td>040000</td>
<td>0.9942</td>
<td>0.9998</td>
<td>$2.51 \times 10^{-5}$</td>
<td>$1.60 \times 10^{-6}$</td>
</tr>
<tr>
<td>080600</td>
<td>0.9999</td>
<td>0.9999</td>
<td>$9.33 \times 10^{-7}$</td>
<td>$1.57 \times 10^{-6}$</td>
</tr>
<tr>
<td>080800</td>
<td>0.9999</td>
<td>0.9999</td>
<td>$9.17 \times 10^{-7}$</td>
<td>$1.62 \times 10^{-6}$</td>
</tr>
<tr>
<td>Portugal</td>
<td>0.9999</td>
<td>0.9702</td>
<td>$6.28 \times 10^{-8}$</td>
<td>$9.95 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

In appendix A.4, the comparison of the data produced by AERIS and the results of the AQM for the relevant SO\textsubscript{2} sectors has been made through scatterplots. From these figures, it can be seen that most points are distributed along the $y = x$ line, and virtually all of them within the FAC2 region (shaded). Although a good agreement can be seen in most cases, the presence of outliers (points outside the FAC2 region) and a somewhat larger dispersion of data is also evident.

5.4.3 Evaluation of the PM source-receptor matrices.

Evaluation of the PM\textsubscript{10} source-receptor matrices.

In line with what has been discussed above, the evaluation of the SRMs of PM\textsubscript{10} indicates that a linear approach is also adequate for modeling this pollutant. In general, the correlation coefficients and the mean values of gamma that have been obtained for each of the analyzed sectors reveal a high degree of linearity between the estimates of AERIS and the results of the AQM. As with the before mentioned cases, the complete set of PM\textsubscript{10} SRMs were validated. The numeric values of the correlation coefficients and the means of gamma are included in table 5.3. The adequateness of the linear approximation for the construction of the SRMs for PM\textsubscript{10} is shown in the figures of appendix A.4. In general, the results of the four simulations ($-90\%$, $-50\%$, $0\%$, $50\%$, $90\%$) for mostly any sector distribute uniformly along the $y = x$ line and always within the FAC2 region. At this point, it is worth noticing that the SRMs for PM\textsubscript{10} (as well as for PM\textsubscript{2.5}) refer only to primary particulate matter (represented as $[G_{PM,j}]_{n \times m}$ in...
Chapter 5. Air quality system validation

Table 5.3: Pearson's correlation coefficients and mean gamma values for $PM_{10}$ SRMs.

<table>
<thead>
<tr>
<th>SNAP group</th>
<th>$r_{01}$</th>
<th>$r_{08}$</th>
<th>$\overline{y}_{01}$ [µg/m$^3$]</th>
<th>$\overline{y}_{08}$ [µg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>020202</td>
<td>0.9996</td>
<td>0.9999</td>
<td>$8.10 \times 10^{-5}$</td>
<td>$5.93 \times 10^{-5}$</td>
</tr>
<tr>
<td>070101</td>
<td>0.9995</td>
<td>0.9999</td>
<td>$1.07 \times 10^{-4}$</td>
<td>$5.71 \times 10^{-5}$</td>
</tr>
<tr>
<td>070103</td>
<td>0.9999</td>
<td>0.9999</td>
<td>$1.56 \times 10^{-5}$</td>
<td>$1.50 \times 10^{-4}$</td>
</tr>
<tr>
<td>070201</td>
<td>0.9975</td>
<td>0.9999</td>
<td>$1.20 \times 10^{-2}$</td>
<td>$4.66 \times 10^{-5}$</td>
</tr>
<tr>
<td>070203</td>
<td>0.9975</td>
<td>0.9999</td>
<td>$1.20 \times 10^{-2}$</td>
<td>$6.64 \times 10^{-5}$</td>
</tr>
<tr>
<td>070301</td>
<td>0.9999</td>
<td>0.9999</td>
<td>$1.01 \times 10^{-4}$</td>
<td>$4.66 \times 10^{-5}$</td>
</tr>
<tr>
<td>070303</td>
<td>0.9999</td>
<td>0.9999</td>
<td>$1.03 \times 10^{-4}$</td>
<td>$5.62 \times 10^{-6}$</td>
</tr>
<tr>
<td>0707/08</td>
<td>0.9996</td>
<td>0.9999</td>
<td>$7.60 \times 10^{-2}$</td>
<td>$5.67 \times 10^{-5}$</td>
</tr>
<tr>
<td>080600</td>
<td>0.9998</td>
<td>0.9999</td>
<td>$1.45 \times 10^{-2}$</td>
<td>$1.01 \times 10^{-4}$</td>
</tr>
<tr>
<td>080800</td>
<td>0.9994</td>
<td>0.9999</td>
<td>$7.09 \times 10^{-4}$</td>
<td>$6.68 \times 10^{-5}$</td>
</tr>
<tr>
<td>100500</td>
<td>0.9986</td>
<td>0.9998</td>
<td>$1.40 \times 10^{-2}$</td>
<td>$1.10 \times 10^{-2}$</td>
</tr>
<tr>
<td>Portugal</td>
<td>0.9992</td>
<td>0.9994</td>
<td>$2.00 \times 10^{-3}$</td>
<td>$6.00 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

section 4.5.2). This means that the contribution of nitrogen and sulfur-emitting sources to the total mass of particulate matter is not considered by the SRMs that are currently assessed. The evaluation of the parameterizations that allowed quantifying the contribution of these species to the total $PM$ mass will be addressed in the following sections.

Evaluation of the $PM_{2.5}$ source-receptor matrices.

As with $PM_{10}$, the SRMs for $PM_{2.5}$ produce estimates that correspond linearly with the outputs of the AQM. This behavior is confirmed by the values of the correlation coefficients and mean

Table 5.4: Pearson's correlation coefficients and mean gamma values for $PM_{2.5}$ SRMs.

<table>
<thead>
<tr>
<th>SNAP group</th>
<th>$r_{01}$</th>
<th>$r_{08}$</th>
<th>$\overline{y}_{01}$ [µg/m$^3$]</th>
<th>$\overline{y}_{08}$ [µg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>020202</td>
<td>0.9995</td>
<td>0.9999</td>
<td>$8.10 \times 10^{-2}$</td>
<td>$7.88 \times 10^{-5}$</td>
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<tr>
<td>070101</td>
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<td>0.9999</td>
<td>$1.06 \times 10^{-4}$</td>
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<td>070103</td>
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<td>0.9999</td>
<td>$1.56 \times 10^{-5}$</td>
<td>$1.52 \times 10^{-4}$</td>
</tr>
<tr>
<td>070201</td>
<td>0.9968</td>
<td>0.9999</td>
<td>$1.20 \times 10^{-2}$</td>
<td>$6.16 \times 10^{-5}$</td>
</tr>
<tr>
<td>070203</td>
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<td>0.9999</td>
<td>$1.20 \times 10^{-2}$</td>
<td>$3.96 \times 10^{-5}$</td>
</tr>
<tr>
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<td>0.9999</td>
<td>$1.01 \times 10^{-4}$</td>
<td>$6.17 \times 10^{-5}$</td>
</tr>
<tr>
<td>070303</td>
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<td>0.9999</td>
<td>$1.03 \times 10^{-4}$</td>
<td>$9.08 \times 10^{-6}$</td>
</tr>
<tr>
<td>0707/08</td>
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<td>0.9999</td>
<td>$7.70 \times 10^{-2}$</td>
<td>$2.65 \times 10^{-5}$</td>
</tr>
<tr>
<td>080600</td>
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<td>0.9999</td>
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<td>$1.24 \times 10^{-4}$</td>
</tr>
<tr>
<td>080800</td>
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<td>0.9999</td>
<td>$3.00 \times 10^{-3}$</td>
<td>$8.72 \times 10^{-5}$</td>
</tr>
<tr>
<td>100500</td>
<td>0.9983</td>
<td>0.9978</td>
<td>$1.30 \times 10^{-2}$</td>
<td>$2.00 \times 10^{-2}$</td>
</tr>
<tr>
<td>Portugal</td>
<td>0.9994</td>
<td>0.9980</td>
<td>$4.00 \times 10^{-3}$</td>
<td>$5.00 \times 10^{-2}$</td>
</tr>
</tbody>
</table>
Table 5.5: Pearson's correlation coefficients and mean gamma values for NH$_3$ SRMs.

<table>
<thead>
<tr>
<th>SNAP group</th>
<th>$r_{01}$</th>
<th>$r_{08}$</th>
<th>$\bar{\gamma}_{01}$ [ppm]</th>
<th>$\bar{\gamma}_{08}$ [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>100101</td>
<td>0.99601</td>
<td>0.9974</td>
<td>4.65×10^{-5}</td>
<td>4.79×10^{-5}</td>
</tr>
<tr>
<td>100102</td>
<td>0.9944</td>
<td>0.9974</td>
<td>2.33×10^{-5}</td>
<td>5.35×10^{-5}</td>
</tr>
<tr>
<td>100500</td>
<td>0.9966</td>
<td>0.9975</td>
<td>3.30×10^{-5}</td>
<td>4.21×10^{-5}</td>
</tr>
<tr>
<td>110000</td>
<td>0.9959</td>
<td>0.9855</td>
<td>2.24×10^{-5}</td>
<td>9.06×10^{-6}</td>
</tr>
<tr>
<td>Portugal</td>
<td>0.9997</td>
<td>0.9999</td>
<td>1.19×10^{-5}</td>
<td>6.25×10^{-5}</td>
</tr>
</tbody>
</table>

gamma values present in table 5.4. In appendix A.4, the scatterplots for PM$_{2.5}$ exhibit good correlation levels with uniformly-distributed points along the one-to-one line ($y = x$) and every point inside the FAC2 region. It should be noted that similar performance levels were observed for PM$_{2.5}$ than for PM$_{10}$, which actually hints on the fact that only primary emissions of particulate matter are being assessed by these SRMs (Ehrlich et al., 2007). In general, it can be said that these behaviors validate the linear approximation between variations in the emissions of primary PM and concentration levels.

5.4.4 Evaluation of the NH$_3$ source-receptor matrices.

As with the rest of pollutants, the linear approach for the parameterization of the relationship between emission variations and concentrations for NH$_3$ seems adequate table 5.5. The value of the correlation coefficients is in every case $r \geq 0.40$ (Thunis et al., 2011). An examination of the scatterplots for the ammonia-relevant sectors in appendix A.4 shows a higher degree of dispersion for this pollutant when compared to the rest. Nevertheless, linearity has also been confirmed and the SRMs for NH$_3$ can be validated.

5.4.5 Evaluation summary

The analysis of the linear approach followed for parameterizing the relationship between emission variation percentages and concentrations has been presented in the before commented sections. In general it was observed that within the studied range $p_i = [-90\%, 90\%]$, emission variations correlate linearly with concentrations proved that the emissions of only one sector and one pollutant are changed. As it was stated in section 5.2.6, the degree of statistical correspondence between the estimates produced by a SRM against the results of the conventional AQM was examined with the Pearson's correlation coefficient ($r$). Furthermore, the mean value of the gamma matrix ($\bar{\gamma}$) was introduced by the author to quantify the degree of deviation between the statistical regression and the AQM when the independent variable equals zero. When contrasting the correlation coefficients with good performance values reported in scientific literature, it becomes clear that the constructed SRMs reproduce reasonably well the results of the AQM and that can be effectively used for calculating concentrations for any variation percentage ($p_i$) that lies within the studied range. From the set of scatterplots
present in appendix A.4, the good-correlation level that has been discussed is also confirmed. Despite the fact that some of these scatterplots (especially those of \( NH_3 \)) do exhibit points that do not distribute along the one-to-one line \( (y = x) \) and even some of them lie outside the \( FAC2 \) region SRMs were generally validated. This by no means indicates that this amount of error is being discarded, but rather taken into consideration for future uncertainty analyses.

### 5.5 Evaluation of the congruence of the modeling approach

In the previous section, the statistical evaluation provided the necessary arguments to validate the constructed SRMs and use them to compute concentrations with enough confidence. However, it is of little interest to calculate the concentrations of only one pollutant as a consequence of changes in the emissions of one sector. Really, a robust IAM should be able to provide answers on the complex interplay between changes in several emission sectors and for different pollutants simultaneously and AERIS was formulated as such (section 4.5). In general lines, AERIS considers that the resulting concentrations of a given pollutant across the domain are the sum of all the marginal variations in concentrations around the baseline scenario produced by those sectors that suffered changes in emissions. Since SRMs have been formulated in terms of independent pollutant and sector-specific response functions it is necessary to evaluate whether the “sum-based”; to this respect an additivity test was conducted.
5.5. Evaluation of the congruence of the modeling approach

The additivity test constitutes a comparison between the total accumulation of error from simulations with sectors varying independently and the total error produced by a simulation in which the same sectors varied simultaneously, since it is uncertain to what extent feedbacks and non-linearities can prevent from a linear addition of reductions computed in an isolated way. This test was applied with guidance from Schöpp et al., (2005) and Bennett et al., (2013). The analysis focused on nitrogen dioxide (NO₂) due to the fact that it is very relevant from the current perspective of air quality and due to the complexity regarding this particular pollutant (an important amount is of secondary nature and it participates in the complex processes of particulate matter and ozone (O₃) formation), so a reasonable idea of the general behaviour of AERIS to this respect can be obtained.

The analysis consisted in defining a simple hypothetical scenario (HS), with a given number of N sectors (S₁, S₂, ... S₅) whose NOₓ emissions were varied when compared to the 2007 baseline scenario. Each of these variations was processed separately with AERIS and the ordinary AQM and their results compared. The full HS was also explicitly simulated by both models and the obtained estimates compared. An assessment on whether the following condition was fulfilled for three different thresholds (t) of 0.5, 1.0 and 1.5 µg/m³ was made:

\[
\sum_{i=1}^{N} |S_{i,AERIS} - S_{i,AQM}| - |HS_{AERIS} - HS_{AQMS}| \leq t \quad t = \{0.5, 1.0, 1.5 \text{µg/m}^3\}
\] (5.5)

The lowest threshold (t = 0.5µg/m³) was selected because it corresponds approximately to the mean error (ME) of NO₂ predicted by AERIS (ME = 0.49µg/m³) for a fully-described emission scenario evaluated in Vedrenne et al., (2013). The other thresholds are twofold and threefold this concentration value respectively. To this respect, the approach was considered adequate enough in those cells below the first threshold, meaning that the accumulation of error due to the independent use of SRMs is analogous to the error associated with the simultaneous use of SRMs. Despite the fact that AERIS is able to provide a variety of air quality indicators, the analysis was carried out using exclusively annual mean concentrations data since is the only metric explicitly computed. Errors and deviations for other parameters would involve not only potential additivity issues but also specific errors in their computation procedure from the annual mean.

5.5.1 Hypothetic scenario for additivity test

The hypothetical emission scenario used for the additivity test (HS) consisted in a number of relevant activity groups, whose emissions changed with respect to the baseline scenario. The variation percentages of NOₓ emissions (pNOₓ,i) in every case were set arbitrarily and do not have any actual relevance because these were chosen to evaluate the model’s response when high variations are applied to the baseline scenario. To this respect, the term arbitrary
refers to the fact that they were not calculated through the comparison of a projected (or future) emission against the baseline scenario. The definition of the hypothetic scenario is presented in Table 5.6. Usually when emission projections are calculated with realistic ancillary information (“real values”), the obtained variation percentages are negative because current trends normally lead to reductions. However, we wanted to examine the behaviour of the approach at high variation percentages that are not likely to occur in reality because these are adequate to have a better view of the model response. Let us not forget that the objective of the additivity test is to analyze the numeric appropriateness of the “sum approach” on which AERIS is based (section 4.5). For this analysis, it is not important to justify whether the variation percentages make sense in terms of future scenarios but to see if the SRMs are able to perform similarly than the AQM to the exact same emission changes in the widest possible range.

### 5.5.2 Results of the additivity test

The additivity test has revealed that for NO₂, the modeling hypotheses implemented during the construction of AERIS seem reasonable. The main question here was assessing whether a combination of the results form isolated SRMs able to reproduce a change in the pollutant concentration in the same way that this change is produced by the AQM along with other varying sectors. The goal of the analysis is to gain insight on the appropriateness of the modeling framework of AERIS. The spatial representation of the threshold agreement is shown in figure 5.3. It can be seen that most cells (4416 - 98.1%) are below the lowest threshold, covering most of the modeling domain while a minority of cells are above $t = 1.0 \, \mu g/m^3$ and $t = 1.5 \, \mu g/m^3$ (73 and 11, 1.6% and 0.2% respectively). Domain-averaged results for the additivity test are presented in Table 5.7 for each of the evaluated sectors. As it can be seen, the resulting NO₂ mean annual concentrations calculated by both models are similar, with low mean absolute errors ($|X_{AERIS} - X_{AQMS}| < 0.5 \mu g/m^3$). It should be noted that the estimates produced by those cells in which $t = 1.5 \, \mu g/m^3$ are not to be discarded due to the fact that the general (domain-wide) performance is considered to be in range. The largest errors (both absolute and relative to emission changes) are related to point sources. To this respect, probably emission dispersion for large point sources is even more meteorology-dependent than for area sources and the larger errors are basically due to reduced accuracy in the computation of the annual from the January and August SRMs.
5.6 Evaluation of secondary pollutants

In the previous sections, the detailed analysis and evaluation of the construction process of the source-receptor matrices (SRMs) that are the fundamental elements of AERIS as an integrated assessment model has been carried out. The general equations of the model presented in section 4.5 make reference to a number of terms who actually do not depend directly on emission variations of the primary pollutant in question. This means that in order to compute concentrations for these pollutants, additional parameterizations had to be made in order to complement the predictive capacity of the initially-obtained SRMs. Such is the case of secondary particles (namely those related to the emissions of $NO_x$, $SO_2$ and $NH_3$) and tropospheric ozone ($O_3$). Equally, the quantification of policy-relevant indicators required numerous assumptions that need to be checked for validity.

Table 5.7: Results of the additivity test expressed as mean values for the entire domain.

| SNAP group | Activity name | $X_{AERIS}$ | $X_{AQM}$ | $|X_{AERIS} - X_{AQM}|$ |
|------------|---------------|-------------|------------|--------------------------|
| 010000     | Coal-fired power plants $\geq 300$ MW | 4.41        | 4.67       | 0.27                     |
| 070101     | Passenger cars - highway driving      | 4.42        | 4.41       | 0.05                     |
| 070103     | Passenger cars - urban driving         | 4.48        | 4.51       | 0.14                     |
| 070303     | Heavy-duty vehicles - urban driving    | 4.43        | 4.44       | 0.01                     |
| $\sum_i^N S_i$ | –                                          | –           | –          | 0.48                     |
| –          | All sectors ($HS$)                      | 4.62        | 4.88       | 0.22                     |

Despite the fact of having a limited number of sectors at the $HS$ and only assessing one pollutant, the basic modeling approach implemented for AERIS seems adequate for representing either individual or group variations. It should be stressed out that this additivity test is able only to provide a rough estimate of the expected deviation between model estimates when different sectors change their emissions simultaneously and only for one pollutant ($NO_2$ in this case). Such a deviation is expected to grow and propagate as the number of sectors as well as the complexity of the evaluation increase. However, the magnitude of the absolute deviations observed in relation to the magnitude of the variations considered in the experiment points out that the actual error for any practical scenario should fall within reasonable limits.
5.6.1 Evaluation of the parameterizations for secondary particulate matter

The formation of secondary particulate matter as a consequence of the emissions of sulfur and nitrogen compounds is a complex process that involves several chemical reactions and equilibria between sulfate, nitrate and ammonium species. Its rigorous description and incorporation into air quality models has been subject of numerous studies (Ansari and Pandis, 1998; Nenes, 1998; Erisman et al., 2003; Erisman and Schaap, 2004; Pankow, 2013). The inherent complexity associated with the description of secondary particles calls for simplifying as much as possible any parameterizations and modeling assumptions in order to effectively incorporate these processes into the general formulation of the IAM. According to the general equations of the model, AERIS estimates the contribution of sulfur and nitrogen (either as NO\textsubscript{x} or NH\textsubscript{3}) to the total mass of particulate matter as a linear relationship between the variation percentages (\(p_i\)) of the so-called precursor gases (Pecorari et al., 2014). This approach has been effectively applied in the formulation of other air pollution integrated assessment models (i.e. GAINS) (Klimont et al., 2009). Namely, for the GAINS model it has been shown that a linear model performs adequately when only marginal changes in emissions around a reference point are considered (Amann et al., 2011).

The modeling hypothesis made for quantifying this specie in AERIS is that the total contribution of a given precursor gas is directly proportional to the total variation of this pollutant in the domain, regardless of the emission sectors that are affected by this variation. As a consequence, in equation 4.6 the terms that quantify the contribution of precursor gases - \([c^{PM}_{NOx}] \cdot p_{NOx}\), \([c^{PM}_{SO2}] \cdot p_{SO2}\), \([c^{PM}_{NH3}] \cdot p_{NH3}\) - have not been modeled as sums but as individual terms. In every case, the terms \([G_i^{PM}]\) are actually secondary matrices of coefficients that have been constructed according to the general methodology used for those related to primary emissions. The construction of these secondary matrices has been made taking into account the related species estimated by CMAQ (which includes the atmospheric chemistry module of the AQM) and they only act as proportionality constants according to Binkowski and Roselle, (2003).

\[
[PM_{NOx}] = [ANO3I] + [ANO3J] = [c^{PM}_{NOx}] \cdot p_{NOx}
\]

\[
[PM_{SO2}] = [ASO4I] + [ASO4J] + [ASO4K] = [c^{PM}_{SO2}] \cdot p_{SO2}
\]

\(^\text{9}\)The term “secondary particulate matter” refers to the amount of the total PM mass that is originated from the emission of NO\textsubscript{x}, SO\textsubscript{2} and NH\textsubscript{3}. Completely separating fractions of secondary aerosol is a complex task and AERIS’s parameterizations only constitute an approximation to the formation of such species. Furthermore, AERIS has not parameterized the formation of secondary organic aerosols.
5.6. Evaluation of secondary pollutants

\[ [PM_{NH3}] = [ANH4I] + [ANH4J] = [G_{NH3}^{PM}] \cdot p_{NH3} \]  

(5.8)

Where species labeled with a \( I \) correspond to the masses of nitrate (\( NO_3^- \)), sulfate (\( SO_4^{2-} \)) and ammonium (\( NH_4^+ \)) in \textit{Aitken mode}. The species labeled with a \( J \) correspond to the masses of the respective compounds in \textit{accumulation mode} while the \( K \) label is associated with \textit{coarse mode} species (Appel et al., 2008). In order to statistically obtain the SRM that correlates the \textbf{total emission variation percentages} of precursor gases and their respective \textbf{total particle contribution} a linear regression was carried out for \( p_i = (-90\%, -50\%, 0\%, 50\%, 90\%) \). As with the ordinary SRMs, the AQM was run for the two conventional months: January and August. The evaluation of the total contributions to particles was carried out according to the usual statistical indicators introduced in \textsection 5.2 and focused on the \textit{linear} correspondence between datasets. To this respect, the scatterplots for each of the before mentioned contributions can be found in \textit{figure} 5.4, while the numeric value of the statistic indicators is shown in \textit{table} 5.8.

In summary, it can be said that the SRMs correlate well with the results yielded by the conventional AQM. From \textit{figure} 5.4, one can see that there is a reasonably good level of statistical correspondence between data pairs, since most points distribute along to \( y = x \) line. The values of the statistical indicators also suggest an acceptable level of performance. The degree of dispersion of the points in \textit{figure} 5.4 for January and August can be attributed to seasonal variations. For example in the case of \( NO_x \) contributions to \( PM \) mass, these seem to be more disperse in the winter when domestic heating and power generation usually register increases (Arsalis and Alexandrou, 2015). To this respect from the values of the \( MB \) and \( NMB \), we see some degree of outlier-compensation which generally biased the AERIS predictions towards underestimation. However, the values of the \( ME \) and \( NME \) indicate that the absolute deviation degree between the full-AQM and the IAM approximation is of 10%. According to previous aerosol-modeling activities, it can be concluded that the SRMs obtained with the general modeling approach of AERIS are \textbf{acceptable} and describe in good terms the aerosol composition

<table>
<thead>
<tr>
<th>Contribution</th>
<th>Month</th>
<th>( r )</th>
<th>( MB - [\mu g/m^3] )</th>
<th>( ME - [\mu g/m^3] )</th>
<th>( NMB(%) )</th>
<th>( NME(%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( [G_{NH3}^{PM}] \cdot p_{NH3} )</td>
<td>January</td>
<td>0.9818</td>
<td>-6.95\times10^{-2}</td>
<td>1.40\times10^{-1}</td>
<td>-5.44</td>
<td>10.99</td>
</tr>
<tr>
<td></td>
<td>August</td>
<td>0.9916</td>
<td>4.54\times10^{-11}</td>
<td>4.46\times10^{-2}</td>
<td>0.01</td>
<td>4.66</td>
</tr>
<tr>
<td>( [G_{NOx}^{PM}] \cdot p_{NOx} )</td>
<td>January</td>
<td>0.9953</td>
<td>-5.03\times10^{-2}</td>
<td>1.08\times10^{-1}</td>
<td>-2.33</td>
<td>5.02</td>
</tr>
<tr>
<td></td>
<td>August</td>
<td>0.9906</td>
<td>-3.47\times10^{-4}</td>
<td>4.95\times10^{-2}</td>
<td>-0.08</td>
<td>11.18</td>
</tr>
<tr>
<td>( [G_{SO2}^{PM}] \cdot p_{SO2} )</td>
<td>January</td>
<td>0.9972</td>
<td>2.86\times10^{-2}</td>
<td>8.21\times10^{-2}</td>
<td>1.30</td>
<td>3.72</td>
</tr>
<tr>
<td></td>
<td>August</td>
<td>0.9913</td>
<td>-3.31\times10^{-1}</td>
<td>3.66\times10^{-1}</td>
<td>-10.12</td>
<td>11.20</td>
</tr>
</tbody>
</table>

Table 5.8: Results of the additivity test expressed as mean values for the entire domain.
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Figure 5.4: $NO_3^-$, $SO_4^{2-}$, and $NH_4^+$ in PM predicted by IAM vs. AQM under the BS.
5.6. Evaluation of secondary pollutants

In the light of the above, it makes sense that AERIS has more difficulties in estimating secondary pollutants as the emission-concentration relationship is not direct.

5.6.2 Evaluation of the parameterization for tropospheric ozone

The secondary parameterization of tropospheric ozone \( O_3 \) is a particularly important element of AERIS, due to the fact that this pollutant is subject to stringent control and yet, it cannot be limited directly since it is not primarily-emitted. The modeling process of tropospheric ozone might not be as straightforward as with the rest of pollutants due the physicochemical processes that describe its formation and atmospheric lifetime (typically longer than the primary pollutants dealt with in previous section). To this respect, the emission-concentration response of \( O_3 \) presents important non-linearities, especially with respect to the emissions of \( NO_x \) (Rypdal et al., 2005; Amann et al., 2011). To deal with these issues, AERIS calculates \( O_3 \) through a non-linear conversion module that correlates the resulting \( NO_2 \) concentrations (expressed as the annual mean concentration of \( NO_2 \) calculated with equation 4.7) and the \( VOC \) emissions with the ambient \( O_3 \) concentration (Carnevale et al., 2012). The expression for estimating the concentrations of \( O_3 \) was adapted from Guariso et al., (2004) and verified with the use of a surface-regression tool in MATLAB® (sftool). The regression coefficients were calculated following a response surface methodology according to Chi et al., (2012). The methodology was analyzed according to the criteria and recommendations published in Heyes et al., (1996) and the re-analysis of the results from the parent AQM model of RAINS (Amann...
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Figure 5.6: IAM vs. AQM scatterplot of the $O_3$ annual mean concentration for the BS.

and Lutz, 2000). The modeling process of the secondary parameterization for tropospheric ozone involved applying the response-surface methodology to the 4500 cells of the domain. Figure 5.5 shows the response surfaces for the three cells of the modeling domain that contain the city centers of Madrid, Barcelona and Seville. From this figure, it is evident that the shape and inclination of the resulting surface depends on the particular conditions of every cell.

The statistical comparison of the predictions of AERIS against the results yielded by the full-AQM for the BS is shown in figure 5.6, where the majority of the data pairs distribute along the $y = x$. For this comparison, the Pearson's correlation coefficient equals $r = 0.9950$ which can be considered good enough to validate the modeling approach. This statistical correspondence is comparable to the one obtained by Amann et al., (2011) for tropospheric ozone (expressed as $SOMO_{35}$) in the GAINS model ($r = 0.9626$). These results suggest that AERIS seems to systematically underpredict $O_3$ against the CMAQ configuration that the AQM incorporates. This tendency towards overprediction by the AQM appears to be offset by the secondary parameterizations of AERIS, as discussed in Vedrenne et al., (2014).

5.6.3 Evaluation of the parameterizations for policy-relevant indicators

In this section, the evaluation of the parameterizations that allow the estimation with AERIS of annual and monthly mean concentrations. According to what has been discussed in section 4.6.2, the quantification of indicators such as percentiles or $AOT_{40}$ require an additional
5.6. Evaluation of secondary pollutants

Figure 5.7: IAM vs. AQM scatterplot for annual mean concentrations for BS.
adjustment that involves mixing AQM outputs and observations. Since at this point the evaluation focuses only on the comparison between AERIS and its parent AQM, the validation of the before mentioned modeling practice will be addressed along with the analysis of AERIS’s performance to real policy scenarios.

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**Evaluation of the annual-mean parameterization**

According to section 4.6.1, the estimation of the annual mean in every case involved calculating a transformation coefficient \( q \) which was derived from a complete annual simulation with the AQM and the respective monthly means of January and August for the 2007 baseline scenario. The computation of the annual mean was the arithmetic mean value between the transformation of the means of January and August for every pollutant. To this respect, the validation of the annual mean parameterization consists in the statistical comparison of the annual means calculated with the AQM outputs and the estimates of AERIS for that are based on the mean monthly concentrations of these two months.

Table 5.9: Statistical indicators for the evaluation of the annual mean parameterization.

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>( r )</th>
<th>( MB - \mu g/m^3 )</th>
<th>( ME - \mu g/m^3 )</th>
<th>( NMB - % )</th>
<th>( NME - % )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( NO_2 )</td>
<td>0.9876</td>
<td>-0.2374</td>
<td>0.4725</td>
<td>-6.18</td>
<td>12.31</td>
</tr>
<tr>
<td>( SO_2 )</td>
<td>0.9639</td>
<td>-0.0284</td>
<td>0.4911</td>
<td>-2.31</td>
<td>14.49</td>
</tr>
<tr>
<td>( PM_{10} )</td>
<td>0.9168</td>
<td>0.7967</td>
<td>1.1563</td>
<td>10.16</td>
<td>14.75</td>
</tr>
<tr>
<td>( PM_{2.5} )</td>
<td>0.9612</td>
<td>0.3107</td>
<td>0.6856</td>
<td>0.33</td>
<td>11.17</td>
</tr>
<tr>
<td>( O_3 )</td>
<td>0.9056</td>
<td>0.8709</td>
<td>0.9896</td>
<td>3.64</td>
<td>4.04</td>
</tr>
<tr>
<td>( NH_3 )</td>
<td>0.6561</td>
<td>0.0194</td>
<td>0.2030</td>
<td>2.95</td>
<td>31.01</td>
</tr>
</tbody>
</table>

The statistical indicators that have been calculated for the assessment of the correspondence between models are shown in table 5.11, while the associated scatterplots are depicted in figure 5.7. In general lines, a good level of statistical correspondence is witnessed between the annual means of the different pollutants under analysis. The best statistical correspondence is observed for \( NO_2 \), \( SO_2 \) and \( PM_{2.5} \), while the worst performance was observed for \( NH_3 \). Although a negative bias indicates a tendency towards underestimation, the low \( MB \) values exhibited by \( NO_2 \) and \( SO_2 \) \(< 1 \mu g/m^3 \) do not suggest that AERIS would substantially worsen annual mean values estimated by CMAQ for these pollutants (Vedrenne et al., 2014). In general, it can be said that AERIS is able to reproduce reasonably well the annual mean concentrations with the assumed parameterization for the six considered pollutants.

**5.6.4 Evaluation summary**

For the purposes of this work, the term secondary parameterization has been defined as an additional data-conditioning process that allows obtaining results of interest that the SRMs are unable to produce under the assumed modeling hypotheses. This was specifically the case...
of secondary particles, tropospheric ozone and mean annual or mean monthly concentrations. The purpose of the evaluation is having an idea about the statistical correspondence between the estimates provided by AERIS and the same type of results yielded by the conventional AQM. In general lines, an evaluation considering a series of statistical indicators that are relevant under a model benchmarking perspective yielded sufficiently good results. The analysis of the parameterizations that allowed quantifying contributions of precursor gases to particles or tropospheric ozone showed that the selected modeling approaches are adequate for their comprehensive description. Specifically for $O_3$ the comparison of the parameterization with the AQM outputs yielded promising results that suggest that the performance of AERIS for predicting the ozone concentrations of the baseline scenario is sufficiently consistent. This fact has been confirmed by its good statistical performance, which was evaluated as reported in scientific literature. As for the mean concentrations (either monthly or annual), adequate levels of statistical correspondence have been witnessed. In every case and for every pollutant, the model performance indicators are within range which also suggests that the level of reproduction of the assumed parameterizations is adequate for the baseline scenario. While in general the Pearson's correlation coefficients are high and the associated accumulated error is low, a much lower degree of correlation was observed for ammonia. This might be imputable to the fact that, in general, $NH_3$ concentrations across the domain are numerically lower than let us say, those of $NO_2$ or $PM_{10}$. An additional source might be the fact that only five sectors for this pollutant are effectively considered in AERIS.

5.7 Evaluation of the performance to a fully-controlled emission scenario

As it has been already explained in section 5.2, the purpose of this evaluation is testing the performance of AERIS (as a complete set of SRMs) against a perfectly-characterized emission scenario. The terms “fully-controlled” or “perfectly-characterized” refer to a given emission scenario in which the number of total sectors whose emissions have varied equals the number of sectors for which SRMs are available in AERIS. In other words, an emission scenario defined in terms of variations of the emissions only for sectors explicitly considered in AERIS. This fully-controlled scenario is obviously an artificial set of emissions that is produced for evaluating model performance for the exact number of sectors. In other words, this sector has been created to have a clear image of the performance level for the considered sectors only. The evaluation of the SRMs and the secondary parameterizations involved individual sectorial changes, while the evaluation at this stage implies considering several and simultaneous sectorial evaluations for different pollutants.

\[
S_{AERIS} = n
\]
\[
S_{AQM} = m
\]
\[
n \geq m
\]
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Table 5.10: Definition of the fully-controlled emission scenario (ES\textsubscript{FC}) - [\text{t/yr}].

<table>
<thead>
<tr>
<th>SNAP code</th>
<th>(E_{SO_2,RS})</th>
<th>(P_{SO_2})</th>
<th>(E_{NO_x,RS})</th>
<th>(P_{NO_x})</th>
<th>(E_{PM_{10},RS})</th>
<th>(P_{PM_{10}})</th>
<th>(E_{NH_3,RS})</th>
<th>(P_{NH_3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>010000</td>
<td>805,700</td>
<td>-88.6%</td>
<td>235,331</td>
<td>-58.8%</td>
<td>17,632</td>
<td>0.0%</td>
<td>0</td>
<td>0.0%</td>
</tr>
<tr>
<td>020020</td>
<td>12,544</td>
<td>-59.7%</td>
<td>24,648</td>
<td>15.5%</td>
<td>23,461</td>
<td>-5.74%</td>
<td>0</td>
<td>0.0%</td>
</tr>
<tr>
<td>030000</td>
<td>83,069</td>
<td>-33.0%</td>
<td>225,942</td>
<td>-58.8%</td>
<td>27,676</td>
<td>0.0%</td>
<td>0</td>
<td>0.0%</td>
</tr>
<tr>
<td>070101</td>
<td>599</td>
<td>0.0%</td>
<td>135,466</td>
<td>-62.1%</td>
<td>5,387</td>
<td>-48.2%</td>
<td>5,225</td>
<td>0.0%</td>
</tr>
<tr>
<td>070103</td>
<td>571</td>
<td>0.0%</td>
<td>75,670</td>
<td>-17.3%</td>
<td>8,052</td>
<td>-67.5%</td>
<td>473</td>
<td>0.0%</td>
</tr>
<tr>
<td>070301</td>
<td>605</td>
<td>0.0%</td>
<td>111,414</td>
<td>-9.9%</td>
<td>4,564</td>
<td>-69.1%</td>
<td>339</td>
<td>0.0%</td>
</tr>
<tr>
<td>0707/08</td>
<td>0</td>
<td>0.0%</td>
<td>0</td>
<td>0.0%</td>
<td>11,621</td>
<td>-17.5%</td>
<td>0</td>
<td>0.0%</td>
</tr>
<tr>
<td>100102</td>
<td>0</td>
<td>0.0%</td>
<td>8,361</td>
<td>0.0%</td>
<td>736</td>
<td>0.0%</td>
<td>110,927</td>
<td>-20.4%</td>
</tr>
<tr>
<td>Portugal</td>
<td>22,918</td>
<td>0.0%</td>
<td>145,250</td>
<td>0.0%</td>
<td>80,563</td>
<td>0.0%</td>
<td>48,970</td>
<td>0.0%</td>
</tr>
</tbody>
</table>

In section 5.4, the adequateness of the assumed linear approaches for the construction of SRMs appeared as a good modeling alternative for integrated assessment. The analysis conducted in section 5.5 revealed that SRMs produce estimates with a small amount of associated error when operating simultaneously and are thus additive. Finally, section 5.6 demonstrated that the secondary parameterizations that were undertaken for the description of pollutants and that are non-dependent of the SRM-approach provide comparable estimates with those ordinarily produced by the AQM. The assessment that is conducted in this section will strongly complement the conclusions taken in the previous sections by analyzing the skills of AERIS for an emission scenario that has the same or less sectors than those considered by the IAM.

5.7.1 Fully-controlled emission scenario

The so-called fully-controlled emission scenario (ES\textsubscript{FC}) outlines a range of emissions likely to occur in Spain and Portugal in year 2014\textsuperscript{10} and is a consequence of the application of technical and non-technical measures to the baseline scenario. Unlike the hypothetical scenario for the additivity test, the fully-controlled emission scenario was estimated and evaluated according to (Lumbreras et al., 2008; 2009b). To this respect, the emissions of four pollutants were followed: \(SO_2\), \(NO_x\), \(PM_{10}\) and \(NH_3\). The variation percentages of the emissions (\(p_i\)) for these pollutants and for the considered sectors are found in table 5.10.\textsuperscript{11} It should be noted that the emissions reported in this table are the emissions of the baseline scenario for the respective pollutants (referred to 2007). In line with the evaluation procedures that have been carried out for the SRMs and secondary parameterizations, the analysis criteria will be the same than those explained in section 5.2. Unlike the hypothetic scenario (\(HS\)), the

\textsuperscript{10}This PhD thesis was prepared between 2011 and 2013, hence 2014 being a “future scenario”. It was developed to represent a situation of emissions derived from a combination of action plans and new legislation implemented between 2007 and 2014 by the National Government.

\textsuperscript{11}Emissions are presented in annual metric tons [\text{t/yr}]. \%VOC = -22.14\%
variation percentages \((p_i)\) that have been obtained are not \textit{arbitrary} but actually represent an abatement scenario based on specific policies and feasible reductions calculated through the use of the Spain's Emission Projection model (SEP) \cite{Lumbreras2008}... For the purposes of the present analysis the specific measures as well as its special characteristics have been omitted as they are considered irrelevant for the discussion at hand.

### 5.7.2 Results of the evaluation

**Table 5.11: Statistical indicators for the evaluation of the fully-controlled scenario.**

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>(r)</th>
<th>(MB - \mu g/m^3)</th>
<th>(ME - \mu g/m^3)</th>
<th>(NMB) ((%))</th>
<th>(NME) ((%))</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO(_2)</td>
<td>0.9841</td>
<td>0.9548</td>
<td>0.4892</td>
<td>4.15</td>
<td>13.11</td>
</tr>
<tr>
<td>SO(_2)</td>
<td>0.9986</td>
<td>0.0944</td>
<td>0.1400</td>
<td>3.35</td>
<td>4.97</td>
</tr>
<tr>
<td>PM(_{10})</td>
<td>0.9966</td>
<td>0.0854</td>
<td>0.2243</td>
<td>1.04</td>
<td>2.73</td>
</tr>
<tr>
<td>(O_3)</td>
<td>0.9654</td>
<td>-0.5892</td>
<td>0.8275</td>
<td>-0.61</td>
<td>0.86</td>
</tr>
<tr>
<td>NH(_3)</td>
<td>0.9810</td>
<td>-0.0406</td>
<td>-0.0877</td>
<td>-6.42</td>
<td>13.85</td>
</tr>
</tbody>
</table>

The validation of AERIS against the conventional AQM is presented in figure 5.8, along with the model benchmarking indicators (table 5.11). It shows that, in most cases, the correspondence between the results of AERIS and the AQM is good. The positive values of \(MB\) and \(NMB\) for NO\(_2\), SO\(_2\) and PM\(_{10}\) suggest that AERIS tends to slightly overestimate the predictions given by AQM (with a 4.15\% maximum deviation). For NH\(_3\) and \(O_3\), the opposite tendency is observed with a maximum 6.42\% underestimation. The values of the Pearson’s correlation coefficients \((r)\) are in general high, while the measure of the absolute error never exceeds 13.8\% indicating that statistical compensation effects due to outliers is kept to a minimum \cite{Thunis2011}... A qualitative inspection of the maps presented in figure 5.8 reveals that AERIS is able to capture hotspots such as cities and important point-sources due to its relatively fine scale (16 \(km\)) and the detail degree of the underlying emission inventories. Additionally, the good statistical correspondence between models for PM\(_{10}\) or \(O_3\) suggests that AERIS implicitly incorporates a description of the formation of secondary pollutants similar to the one provided by the ordinary AQM. An interesting issue to highlight is that AERIS is able to deal with the emissions of several sectors and pollutant simultaneously. However, it should also be noted that the results provided by AERIS have an explicit confidence interval of emission variation percentages within \([-90\%, +90\%]\) of the baseline scenario. Additionally, a limitation that AERIS presents is the fact that any simulation must be referred to the specific \textit{baseline scenario}, which impedes using any custom baseline scenario directly.
Figure 5.8: a) AERIS Mean annual concentrations. b) AERIS vs. AQM scatterplots.
5.8 Evaluation of the performance to a real-policy emission scenario

According to section 5.2, evaluating the performance of AERIS against a real-policy emission scenario (ESRP) is very useful for analyzing the abilities of the IAM to a given emission scenario that is actually of policy-making interest. The real-policy scenario corresponds to a given emission scenario in which the number of total sectors whose emissions have varied is higher the number of sectors for which SRMs are available in AERIS, and which is usually a consequence of an integral air-quality plan. As a result, some degree of deviation between the results produced by the AQMS and AERIS is to be expected. In a broader sense, this analysis should indicate about the suitability of AERIS as a screening tool whose results are comparable to those of the AQM. Analysis focused on different policy-relevant indicators for NO\textsubscript{2}, SO\textsubscript{2}, PM\textsubscript{2.5}, NH\textsubscript{3}, and O\textsubscript{3} produced by one year-run of AERIS and the AQM respectively.

\[ S_{AERIS} = n \]
\[ S_{AQM} = m \]
\[ n < m \]

The goal of this section is analyzing through a concurrent comparison the general skills of AERIS while reproducing: (a) the predictions of the AQM (for a future scenario - 2014) and (b) air-quality observations (for a past scenario - 2011)\textsuperscript{12} in order to justify its use while also aiming to recognize its limitations (Bennett et al., 2013). The validation rationale is based on model performance criteria according to Boylan and Russell (2006), USEPA (2007) and Chemel et al., (2010).

5.8.1 Validation against air-quality observations

The objective of validating the outputs of AERIS against air quality observations is analyzing the goodness of the secondary parameterizations that were undertaken for the description of policy-relevant indicators (section 4.6.2). To this respect, modeled concentrations by AERIS were compared against measurements from the EMEP monitoring network (www.emep.int) located in Spain and Portugal for year 2011 (table 5.12). The spatial coverage of the monitoring network is shown in figure 5.9, being composed only of urban and rural background stations whose measurements are deemed representative of the spatial scale of AERIS (16 km). Although this methodology has little discriminating power to understand model behaviour, the objective of the validation practice is determining whether AERIS is able to replicate observed values. Comparisons were made exclusively for NO\textsubscript{2}, O\textsubscript{3}, PM\textsubscript{2.5}, and SO\textsubscript{2} and for the following relevant indicators: the 19\textsuperscript{th} highest hourly concentration of NO\textsubscript{2},

\textsuperscript{12}The emission scenario of year 2011 was created to produce air quality estimates with AERIS that could be compared with an independent dataset (observations). When this thesis was being prepared, there were no values reported for 2014.
Chapter 5. Air quality system validation

Table 5.12: Selected monitoring locations for model validation.

<table>
<thead>
<tr>
<th>Country</th>
<th>Station Name</th>
<th>Code</th>
<th>Longitude</th>
<th>Latitude</th>
<th>Measured Pollutants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spain</td>
<td>Barcarrota</td>
<td>BRCR</td>
<td>6°55’14”W</td>
<td>38°28’22”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Cabo de Creus</td>
<td>CCRE</td>
<td>3°18’56”E</td>
<td>42°19’09”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Campisábalos</td>
<td>CAMP</td>
<td>3°08’33”W</td>
<td>41°16’27”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Doñana</td>
<td>DONA</td>
<td>6°33’19”W</td>
<td>37°03’06”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Els Torms</td>
<td>ELTR</td>
<td>0°44’04”E</td>
<td>41°23’38”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Mahón</td>
<td>MAHN</td>
<td>4°19’26”E</td>
<td>39°52’33”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Niembro</td>
<td>NMBR</td>
<td>4°50’60”W</td>
<td>43°26’21”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Noia</td>
<td>NOIA</td>
<td>8°55’24”W</td>
<td>42°43’14”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>O Saviñao</td>
<td>OSAV</td>
<td>7°42’16”W</td>
<td>42°38’14”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Peñausende</td>
<td>PENS</td>
<td>5°53’51”W</td>
<td>41°14’20”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Risco Llano</td>
<td>RSLL</td>
<td>4°21’11”W</td>
<td>39°31’15”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Víznar</td>
<td>VIZN</td>
<td>6°32’03”W</td>
<td>37°14’13”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Spain</td>
<td>Zarra</td>
<td>ZARR</td>
<td>1°06’03”W</td>
<td>39°04’58”N</td>
<td>NO_2, O_3, SO_2</td>
</tr>
<tr>
<td>Portugal</td>
<td>Camarinha</td>
<td>CAMH</td>
<td>9°02’51”W</td>
<td>38°26’49”N</td>
<td>NO_2, O_3, SO_2, PM_2.5</td>
</tr>
<tr>
<td>Portugal</td>
<td>Douro Norte</td>
<td>DOUN</td>
<td>7°47’44”W</td>
<td>41°22’27”N</td>
<td>NO_2, O_3, SO_2, PM_2.5</td>
</tr>
<tr>
<td>Portugal</td>
<td>Olivais</td>
<td>OLIV</td>
<td>9°06’25”W</td>
<td>38°46’12”N</td>
<td>NO_2, O_3, SO_2, PM_2.5</td>
</tr>
<tr>
<td>Portugal</td>
<td>Reboleira</td>
<td>REBL</td>
<td>9°13’50”W</td>
<td>38°45’15”N</td>
<td>NO_2, O_3, SO_2, PM_2.5</td>
</tr>
</tbody>
</table>

the daylight AOT_{40} of O_3, the mean annual concentration of PM_{2.5} and the 25^{th} highest hourly concentration SO_2.

5.8.2 Real-policy emission scenarios

Past emission scenario - 2011

The emission scenario of year 2011 (ES_{RP11}) was created to produce air quality estimates with AERIS, expressed as policy-relevant indicators, that were further compared with observations. This was accomplished by using emission values of the considered sectors reported by the Spanish and Portuguese Emission Inventories (SNEI, PNEI) of the same year (Costa-Pereira et al., 2013; MAGRAMA, 2013). These values were introduced into AERIS in order to quantify the corresponding variation percentages of emissions (p_i) of the relevant pollutants (NO_x, SO_2, PM_{10}, PM_{2.5}, NH_3, VOC) and subsequently run the model. The variation percentages for ES_{RP11} are shown in table 5.13.

Future emission scenario - 2014

The future scenario of emissions (ES_{RP14}) was developed to represent as accurately as possible the situation of emissions in year 2014 in Spain for NO_x, SO_2, PM_{10}, PM_{2.5}, NH_3 and VOC. The variations in each of the considered sectors are a consequence of the adoption of a set
5.8. Evaluation of the performance to a real-policy emission scenario

Figure 5.9: Geographic representation of the modeled domain and monitoring locations used for validation.

...of feasible technical and non-technical measures on a national scale (table 5.13). Most of these actions were derived from a combination of action plans and new legislation implemented between 2007 and 2014 by the Spanish Government and the Municipality of Madrid (AM, 2012). Examples of these actions are the application of limits to fuel compositions, the introduction of more efficient combustion devices, the implementation of best-available techniques (BATs), progressive changes to renewable energy sources, mobility and traffic restrictions in cities, etc. The \( ES_{RP14} \) was elaborated with the SEP model and evaluated according to Lumbreras et al., (2008; 2009b). It should be noted that \( ES_{RP14} \) exhibits variations in the emissions of many more sectors (162 sectors) than those represented by the SRMs of AERIS. However, we consider that the sectors simulated by AERIS are representative enough to provide a good picture of the air quality situation in the Iberian Peninsula.

5.8.3 Results of the Evaluation

The concentration fields provided by AERIS are presented in terms of the most relevant indicators in terms of their significance with European-level policy: the 19\(^{th}\) highest hourly concentration of \( NO_2 \), the daylight \( AOT_{40} \) of \( O_3 \), the annual mean concentration of \( PM_{2.5} \) and the 25\(^{th}\) highest daily concentration (\( SO_2 \)). The spatial representation of these indicators is shown in figure 5.10. From a qualitative point of view, these concentration maps clearly
Figure 5.10: Concentration results of the real policy scenario (2014) a) 19th highest hourly concentration - $NO_2 [\mu g/m^3]$ b) daylight $AOT_{40} - O_3 [\mu g/m^3 h]$ c) annual mean concentration - $PM_{2.5} [\mu g/m^3]$ d) 25th highest hourly concentration - $SO_2 [\mu g/m^3]$. 
### Table 5.13: Definition of the real-policy emission scenarios (ES\(_{RP}\)) - (%).

<table>
<thead>
<tr>
<th>SNAP code</th>
<th>(\text{NO}<em>x) (P</em>{2011})</th>
<th>(\text{NO}<em>x) (P</em>{2014})</th>
<th>(\text{SO}<em>2) (P</em>{2011})</th>
<th>(\text{SO}<em>2) (P</em>{2014})</th>
<th>(\text{PM}<em>{10}) (P</em>{2011})</th>
<th>(\text{PM}<em>{10}) (P</em>{2014})</th>
<th>(\text{PM}<em>{2.5}) (P</em>{2011})</th>
<th>(\text{PM}<em>{2.5}) (P</em>{2014})</th>
<th>(\text{NH}<em>3) (P</em>{2011})</th>
<th>(\text{NH}<em>3) (P</em>{2014})</th>
</tr>
</thead>
<tbody>
<tr>
<td>010000</td>
<td>-53.3</td>
<td>-58.8</td>
<td>-85.0</td>
<td>-88.2</td>
<td>-78.6</td>
<td>-74.9</td>
<td>-81.9</td>
<td>-78.9</td>
<td>-97.9</td>
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</tr>
<tr>
<td>020202</td>
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<td>-32.3</td>
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<td>-67.5</td>
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<td>-87.0</td>
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<td>-95.1</td>
<td>-93.7</td>
<td>-85.2</td>
<td>-90.1</td>
<td>-85.2</td>
<td>-90.1</td>
<td>-75.6</td>
<td>-46.0</td>
</tr>
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<td>-69.1</td>
<td>-18.4</td>
<td>9.1</td>
</tr>
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<td>-93.81</td>
<td>-91.6</td>
<td>-85.1</td>
<td>-88.6</td>
<td>-85.1</td>
<td>-88.6</td>
<td>-67.8</td>
<td>-68.3</td>
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<tr>
<td>070708</td>
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<td>0.0</td>
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<td>33.3</td>
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<td>0.0</td>
<td>0.0</td>
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<tr>
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<td>-40.2</td>
<td>-85.7</td>
<td>-90.6</td>
<td>-90.4</td>
<td>-90.6</td>
<td>-90.4</td>
<td>46.1</td>
<td>42.1</td>
</tr>
<tr>
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<td>-85.2</td>
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<td>-90.1</td>
<td>-50.5</td>
<td>0.0</td>
<td>33.8</td>
</tr>
<tr>
<td>100101</td>
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<td>-66.7</td>
<td>0.0</td>
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<td>0.0</td>
<td>0.0</td>
<td>-4.8</td>
<td>-20.4</td>
</tr>
<tr>
<td>100102</td>
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<td>130.0</td>
<td>0.0</td>
<td>0.0</td>
<td>-15.5</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>5.4</td>
<td>-11.1</td>
</tr>
<tr>
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<td>0.0</td>
<td>0.0</td>
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<td>22.6</td>
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<td>38.7</td>
<td>-5.8</td>
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<td>5.3</td>
<td>12.8</td>
<td>172.5</td>
<td>11.4</td>
<td>-100.0</td>
<td>17.3</td>
<td>0.0</td>
<td>0.0</td>
<td>-96.5</td>
<td>-12.3</td>
</tr>
<tr>
<td>Portugal</td>
<td>-24.4</td>
<td>0.0</td>
<td>-40.5</td>
<td>0.0</td>
<td>-13.7</td>
<td>0.0</td>
<td>-12.3</td>
<td>0.0</td>
<td>-4.6</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Identify pollution hotspots such as cities (i.e. Madrid, Barcelona) or areas influenced by large point-sources as a consequence of the implemented finer resolution of the modelled domain and the detailed emission inventories (when compared to European-level IAMs). For the concrete case of \(O_3\), high-concentration zones are evident in regions that are typically affected by summer events such as the Mediterranean coast of Spain (de Andrés et al., 2012). The fact of presenting concentrations using these indicators is useful for assessing whether some specific locations might attain European and National legislation limits for future emission scenarios. Moreover, these indicators can be easily related with impacts or exposure levels and are certainly useful for the future construction of health and ecosystems-related modules discussed in the following chapters.

### Validation of AERIS against the AQM

The statistical comparison of the AERIS estimates and the AQM-outputs by the means of benchmarking indicators is shown in table 5.10. The estimates provided for \(\text{NO}_x\) are characterized by slight tendencies towards overprediction as evidenced by the \(MB\) and the \(NMB\).
values, while the total error ($ME$) roughly reaches 0.35 $µg/m^3$. However, the accuracy of $NO_2$ predictions might be slightly compromised since $NMB = 19.82\%$ indicates overprediction (being above the recommended threshold of $|NMB| \leq 15\%$) (Russell and Dennis, 2000).

A similar behaviour is observed for $SO_2$, where the same tendencies exist but with a lower error presence ($NME = 17.14\%$). The overpredictive character of AERIS for these pollutants, whose SRMs do not account for the totality of emission sectors present in the $ES_{RP\text{14}}$, might be explained by the loss of accuracy that is inherent to any statistical parameterization and the fact that the emission reductions might be concentrated in those sectors for which the IAM has considered a SRM.

Table 5.14: Comparison indicators between AERIS and the conventional AQM for $ES_{RP\text{14}}$.

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>$r$</th>
<th>$MB - [µg/m^3]$</th>
<th>$ME - [µg/m^3]$</th>
<th>$NMB - (%)$</th>
<th>$NME - (%)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$NO_2$</td>
<td>0.9787</td>
<td>0.32</td>
<td>0.35</td>
<td>19.82</td>
<td>21.96</td>
</tr>
<tr>
<td>$SO_2$</td>
<td>0.9806</td>
<td>0.32</td>
<td>0.47</td>
<td>11.49</td>
<td>17.14</td>
</tr>
<tr>
<td>$PM_{2.5}$</td>
<td>0.9891</td>
<td>-0.34</td>
<td>0.43</td>
<td>-5.39</td>
<td>6.81</td>
</tr>
<tr>
<td>$NH_3$</td>
<td>0.9851</td>
<td>-0.02</td>
<td>0.06</td>
<td>-4.35</td>
<td>10.38</td>
</tr>
<tr>
<td>$O_3$</td>
<td>0.9706</td>
<td>-0.26</td>
<td>-0.76</td>
<td>-0.27</td>
<td>0.78</td>
</tr>
</tbody>
</table>

For the rest of pollutants, the opposite behaviour was witnessed. For instance, $PM_{2.5}$ shows a general underpredictive trend, which is also the highest among the studied species ($NMB = -5.39\%$). This deficit in $PM_{2.5}$ predictions might be explained by the fact that not all the emission sectors are actually simulated by AERIS. The parameterization of the secondary component of $PM_{2.5}$ might also be a cause of this behavior. Additionally, the $O_3$ estimates were calculated by an additional parameterization that depends on the $NO_2$ SRMs so an additional component for statistical mismatch is to be expected for this pollutant.

Validation of AERIS against observations

Unlike previous validation exercises, this section will address the validation of AERIS against independent observations and therefore the magnitude and sign of deviations are not comparable to the results shown previously. In general, the correspondence of AERIS with air quality observations from the selected network is adequate, according to the considered model validation criteria (Thunis et al., 2011). Special attention needs to be put on the statistical metrics for $PM_{2.5}$ since only four monitoring stations were used (all of them in Portugal). Although the correspondence between datasets is the best among the analyzed pollutants, any interpretations on model skills for $PM_{2.5}$ need to be put into perspective. In every other case, the Pearson correlation coefficient ($r$) is above $r = 0.65$ which hints on the linear correspon-
5.8. Evaluation of the performance to a real-policy emission scenario

Figure 5.11: Comparison of the selected policy-relevant indicators calculated with AERIS against observations for the 2011 real policy scenario ($ES_{RP11}$). Units for $NO_2$, $PM_{2.5}$, $SO_2$: [µg/m$^3$], $O_3$: [µg/m$^3\cdot$h].

dence between values (figure 5.11). Additionally, one can see that AERIS has a tendency for overpredicting air quality levels from the fact that the $MB$ and $NMB$ values for every pollu-
tant are positive, of which only \( NO_2 \) is in the range \( |NMB| \leq 15\% \) (Boylan and Russell, 2006).

Table 5.15: Statistic indicators of comparison between AERIS and observations for \( ES_{RP11} \).

<table>
<thead>
<tr>
<th>Indicator</th>
<th>( r )</th>
<th>( MB ) ( [\mu g/m^3] )</th>
<th>( ME ) ( [\mu g/m^3] )</th>
<th>( NMB ) ( (%) )</th>
<th>( NME ) ( (%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max19\textsuperscript{th} – ( NO_2 )</td>
<td>0.8163</td>
<td>1.75</td>
<td>6.75</td>
<td>6.52</td>
<td>25.18</td>
</tr>
<tr>
<td>( AOT_{30} ) – ( O_3 )</td>
<td>0.7852</td>
<td>4489</td>
<td>4808</td>
<td>23.27</td>
<td>24.92</td>
</tr>
<tr>
<td>Ann.\textsuperscript{Mean} – ( PM_{2.5} )</td>
<td>0.9973</td>
<td>0.27</td>
<td>0.31</td>
<td>9.82</td>
<td>11.25</td>
</tr>
<tr>
<td>Max25\textsuperscript{th} – ( SO_2 )</td>
<td>0.7432</td>
<td>4.64</td>
<td>4.97</td>
<td>77.84</td>
<td>83.27</td>
</tr>
</tbody>
</table>

This fact is especially evident for \( SO_2 \), \( (NMB = 77.8\%, \text{FAC2} = 58\%) \) indicating that the SRMs might not be able to capture all the effective reductions in emissions that took place between the baseline scenario and 2011 (table 5.15). An example of this could be the substitution of coal for other fuels by some coal-power plants in northern Spain as a consequence of the introduction of fuel composition limits immediately after 2007. In the same line, an additional explanation for this deviation could be the fact that \( SO_2 \) greatly depends on local sources and other factors (i.e. emissions from industries) (Georgoulias et al., 2009). In the case of \( O_3 \), the slighter overpredictive character is observed although the value of \( NME (24.9\%) \) lies below the \( NME \leq 35\% \) model performance threshold (Russell and Dennis, 2000). To this respect, the parent-AQM of AERIS (WRF-SMOKE-CMAQ) also exhibits some bias towards overprediction for ozone, as shown in de Andrés et al., (2012).

It is worth noting that the number of chosen monitoring locations is limited, due to the fact that a geographically well-distributed network of rural background stations was preferred in order to have observations that might not be influenced by local gradients and that would be representative of the 16 \( km \)-scale of AERIS. In general, another issue that needs to be kept in mind is the fact that SRMs were built using meteorological fields from year 2007 so a deviation between model predictions and observations was to be expected. Despite the fact that 2011 was not considered atypical in the meteorological sense (AEMET, 2012), any conclusions drawn from a direct comparison with observations should be handled with care.

### 5.9 Validation of AERIS air quality system: final remarks

The previous sections of this chapter have been devoted entirely to evaluating AERIS in terms of its outputs and its performance when compared to its parent-AQM or observations under different circumstances. The performance analysis of AERIS is a central issue to determine its capabilities and recognize its limitations. To this effects, a quantitative analysis of performance as well as an intense model benchmarking process was carried out in order to point out where models differ from each other, as well as identifying the causes for such differences in output quality (Bennett et al., 2013). Taking into account the behavior of AERIS
under the different evaluation techniques that were applied to its outputs, it can be said with sufficient confidence that its estimates reproduce in a reasonable way the performance of a traditional AQM such as the WRF-SMOKE-CMAQ system. This validation exercise allowed gaining enough knowledge on the potential “amounts of error” that are associated with the estimates that AERIS produces under normal operation conditions. Particularly, the model has been contrasted against performance thresholds that have been normally agreed-upon (Denby et al., 2009). This was made with the objective to endow our model with enough credibility, especially to give the feeling that its results meet the standards of scientific plausibility and technical adequacy while reducing the level of complexities as much as possible (Cash et al., 2003). Studying the reduction pathways of these uncertainty levels could be developed as a future line of research.

The general position of the author and the people involved in the formulation and development of the AERIS model is that “the evaluation of models should be a central part of the model development process, not an afterthought” (Crout et al., 2009; Alexandrov et al., 2011).
The process of atmospheric deposition of emitted pollutants is part of the intrinsically complex air pollution problem that needs to be sufficiently described under an integrated assessment perspective. As with the ambient air quality levels that have been described in section 4, the quantification of the deposition rates of pollutant species is relevant in the light of the potential impacts that might be produced in nature. The purpose of this section is the description of the methodological framework that allowed constructing the atmospheric deposition module of AERIS, which is related to the general formulations of the emission module and the air quality system (section 2). It is worth noting that despite negative effects may be associated to the deposition of chemicals (i.e. heavy metals, organic compounds, etc.), the present section only focuses on nitrogen and sulfur compounds. This module was developed to be able to quantify the impacts of air pollution on ecosystems due to atmospheric deposition.

6.1 Theoretical background

The atmospheric deposition of nitrogen (N) and sulfur (S) is a typical environmental concern that has captured the attention of policymakers in the world, and especially in Europe, for the last two decades (Cornell, 2011). The deposition of these compounds is generally a consequence of both natural and anthropogenic sources that lead either to benefits (fertilization) or most commonly, drawbacks among which acidification and accumulation of excess nutrients are the most relevant (Driscoll et al., 2003; Im et al., 2013). These drawbacks have a direct and sometimes irreversible impact on the natural sulfur and nitrogen cycles, making them highly man-affected (Hultberg et al., 1994). Under an emission-control perspective, the deposition of nitrogen species are differentiated in reduced and oxidized nitrogen ($N_{\text{red}}$ and $N_{\text{ox}}$ respectively). The distinction between species is especially important nowadays, due to the fact that in Europe, sulfur and oxidized nitrogen emissions are more easily-controllable than those of reduced nitrogen due to the nature of the emission sources that produce them (Dentener et al., 2006).
As a consequence of the deposition-related impacts, control strategies throughout Europe have been taken in the last decades which led in the first place to the Gothenburg protocol derived under the Convention on Long-Range Transboundary Air Pollution of the UN Economic Commission for Europe. Within the European Union, the European Parliament and the Council adopted the National Emission Ceilings (NEC) Directive regulating EU member state emissions of acidifying and eutrophying pollutants which were supposedly attained by 2010 (ApSimon et al., 2003).

These objectives (or ceilings) were set with the support of scientific methodologies and datasets available until 2001, and further processed with air quality models for the computation of atmospheric dispersion and deposition of nitrogen and sulfur compounds. (Hettelingh et al., 2013). This step is particularly relevant because the entire atmospheric deposition process is heavily determined by very complex interactions between meteorology and atmospheric chemistry, being species transported over long distances and deposited to aquatic and terrestrial ecosystems together with other pollutants.

Additionally, the deposition of nitrogen and sulfur compounds has a direct impact in the general atmospheric chemistry state, affecting or enhancing the formation of aerosols, tropospheric ozone and changing the final concentration of the associated precursor gases (NOx, NH3 and SO2) (Sotiropoulou et al., 2004). Due to the inherent complexity involved with these processes, relying on air quality models (AQMs) is useful in order to provide integrated views of the temporal and spatial variations of the atmospheric deposition processes at regional scales (Im et al., 2013).

6.2 Modeling approach

As with the estimation of the concentrations, the formulation of the atmospheric deposition module in AERIS relied on its parent-AQM, namely the WRF-SMOKE-CMAQ modeling system. Similar configurations of the parent-AQM have been applied and validated for the estimation of deposition budgets in various case studies in Europe and North America (Ganev et al., 2008; Appel et al., 2012; Im et al., 2013). The particular formulation of CMAQ involves describing two types of deposition: wet deposition and dry deposition as shown in figure 6.1 (Dennis, 2009).

According to Im et al., (2013), CMAQ calculates dry deposition by considering turbulent air motion and by direct gravitational sedimentation of large particles according to a resistance model developed by (Wesely and Hicks, 1977) while the velocities of particle deposition under this mechanism are calculated with the Meteorology and Chemistry Interface Processor (MCIP). Wet deposition is calculated in a special module of CMAQ called the “cloud-module”, which determines deposition as a function of the Henry’s Law constant of the gaseous tracer.
or the scavenging rate of the aerosol mode and component. For its quantification, CMAQ considers an algorithm that allocates precipitation amounts to individual layers taking into consideration precipitation rates, sum of hydrometers (rain, snow and graupel) and layer thickness (Foley et al., 2010).

The basic modeling approach that was followed in order to incorporate the description of atmospheric deposition in AERIS is essentially the same as the one applied for determining annual means as a function of the mean monthly concentrations of January and August. The fact of relying on this parameterization obeys to the fact that constructing specific source-receptor matrices (SRMs) from hourly deposition values for each of the relevant species is a time and resource-consuming procedure that can be effectively substituted by the selected approach. Namely, the mean monthly concentrations of the summer and winter representative months (January and August) of any precursor gas \( i \) were transformed into the accumulated atmospheric deposition per unit of area \( D_{acc}^v \) of a given specie \( v \) by the means of a transformation matrix \( \{Q_{dep}\} \) which will act as a proportionality constant between both concentrations (equations 6.1, 6.2):

\[
[D_{acc}^v]_{n \times m} = [Q_{Dep,01}]_{n \times m} \cdot [C_{i,01}]_{n \times m}
\] (6.1)

\[
[D_{acc}^v]_{n \times m} = [Q_{Dep,08}]_{n \times m} \cdot [C_{i,08}]_{n \times m}
\] (6.2)
6.2. Modeling approach

Table 6.1: Description of the species subject to atmospheric deposition.

<table>
<thead>
<tr>
<th>Generic deposition</th>
<th>AERIS name</th>
<th>CMAQ name</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxidized nitrogen - (N_{ox})</td>
<td>(D_{NO2})</td>
<td>([NO2])</td>
<td>Nitrogen dioxide</td>
</tr>
<tr>
<td></td>
<td>(D_{NO})</td>
<td>([NO])</td>
<td>Nitrogen monoxide</td>
</tr>
<tr>
<td></td>
<td>(D_{HONO})</td>
<td>([HONO])</td>
<td>Nitrous acid</td>
</tr>
<tr>
<td></td>
<td>(D_{NO2})</td>
<td>([NO2])</td>
<td>Dinitrogen pentoxide</td>
</tr>
<tr>
<td></td>
<td>(D_{NO3})</td>
<td>([NO3])</td>
<td>Semivolatile nitrate</td>
</tr>
<tr>
<td></td>
<td>(D_{AN03I})</td>
<td>([AN03I])</td>
<td>Nitrate in Aitken mode</td>
</tr>
<tr>
<td></td>
<td>(D_{AN03J})</td>
<td>([AN03J])</td>
<td>Nitrate in accumulation mode</td>
</tr>
<tr>
<td></td>
<td>(D_{HNO3})</td>
<td>([HNO3])</td>
<td>Nitric acid</td>
</tr>
<tr>
<td>Reduced nitrogen - (N_{red})</td>
<td>(D_{NH3})</td>
<td>([NH3])</td>
<td>Ammonia</td>
</tr>
<tr>
<td></td>
<td>(D_{ANH4I})</td>
<td>([ANH4I])</td>
<td>Ammonium in Aitken mode</td>
</tr>
<tr>
<td></td>
<td>(D_{ANH4J})</td>
<td>([ANH4J])</td>
<td>Ammonium in accumulation mode</td>
</tr>
<tr>
<td>Sulfur - (S)</td>
<td>(D_{SO2})</td>
<td>([SO2])</td>
<td>Sulfur dioxide</td>
</tr>
<tr>
<td></td>
<td>(D_{SULF})</td>
<td>([SULF])</td>
<td>Sulfuric acid</td>
</tr>
<tr>
<td></td>
<td>(D_{ASO4I})</td>
<td>([ASO4I])</td>
<td>Sulfate in Aitken mode</td>
</tr>
<tr>
<td></td>
<td>(D_{ASO4J})</td>
<td>([ASO4J])</td>
<td>Sulfate in accumulation mode</td>
</tr>
<tr>
<td></td>
<td>(D_{ASO4K})</td>
<td>([ASO4K])</td>
<td>Sulfate in coarse mode</td>
</tr>
</tbody>
</table>

With \([C_{i,01}]_{n \times m}\) and \([C_{i,08}]_{n \times m}\) being the mean monthly concentrations of January and August respectively of \(NO_2\), \(SO_2\) or \(NH_3\), and \([Q_{Dep,01}]_{n \times m}\), \([Q_{Dep,08}]_{n \times m}\) the respective concentration-deposition transformation matrices. For calculating the numeric value of the transformation matrices, a complete annual run of the baseline scenario was carried out with the AQM. Assuming that the mathematical relationship between the mean monthly and mean annual concentrations for this annual run can also be described by equations 6.1 and 6.2, the transformation matrices were estimated accordingly.

\[
[Q_{Dep,01}]_{n \times m} = \left[ D_{acc}^{v,2007} \right]_{n \times m} / [C_{i,01,2007}]_{n \times m}
\]

\[
[Q_{Dep,08}]_{n \times m} = \left[ D_{acc}^{v,2007} \right]_{n \times m} / [C_{i,08,2007}]_{n \times m}
\]

Since the two transformation matrices produce annual accumulated atmospheric depositions per unit of area, the representativeness of this values can be increased by calculating the arithmetic mean of the estimates produced by the January and August equations (equations 6.3). Due to the fact that these transformation matrices have been calculated using the baseline scenario of AERIS with the same AQM, they can be considered valid for any future scenarios provided that these are modeled as deviations from this baseline scenario.

\[
[D_{acc}^{v}]_{n \times m} = 0.5 \cdot \left( [Q_{Dep,01}]_{n \times m} \cdot [C_{i,01}]_{n \times m} + [Q_{Dep,08}]_{n \times m} \cdot [C_{i,08}]_{n \times m} \right)
\]
Chapter 6. Atmospheric deposition module

The estimation of the annual accumulated atmospheric deposition per unit of area for reduced nitrogen, oxidized nitrogen and sulfur for the annual run of baseline scenario had to be derived from a series of methodological assumptions, following the general methodology presented in Ganev et al., (2008) and modified for the particular conditions of the Iberian Peninsula according to Martín et al., (2011). The atmospheric deposition outputs of CMAQ for this annual simulation consist in a dry deposition and a wet deposition file, DRYDEP and WETDEP respectively. These files contained hourly values of atmospheric deposition for a several nitrogen and sulfur species that are quantified by CMAQ according to the chemical processes it considers (figure 6.1) and for each of the 4500 cells of the modeling domain. The total amount of sulfur that is deposited \( D_S \) in each cell can be quantified with equation 6.4) in kilograms of elemental sulfur per hectare, [kgS/ha], considering the mass-contribution of each of the sulfur-related species that appear in the equation (table 6.1). The coefficients correspond to the species-to-total sulfur mass ratios.

\[
D_S = 0.5 \cdot D_{SO2} + 0.326 \cdot D_{SULF} + 0.333 \cdot (D_{ASO4I} + D_{ASO4J} + D_{ASO4K}) \quad (6.4)
\]

Where:

\[
D_u = D_{u,WETDEP} + D_{u,DRYDEP} \quad (6.5)
\]

In a similar way, the equations that quantify the total amount of oxidized and reduced nitrogen that are deposited \( \{ D_{Nox} \} \) and \( \{ D_{Nred} \} \) in [kgN/ha] can be written considering the relevant species, as follows (equations 6.6, 6.7). The coefficients correspond to the species-to-total nitrogen (oxidized, reduced) mass ratios.

\[
D_{Nox} = 0.304 \cdot D_{NO2} + 0.467 \cdot D_{NO} + 0.297 \cdot D_{HONO} + 0.259 \cdot D_{N2O5} + 0.225 \cdot (D_{NO3} + D_{ASO4I} + D_{ASO4J}) + 0.222 \cdot D_{HNO3} \quad (6.6)
\]

\[
D_{Nred} = 0.823 \cdot D_{NH3} + 0.777 \cdot (D_{ANHAI} + D_{ANHAJ}) \quad (6.7)
\]

Each of the terms that allow quantifying the total deposition of sulfur and nitrogen compounds correspond to direct output-species generated by CMAQ. The name of each of these species and their correspondence with the CMAQ outputs can be seen in table 6.1. Such a classification was done according to what is published in Binkowski and Roselle, (2003), Ganev et al., (2008) and Im et al., (2013). The terms \( D_S \), \( D_{Nox} \) and \( D_{Nred} \) correspond to the hourly
depositions per unit of area for the annual simulation of the baseline scenario. However, in order to obtain the annual accumulated deposition per unit of area, the accumulated sum for the entire set of hourly values in a year (8760 hours) needs to be calculated according to equation 6.8.

$$[D_{\text{acc}}^v]_{n \times m} = \sum_{t=1h}^{8760h} D_v \cdot \Delta t$$

(6.8)

For the concrete case of the 2007 baseline scenario, the term in the left side of equation 6.8 can be immediately substituted by the term $[D_{\text{acc}}^v]_{n \times m}$ to be further introduced in equation 6.1 or equation 6.2 in order to calculate the value of the concentration-deposition transformation matrices. Once the concentration-deposition transformation matrices have been obtained, these can be widely used for converting annual mean concentration values into annual accumulated depositions per unit of area. The fact of presenting atmospheric deposition values referred to a unit of area is of special relevance when quantifying impacts on ecosystems, vegetation or soils and to properly assess their spatial extension. In summary, the general modeling approach for the estimation of atmospheric deposition is based on the fact that deposition rates are proportional to concentration levels of precursor gases and therefore, proportional to emissions. In the following sections, the evaluation of the present modeling approach will be undertaken.

6.3 Evaluation of the modeling approach

In line with what has already been carried out for the emission and air quality system modules, an evaluation of the atmospheric deposition module is very necessary in order to have enough confidence on the estimates of AERIS when used for policy making. Although far less ambitious than the evaluation procedure for the air quality system presented in chapter 5, the assessment of this module will be based in the comparison of the deposition estimates of AERIS against the (i) deposition results generated by the parent-AQM and (ii) the outputs of a completely-independent model which is often used as reference in European contexts: the EMEP model. The first evaluation is carried out in order to validate if the parameterization of atmospheric deposition in AERIS corresponds to the results that the AQM yields normally. The comparison against the EMEP model was made to judge on the order of magnitude of the IAM outputs, as well as on their representativeness to a much coarser spatial resolution. It is worth noting that the evaluation will be carried out for the baseline scenario of 2007 in both cases.
Figure 6.2: Annual accumulated depositions per unit of area of AERIS and the ordinary AQM.
6.3. Evaluation of the modeling approach

6.3.1 Evaluation of AERIS against the AQM

As it was already stated, this evaluation will center on the ability of AERIS to reproduce the deposition estimates of the ordinary AQM (namely CMAQ). Following the validation rationale that was used for examining the performance of the air quality system (section 5.1), the statistical comparison between models is based on indicators such as the Pearson correlation coefficient \( r \), the Mean Bias \( MB \), the Mean Error \( ME \), the Normalized Mean Bias \( NMB \) and the Normalized Mean Error \( NME \).

The spatial profile of the annual accumulated deposition per unit of area of the nitrogen and sulfur species according to AERIS and the AQM is shown in figure 6.2. A qualitative comparison of this figure reveals that the spatial representation of both models for each of the deposited species is very similar, depicting high deposition levels in Northern Spain and in the Pyrenees, being sulfur deposition especially relevant for the north-western regions of the Peninsula. The results of the quantitative comparison related to the statistical evaluation have been listed in table 6.2, while the linear correspondence between AERIS and AQM-outputs is shown as scatterplots in figure 6.3.

Table 6.2: Statistical indicators for the evaluation of annual depositions (AERIS vs. AQM).

<table>
<thead>
<tr>
<th>Species</th>
<th>( r )</th>
<th>( MB - [mg/m^2 yr] )</th>
<th>( ME - [mg/m^2 yr] )</th>
<th>NMB - (%)</th>
<th>NME - (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_{ox} )</td>
<td>0.9966</td>
<td>-1.89</td>
<td>4.13</td>
<td>-2.84</td>
<td>6.20</td>
</tr>
<tr>
<td>( N_{red} )</td>
<td>0.9956</td>
<td>-6.83</td>
<td>7.11</td>
<td>-7.89</td>
<td>8.31</td>
</tr>
<tr>
<td>S</td>
<td>0.9952</td>
<td>3.93</td>
<td>8.76</td>
<td>3.16</td>
<td>7.04</td>
</tr>
</tbody>
</table>

In general, it can be seen that the parameterization correlates well with the rigorous outputs of the AQM as evidenced by the numeric values of the indicators in table 6.2 (units of \( MB \) and \( ME \) - [mg/m\(^2\) yr]). The value of the Pearson correlation coefficients in every case is above \( r > 0.99 \), which is certainly an indicator of a good statistical correspondence. In the same line, the data points in each of the scatterplots (figure 6.3) distribute uniformly along the \( y = x \) line. The values of these correlation coefficients are similar to the ones obtained for nitrogen and sulfur deposition when analogously compared against the EMEP model (namely \( r = 0.9985 \) and \( r = 0.9976 \), respectively) (Amann et al., 2011). Additionally, it can be seen that the tendencies towards under or overprediction are small while the total amount of associated error does not exceed 9% in the worst case. While no evaluation thresholds or criteria were established for assessing the performance of models when addressing atmospheric deposition processes, the indicators obtained before are presumably low according to common statistical ranges of "correspondence".
Chapter 6. Atmospheric deposition module

Figure 6.3: IAM vs. AQM and IAM vs. EMEP scatterplots for annual accumulated depositions per unit of area.
6.3. Evaluation of the modeling approach

6.3.2 Evaluation of AERIS against the EMEP model

The objective of evaluating the estimates of the AERIS model against the outputs of the EMEP model is contrasting their orders of magnitude. To this respect, the EMEP model is the parent-AQM of GAINS and a highly-credited diagnosis tool for policymaking in the European context so its comparison against the AERIS outputs might provide important information about similarities in modeling approaches as well as on the adequateness of the contrasted outputs for national or regional scale (in this case, the Iberian Peninsula). However, it should be taken into account that the different spatial resolution will bring about errors and biases even if the average levels by both models were identical.

The so-called EMEP model is the common name of the EMEP MSC-W Unified Eulerian model which incorporates Europe-wide emissions and a series of parameterizations that are documented in Simpson et al., (2003) and Fagerli et al., (2004). The performance of the EMEP model is considered acceptable enough for estimating the atmospheric deposition of nitrogen species since it has been validated against measurements throughout Europe (Simpson et al., 2006). For the concrete case of this evaluation, data of the total deposition of oxidized nitrogen, reduced nitrogen and oxidized sulfur were directly obtained from the website of the EMEP/Meteorological Synthesizing Centre - West (MSC-W) for Spain, Portugal and France (figure 6.4). These data are referred to the 2008 extended version of the EMEP grid, which is a European-scale spatial reference with a cell-resolution of 50 km.

In order to consistently compare the two models, these must be referred to the same grid. As a consequence, the outputs of AERIS (16 km) were aggregated to the scale of the EMEP model (50 km), whose cell-spatial extent is approximately 10 times the size of the AERIS equivalent. The cell-aggregation procedure was carried out according to what is published in Boulton et al., (2002) and allowed converting the 4500 cells of the AERIS modelling domain into 494

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Figure 6.4: Annual accumulated deposition per unit of area for $N_{ox}$, $N_{red}$ and $S$ estimated by EMEP.

[Diagram showing annual accumulated deposition per unit of area for $N_{ox}$, $N_{red}$, and $S$.]
Chapter 6. Atmospheric deposition module

EMEP-size cells. The spatial extension of the EMEP outputs was limited to that of the AERIS modeling domain by the application of GIS-based techniques.

The resulting statistical indicators from the comparison between the outputs of AERIS and the EMEP model can be seen in Table 6.3 and have been computed according to what was presented in Chapter 5. In total disagreement with the good correspondence between AERIS and its parent-AQM, the comparison with the EMEP model shows a poor level of reproduction, especially by examining the value of the Pearson correlation coefficients and the scatterplots. Yet, a priori this need not be a negative aspect due to the fact that two different models, whose ancillary parameterizations for the description of the atmospheric deposition are different do not have to perform identically. In addition, the difference in the original spatial scale of both simulations necessarily have an impact as mentioned before.

Table 6.3: Statistical indicators for the evaluation of the annual depositions per unit of area (AERIS vs. EMEP).

<table>
<thead>
<tr>
<th>Species</th>
<th>r</th>
<th>MB [mg/m² yr]</th>
<th>ME [mg/m² yr]</th>
<th>NMB (%)</th>
<th>NME (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nox</td>
<td>0.2910</td>
<td>-195.85</td>
<td>201.31</td>
<td>-64.06</td>
<td>65.84</td>
</tr>
<tr>
<td>Nred</td>
<td>0.3981</td>
<td>-217.11</td>
<td>226.85</td>
<td>-61.75</td>
<td>64.52</td>
</tr>
<tr>
<td>S</td>
<td>0.4286</td>
<td>-179.94</td>
<td>205.23</td>
<td>-45.95</td>
<td>52.41</td>
</tr>
</tbody>
</table>

As it was already stated, the main objective of this comparison was to examine the correspondence in orders of magnitude. By examining the values of the normalized mean error, it can be said that the total amount of error associated is 66% in the worst case (oxidized nitrogen). When analyzing the values of the normalized mean bias, one can see that these are quite similar to the values of the NME revealing the presence of systematic errors (Jolliff et al., 2009). By the sign of the bias values, it is evident that the EMEP outputs are, in average, higher than the estimates given by AERIS. This behavior can be interpreted as an expected performance between AERIS and EMEP of around ± 66% for oxidized nitrogen, ± 65% for reduced nitrogen and ± 50% for sulfur dioxide (approximately). It is also worth noting that the spatial aggregation procedure applied to the outputs of AERIS might also be responsible for the lack of statistical match between datasets, being actually difficult to quantify the extent of this influence.

The annual total deposition of oxidized and reduced nitrogen as well as sulphur estimated according to AERIS and EMEP are shown in Table 6.4. This table suggests that the estimates provided by AERIS are significantly lower than those calculated for Spain by EMEP, being approximately half for each of the deposited species. It is worth noting that the results of the comparison between these two models are totally-objective performance indicators. The way in which the respective outputs were produced is very different in each case, so as it was
6.3. Evaluation of the modeling approach

Figure 6.5: Annual accumulated depositions per unit of area of AERIS and the EMEP model.
Table 6.4: Annual deposition estimated for Spain with AERIS and EMEP for 2007.

<table>
<thead>
<tr>
<th>Species</th>
<th>AERIS ([-t/yr])</th>
<th>EMEP ([-t/yr])</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{ox}$</td>
<td>53,956</td>
<td>125,634</td>
</tr>
<tr>
<td>$N_{red}$</td>
<td>64,578</td>
<td>139,257</td>
</tr>
<tr>
<td>$S$</td>
<td>77,491</td>
<td>166,245</td>
</tr>
</tbody>
</table>

already said this comparison was only carried out to examine any correspondence in orders of magnitude. The results of the IAM are the product of the parameterization of an AQM that has been run with specific initial and boundary conditions and with a series of models that address meteorology, dispersion and chemistry in a particular way (WRF-CMAQ) and for a smaller-scale geographic domain (Iberian Peninsula). On its behalf, the EMEP model has its own particularities too and run for a higher-scale domain (Europe) as well as coarser resolution.

The quality of the deposition estimates of EMEP model is usually a function of the meteorology of every year, especially of precipitation fields for wet deposition. Year-to-year variations in model evaluation can be large and cannot be assumed to be representative of general model performance. Additionally, model performance varies strongly among pollutants for this model and often in an uncorrelated way. It has been estimated that EMEP overestimates sulfur-related deposition in approximately 23% (Simpson et al., 2013; Gauss et al., 2014).

6.4 Validation of AERIS atmospheric deposition module: final remarks

In this section, the atmospheric deposition module that was constructed for its integration into AERIS has been explained and validated. An evaluation of the parameterization that allowed quantifying the annual accumulated deposition per unit of area of reduced and oxidized nitrogen and sulfur species revealed that, when compared to its parent-AQM of AERIS for the baseline scenario of 2007, the statistical correspondence was very good. This was evidenced by the linear correspondence observed in the respective scatterplots and the numeric value of the statistical indicators that were selected for quantitative analysis. When analyzing the performance of AERIS against the EMEP model for the same baseline scenario, a poor statistical correspondence was observed which is a consequence of the underlying differences in model formulation and of the spatial aggregation process that allowed comparing outputs at the same scale. In general, it can be said that the deviations between AERIS and EMEP are in range and that the undertaken parameterization performs adequately for describing atmospheric deposition processes.
Protection of ecosystems module

The protection of ecosystems module is completely dedicated to the analysis of the potential impacts that air pollution may have on ecosystems as a consequence of the atmospheric deposition process. It is therefore interesting to be able to quantify the extent of the impact caused by these deposition processes on the ecosystems present in the modeling domain in order to undertake actions oriented to their protection and conservation. Due to the fact that this module describes the impacts associated with atmospheric deposition, its estimates feed from the results of the deposition module which has been described in section 6. The objective of this chapter is the description of the methodology that was followed in order to construct this module, which focuses on the impacts produced by nitrogen and sulfur species on ecosystems and soils. Although other pollutants and chemical species may cause impacts on ecosystems (i.e. heavy metals, organic compounds, etc.), only nitrogen and sulfur species have been described.

7.1 Theoretical background

The atmospheric deposition processes have direct consequences in the environmental equilibria of ecosystems by altering the naturally-occurring biogeochemical cycles of nitrogen and sulfur. Impacts are caused by the deposition of species in surface-air masses and by the direct contact with droplets from fog and clouds on the ground vegetation and forest in mountainous areas (Hultberg et al., 1994).

Nitrogen in particular is a compound that plays a crucial role being an essential nutrient that directly intervenes in the biological functions of ecosystems as it is one of the most important abiotic factors that determine plant species composition. Moreover, it is a limiting nutrient for plant growth in many natural and semi-natural ecosystems. To this respect, nitrogen impacts can be manifested through three principal mechanisms: eutrophication, acidification and direct toxicity (Bobbink et al., 2010; Jones et al., 2013). The sulfur cycle and its disturbance is strongly affected by anthropogenic emissions, their associated dispersion and deposition
processes. It is therefore critical to quantify the total sulfur input via deposition at the catch-
ment level, aiming to characterize part of the biogeochemical cycling of sulfur (Sanderson
et al., 2006). It is well known that the elevated atmospheric deposition of anthropogenic
sulfur combined with the lack of retention mechanisms produces acidification over large
areas, as well as nutrient losses and possibly forest decline (Hultberg et al., 1994; Posch, 2002).

Both acidification and eutrophication of ecosystems and soils due to the deposition of sulfur
and nitrogen has gained increased attention in Europe since it is a direct consequence of
the transboundary environmental problem. In year 2001 the European Parliament and the
Council adopted the National Emission Ceilings Directive (NEC) regulating EU member state
emissions of acidifying and eutrophying pollutants (Hettelingh et al., 2013). The so-called
ceilings or objectives were set with the support of scientific methodologies available until
2001 for the computation of atmospheric dispersion by sophisticated models as well as on
the determination of critical loads for the deposition of the before mentioned compounds.
The term critical load is crucial for the definition of impacts on ecosystems produced by
deposition processes as well as under a policy making point of view. The following section is
devoted to its definition and to a detailed explanation of its relevance for the construction of
AERIS, especially in the light of the new NEC Directive.

7.2 Critical loads: concept and definitions

The concept of critical load (CL) is a central issue that is essential for the correct estimation of
deposition-associated impacts on ecosystems. Formally, a critical load is defined as “a quanti-
tative estimate of an exposure to one or more pollutants below which significant harmful effects
on specified sensitive elements of the environment do not occur according to present knowledge”
(Nilsson and Grennfelt, 1988). This critical-load approach is based on the assumption that a
pollution load exists below which no harmful effects occur. To this respect, defining critical
loads require different chemical criteria. Since the maximum tolerable load is usually wanted,
the calculation should assume a steady state simulation where in principle the system is held
at the limit for adverse effects. Any slight increase should imply further damage and thus a
violation of the critical load. In conclusion, the estimation of the critical load is necessary
for the evaluation of acceptable levels of deposition throughout a geographic domain as well
as for balancing the acidification-nutrient stress imposed on ecosystems by land use. The
ultimate goal of these critical loads is to set objectives for future deposition rates such that the
environment is protected (Sverdrup and De Vries, 1994).

The critical loads of sulfur and nitrogen have been widely used as indicators of ecosystem
sensitivity to the potential impacts caused by acidification and eutrophication under the
framework imposed by the Convention of Long-range Transboundary Air Pollution (CLRTAP)
and the revision of the National Emission Ceilings (NEC) Directive (Reinds et al. 2008). As
a consequence, and due to the fact that the deposition processes of other pollutants are not presently quantified, only these critical loads will be effectively introduced into the modeling framework of AERIS resulting in two categories, namely those related to eutrophication or nutrient nitrogen and acidification.

The critical load of nutrient nitrogen ($CL_{nut}(N)$) is a single number while the acidity critical loads for a given ecosystem are defined by a critical load function characterized by three quantities: $CL_{max}(S)$, $CL_{min}(N)$ and $CL_{max}(N)$ which correlate through a trapezoidal function in the nitrogen-sulfur deposition plane and which indicate the maximum and/or minimum loads of sulfur and nitrogen that an ecosystem can receive without suffering damage. These quantities are computed from parameters and chemical criteria that need to be clearly defined for every ecosystem type (Posch et al. 2001; Reinds et al., 2008). The function that allows quantifying the critical loads for acidification is shown in figure 7.1, where the gray-shaded area indicates combinations of nitrogen and sulfur depositions ($D_N, D_S$) that do not lead to the exceedance of critical loads.

In every case, critical loads link deposition to ecosystem effects through the incorporation of chemical criteria (fundamentally those related to soils) that determine the critical limits. These limits are quantified in terms of dose-response relationships between the particular chemical characteristics and the overall ecosystem functioning at steady state. As a result, choosing an adequate chemical criterion in order to derive a critical load is crucial since it has to be targeted to a given negative effect that one wants to avoid (Posch, 2002).
7.3 General modeling approach

Despite the fact that this module quantifies impacts on ecosystems and soils separately, the modeling methodology is the same and only the receptors are changed accordingly. The degree of vulnerability of a given receptor is measured by the exceedance of the critical load \((E_x)\) by a deposition rate in a geographic domain of interest. According to Posch et al., (2001),

\[
E_x = \max(D - CL, 0)
\]  

(7.1)

The exceedance of a nutrient nitrogen \((CL_{nut}(N))\) critical load is simply the difference between such value and the deposition of reduced nitrogen according to equation 7.1. However, the exceedance of an acidity critical load should take into consideration the trapezoidal function defined by \(CL_{max}(S), CL_{min}(N)\) and \(CL_{max}(N)\). This calculation process should include the exceedances associated to sulfur and nitrogen respectively \((E_{xN}, E_{xS})\) and add them up (equation 7.2).

\[
E_{xAC} = E_{xAC,N} + E_{xAC,S}
\]  

(7.2)

When comparing present with future deposition scenarios, uniform percentage reductions of the excess depositions were agreed upon by integrated assessment modelers for the definition of the reduction scenarios. These percentage reductions, the so-called gap closures were decided because of the difficulties in attaining non-exceedance in some points of the modeling domain. As a result, a more refined concept such as the ecosystem area gap closure was introduced, in which critical loads are moderated by the extent of the areas \(\left(A_i\right)\) of their respective ecosystems. To this respect, the average accumulated exceedance \((AAE)\) for every cell has been introduced and defined according to equation 7.3 (Posch et al., 2001).

\[
AAE = \frac{\sum_{i=1}^{N} A_i \cdot E_{x_i}}{\sum_{i=1}^{N} A_i}
\]  

(7.3)

It is worth noting that quantifying the critical loads is not an easy procedure and, as it has been already stated, requires ecosystem-specific data. According to Posch et al., (1999), in one 150x150 km² cell, up to 100,000 ecosystems can be found so it is obvious that its calculation is a data-intensive process. The differentiation between exceedances on ecosystems and...
soils relied precisely on the different methodological approaches that were followed for the quantification of the respective critical loads. In the following sections, a brief description of the methodology for quantifying the critical loads is given in terms of their ancillary data and their representativeness.

7.4 Estimation of the critical loads

7.4.1 Critical loads of ecosystems

The quantification of the critical loads of ecosystems focused on eutrophication and acidification in a process that was not directly made by the author of this work. These critical loads were rather derived from atmospheric deposition estimates produced by GAINS model (IIASA) and the Coordination Centre for Effects (CCE) for a given emission scenario and further processed statistically. This alternative was chosen in agreement with the before mentioned methodological aspects that were also used for the formulation of the GAINS model (Posch et al., 2001; Hettelingh et al., 2007).

The basic idea behind this procedure involved assuming that the critical loads are intrinsic “properties” of the ecosystem, regardless of the scale of the cell on which it is located. This fact however, is not completely true since the scale of the domain may condition the quality and representativeness of the data. In this sense, AERIS should provide much more meaningful results than GAINS since it resolution is much finer and therefore it is possible to produce more specific and representative information for every grid cell in the modelling domain.

An additional aspect that needs to be taken into consideration is the fact that the GAINS model provided outputs referred to a 50 km cell size, whereas the scale of the domain of AERIS is 16 km. In order to translate data from one scale to the other, a spatial disaggregation procedure through a GIS-based technique was made with its potential associated “quality loss”. An example of this scale-change process is shown for in figure 7.2 in which the values of the critical loads are reflected in their native 50 km scale and in the AERIS scale of 16 km. The scale-change process that was carried out for the estimation of the critical loads is exactly the same than the one presented in section 6.3.2. In a more general perspective, the critical load values that have been obtained for the modeling domain of AERIS from GAINS-CCE estimates are of an all-ecosystem nature. In other words, these values include critical loads of forests, natural and semi-natural vegetation and surface waters. This process was carried out through the combination of maps of soils, land cover and forest growth regions (Hettelingh et al., 2007). More specifically, these estimates were produced with the Global Land Cover 2000 project map at 1 km resolution (Bartholome et al., 2002), the European Soil database (EUSOIL) (Panagos et al., 2011), and the European Forest Institute database (Schelhaas et al., 1999). The statistical derivation of the acidification and eutrophication critical loads is presented along with the equivalent values determined by the CCE in figure 7.2. Although no quantitative comparison (through statistical procedures) is whatsoever done, a
Figure 7.2: Critical loads of ecosystems according to a) GAINS - CCE b) GAINS - AERIS c) AERIS – \( \text{eq/ha yr} \).
7.4. Estimation of the critical loads

Figure 7.3: Predominant soil classes in the modeling domain of AERIS.

qualitative inspection reveals some differences for the case of the maximum sulfur critical loads \( CL_{max}(S) \), while for nutrient nitrogen \( CL_{nut}(N) \) the differences are less noticeable and within the presented color range. To this respect, the author should acknowledge that the present derivation procedure of the critical loads of ecosystems does not follow the most orthodox modeling guidelines but it was applied due to the limited degree of information and to the complexity and extent of the present project.

7.4.2 Critical loads of soils

The estimation of the critical loads of soils, unlike that of ecosystems, has been carried out through a simple mass balance (SMB) model according to the general methodology explained in Reinds et al., (2008)... This is the most practical and suitable modeling approach for calculating critical loads, due to the fact that SMB methods assume that soil processes are in equilibrium with depositions. Due to the fact that determining the critical loads for soil acidification is a complex task that involves several calculations, the determination of these values was carried out through the application of the Very Simple Dynamic (VSD) model. The VSD model is the simplest extension of steady-state models for critical load calculations with an eye on regional applications (Posch and Reinds, 2009)... In order to determine the respective critical loads, this model requires specific information on the soil types and its physico-chemical properties. Due to the fact that the VSD model is not able to quantify critical
loads of nutrient nitrogen, these magnitudes were not calculated for soils in the current version of AERIS. The first step in the collection process of the physico-chemical properties of soils is its identification in soil classes. To this respect, soil covers were needed to spatially locate such predominant soil classes within the modeling domain. Soil covers from the European Soil database at a scale 1:1 M were obtained for Spain, Portugal, Andorra and France (Panagos et al., 2011), while in the case of Morocco and Algeria, soil covers came from the FAO digital soil map of the world with a 1:5 M scale (FAO, 2003) following the recommendations of Reinds et al., (2008). The soil class cover in the modeling domain is presented in figure 7.3. The soil classification nomenclature that was used in this modeling process is the so-called World Soil Classification proposed by FAO which offers useful generalizations about soils pedogenesis in relation to the interactions with the main soil-forming factors (FAO, 1988). The processing of the before mentioned soil covers revealed that there are 36 predominant soil types in the modeling domain of AERIS, of which cambisols are the most common soil classes (Be, Bh, Bk) while the rest of soil classes are presented in table 7.1.

Table 7.1: Predominant soil classes in the modeling domain of AERIS.

<table>
<thead>
<tr>
<th>Code</th>
<th>Soil class name</th>
<th>Code</th>
<th>Soil class name</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bc</td>
<td>Chromic Cambisol</td>
<td>Ne</td>
<td>Eutric Nitosol</td>
</tr>
<tr>
<td>Bd</td>
<td>Dystric Cambisol</td>
<td>Ph</td>
<td>Humic Podzol</td>
</tr>
<tr>
<td>Be</td>
<td>Eutric Cambisol</td>
<td>Po</td>
<td>Orthic Podzol</td>
</tr>
<tr>
<td>Bg</td>
<td>Gleyic Cambisol</td>
<td>Qc</td>
<td>Cambic Arenosol</td>
</tr>
<tr>
<td>Bh</td>
<td>Humic Cambisol</td>
<td>Re</td>
<td>Eutric Regosol</td>
</tr>
<tr>
<td>Bk</td>
<td>Calcic Cambisol</td>
<td>U</td>
<td>Ranker</td>
</tr>
<tr>
<td>E</td>
<td>Rendzina</td>
<td>Vc</td>
<td>Chromic Vertisol</td>
</tr>
<tr>
<td>I</td>
<td>Lithosol</td>
<td>Vp</td>
<td>Pellic Vertisol</td>
</tr>
<tr>
<td>Jc</td>
<td>Calcic Fluvisol</td>
<td>Wd</td>
<td>Dystric Planosol</td>
</tr>
<tr>
<td>Je</td>
<td>Eutric Fluvisol</td>
<td>WR</td>
<td>Molllic Planosol</td>
</tr>
<tr>
<td>Kk</td>
<td>Calcic Kastanozem</td>
<td>Xk</td>
<td>Calcic Xerosol</td>
</tr>
<tr>
<td>Lc</td>
<td>Chromic Luvisol</td>
<td>Xy</td>
<td>Gypsic Xerosol</td>
</tr>
<tr>
<td>Lf</td>
<td>Ferric Luvisol</td>
<td>Yh</td>
<td>Haplic Yermosol</td>
</tr>
<tr>
<td>Lg</td>
<td>Gleyic Luvisol</td>
<td>Yk</td>
<td>Calcic Yermosol</td>
</tr>
<tr>
<td>Lo</td>
<td>Orthic Luvisol</td>
<td>Yy</td>
<td>Gypsic Yermosol</td>
</tr>
<tr>
<td>Lv</td>
<td>Vertic Luvisol</td>
<td>Zg</td>
<td>Gleyic Solonchak</td>
</tr>
</tbody>
</table>

For each of the before mentioned soil classes, a comprehensive set of parameters need to be collected and further introduced into the VSD model. This data collection process is a very complex activity because the necessary parameters are not usually available since they are derived from on-site measurements. To this respect, most of these parameters were obtained from the Soil Profile Analytical Database for Europe (SPADE) of the Joint Research Centre (JRC) (Hiederer et al., 2006). This database contains soil physico-chemical properties for 25 locations in Spain, 7 locations in Portugal and 3 locations in southern France. The exact
7.4. Estimation of the critical loads

The location of the measurement sites is shown in Figure 7.4. According to the documentation of the VSM model, the necessary data for estimating soil critical loads are listed as follows.

- Thickness of the soil top layer \((z_{top})\) - [m]. Obtained from SPADE measurements.
- Bulk density of the top layer \((\rho_{top})\) - \([g/cm^3]\). Obtained from SPADE measurements.
- Volumetric water content of the soil \((\theta)\) - \([m^3/m^3]\). Estimated as a function of the average clay content according to equation 7.4 as specified in Spranger et al., (2004).

\[
\theta = 0.04 + 0.0077 \cdot \%_{clay}
\]  

- Soil acidity - \(pH\) in the soil solution. Obtained from SPADE measurements.
- Carbon dioxide pressure in the soil solution \((p_{CO2})\) - \([atm]\). It was assumed that the top soil layers are systems open to the atmosphere, for which a mean value of \(3.7 \times 10^{-4} \text{ atm}\) was chosen (ibid.).
• Average potential cation exchange capacity of the soil \((CEC) - [meq/kg]\). Obtained from SPADE measurements.

• Initial base cations saturation \((E_Bc)\). Assumed as \(E_Bc = 0\) for sandy soils and \(E_Bc = 0.297\) for clay and loess-type soils (ibid.)..

• Aluminium - Base cations selectivity constant \((\log_{10} K_{AlBc})\). Assumed as \(\log_{10} K_{AlBc} = 4.116\) for sandy soils, \(\log_{10} K_{AlBc} = 1.139\) for loess soils and \(\log_{10} K_{AlBc} = 0.3\) for clay soils under the Gaines-Thomas cation exchange model according to de Vries and Posch., (2003).~

• Acid - Base cations selectivity constant \((\log_{10} K_{HBc})\). Assumed as \(\log_{10} K_{HBc} = 6.04\) for sandy soils, \(\log_{10} K_{HBc} = 5.569\) for loess soils and \(\log_{10} K_{HBc} = 6.579\) for clay soils under the Gaines-Thomas cation exchange model (ibid.).

• Aluminium equilibrium constant \((\log_{10} K_{Al})\). For sandy soils, a value of \(\log_{10} K_{Al} = 5.59\) was selected while for loess and clay soils, values of \(\log_{10} K_{Al} = 3.14\) and 4.68 respectively as specified in Spranger et al., (2004).~

• Proportionality constant of the \(pH\) - \(pAl\) relationship \((a)\). Considered \(a = 2.68\) for sandy soils, \(a = 2.15\) for loess soils and \(a = 1.83\) for clay soils (ibid.).

• Minimum rate of immobilized nitrogen \((N_{i,min}) - [eq/m^2 yr]\). Due to the complexity in estimating this parameter, it was assumed constant for every soil class, namely \(N_{i,min} = 0.0071428\ eq/m^2 yr\) according to Posch and Reinds, (2009).~

• Average soil temperature \(T_{soil} - [\degree C]\). Although this is a parameter that changes with time, it has been assumed as \(T_{soil} = 8\ \degree C\) as a mean value in the Iberian Peninsula (Gascó et al., 2003).~

• Weathering rates of calcium \((Ca_{we})\), magnesium \((Mg_{we})\) and potassium \((K_{we}) - [eq/m^3 yr]\). The weathering rates of the before mentioned cations were estimated as a function of texture and parent material classes (acidic, intermediate, basic and organic) according to Posch et al., (2003).~The actual weather rate for a non-calcareous soil of depth \(z_{soil}\) is computed according to equation 7.5.

\[
BC_{we} = 500 \cdot z_{soil} \cdot (WR - 0.5) \cdot \exp \left(12.81 - \frac{3600}{273 + T_{soil}}\right) \tag{7.5}
\]

• Initial amount of carbon in top layer per unit of area \((C_{pool}) - [g/m^2]\). Generally obtained from SPADE measurements. When missing, a generic value of \(C_{pool} = 4,000\) was used according to Posch and Reinds, (2009).~

• Initial carbon-nitrogen ratio in topsoil \((CN_i)\). Generally obtained from SPADE measurements and assumed as \(CN_i = 0.279\) when missing according to Spranger et al., (2004).~
7.4. Estimation of the critical loads

- Precipitation surplus \( (p_{\text{surplus}}) \) - \([\text{m/yr}]\). This value was supposed to be 0.15 according to the recommendations presented in Gascó et al., (2003) for the Iberian Peninsula.

The critical loads for soils that were obtained with the VSD model, \( CL_{\text{max}}(N) \) and \( CL_{\text{max}}(S) \), are presented in figure 7.5. The trapezoidal nitrogen-sulfur functions are presented for the total soil classes in appendix A.5. In general, most of the critical loads within the modeling domain of AERIS are above 1000 \( eq/ha \text{ yr} \) (dark green) which indicates that according to the modeling methodology that was followed, most soils are not in a delicate situation with respect to deposition of nitrogen and sulfur. Yet there are of course, large extents of soils whose critical loads are below 200 \( eq/ha \text{ yr} \) (red); the most sensitive regions in the modeling domain are the Guadalquivir valley in south-western Spain, the Garonne basin in south-eastern France and several regions in Northern Africa. The actual damage will eventually depend on the total atmospheric deposition of nitrogen and sulfur species (Gaudio et al., 2014).

In order to bear out that the estimated critical loads for soils are within the “expected range”, the critical load maps of sulfur that are presented in figure 7.5 can be compared to the estimates produced by Posch et al., (2003) for the European scale (CCE) as well as to the map of critical loads elaborated for Spain by Macías-Vásquez et al., (2002). These comparison maps are presented in figure 7.6. Due to the fact that no raw numeric values for each of the critical loads at cell or polygon level in the maps of figure 7.6 were whatsoever given, only a qualitative comparison is relevant at this point. When comparing the \( CL_{\text{max}}(S) \) map of AERIS against the European map it can be seen that the critical loads estimated by Posch et al., (2003) are higher than those of AERIS, being most of them above a value of 1500 \( eq/ha \text{ yr} \). However, critical loads in the central - western part of the Iberian Peninsula are within magnitude order (400 - 700 \( eq/ha \text{ yr} \) for both, AERIS and CCE). The differences are related with the ecosystems covers and physicochemical properties of the considered soils.

A better qualitative correspondence appears to exist with the critical load map estimated by Macias-Vásquez et al., (2002), in which the vast majority of the territory presents a critical load value between 1000 and 1500 \( eq/ha \text{ yr} \). A similar correspondence is observed for the central - western part of the peninsula, where the values of AERIS are below 700 \( eq/ha \text{ yr} \), while the values of ibid. lie between 500 and 1000 \( eq/ha \text{ yr} \). The comparison before was carried out exclusively for \( CL_{\text{max}}(S) \) due to the fact that, according to the particularities of the modeling approach that was applied to the determination of critical loads, it controls most of the acidification-related impacts. This fact is a direct consequence of considering a constant minimum rate of immobilized nitrogen \( (N_{\text{min}}) \) which is the main parameter that determines the magnitude of the minimum critical load of nitrogen \( (CL_{\text{min}}(N)) \). In other words, this assumption renders the maximum critical load of nitrogen directly proportional to the maximum critical load of sulfur. Being this so, whenever acidification impacts on soils are being assessed it should be taken into consideration that \( E_{AC} \approx E_{AC,S} \).
Figure 7.5: Resulting $CL_{max}(N)$ and $CL_{max}(S)$ values for soils in the modeling domain.
In order to present some results on the capabilities and skills of AERIS when determining impacts on ecosystems and soils, these were estimated for the baseline scenario of 2007 in terms of exceedances \((Ex_i)\) and for the concrete case of nutrient nitrogen, as an average accumulated exceedance \((AAE)\). The results are presented in figure 7.7. The exceedance of critical loads of nutrient nitrogen are basically located in north-eastern Spain, particularly around the Pyrenees and the adjacent valleys as well as on the southern coast of Spain. When representing the same impact as the average accumulated exceedance, exceedances seem to increase due to the fact that impacts are weighed by the area and sensitivity of the ecosystems contained within the modeling cell. This behavior is particularly evident in the eastern coast of Spain, the southern coast of France and the western coast of Portugal, which might hint on the vulnerability of coastal ecosystems to air pollution.

When analyzing the exceedance of sulfur critical loads a lower level of impact can be seen, where a much smaller number of cells present a certain degree of vulnerability. The analysis of acidity exceedances on soils shows affected locations that occur at the most sensitive regions (lowest critical loads) located in Algeria as well as in the Guadalquivir valley. A similar behavior is observed for the exceedance of critical loads of sulfur for ecosystems. Affected zones are shown in along the Atlantic coast of Morocco and the southern coast of Spain. Unlike with nutrient nitrogen, ecosystems and soils in the modeling domain exhibit a lesser degree of impact from sulfur due to the purported decrease in sulfur emissions that has been attained in Europe in the last 10 years \((Fenger, 2009)\). ...

7.5 Final remarks on protection of ecosystems evaluation

In line with the European criteria for evaluating air pollution impacts on nature, the degree of protection of ecosystems is measured through the concept of an exceedance of a critical load. To this respect, estimating critical loads is per se a complex modeling activity that
Chapter 7. Protection of ecosystems module

Figure 7.7: Resulting critical load exceedances for nitrogen and sulfur in the modeling domain.
7.5. Final remarks on protection of ecosystems evaluation

requires introducing a great amount of data in the form of spatial covers and physico-chemical parameters. Due to this data intensive nature, a critical load estimate may contain a substantial amount of uncertainty especially when data are subject to scale-change processes or come from non-homogeneous data sources (such as the difference in soil-class covers). However, the current results that AERIS is able to produce actually possess a good level of interpretative value and are helpful to identify areas subjected to excessive pollution loads and areas that might be vulnerable to air pollution in the future. Although not in an incontestable way, the critical loads that were determined for soils have been compared to those reported by other authors for different scales in order to stay confident that results will be in order of magnitude. Up to now, no strict validation procedures for the protection of ecosystems module has been made. However, a performance comparison against the GAINS model has been carried out and is presented in chapter 10.
8 Crops & vegetation impacts module

It is widely known that air pollution has a direct impact on trees and plants, which in many cases are sources of food and natural resources. Therefore it is interesting and necessary under a policy making point of view that the impacts produced on vegetal species by air pollutants are kept to a minimum and therefore, they need to be adequately characterized and quantified. A considerable amount of effort has been carried out by research groups and government bodies to quantify through the use of empirical models the cause-effect relationship between air pollution and adverse effects on terrestrial vegetation. As a consequence, such resources were introduced in AERIS where relevant through the construction of a crops and vegetation impacts module. This module is based on the air quality system that has been widely explained and validated in sections 4 and 5. The present section is devoted to the explanation of the modeling methodology that permitted constructing the module which only focuses on damage to forests caused by the exceedance of critical levels of nitrogen dioxide ($NO_2$) and sulfur dioxide ($SO_2$). Additionally, AERIS describes damage to crops produced by tropospheric ozone ($O_3$) and sulfur dioxide for the most relevant plant species, according to the scientific literature available on the matter. The damaged produced on forests by $O_3$ is not explicitly considered by AERIS, but rather addressed by $AOT_{40}$ as calculated in chapter 4.

8.1 Theoretical background

The association between air pollution and its detrimental effects on vegetal species is well established. Pollutants such as tropospheric ozone ($O_3$), sulfur dioxide ($SO_2$), nitrogen oxides ($NO_x$), peroxyacetyl nitrate ($PAN$) and many volatile organic compounds ($VOC$) are potential vegetation-damaging agents (Tong et al., 2007). Among them, $O_3$ either alone or together with acid rain precursors accounts for up to 90% of the total crop losses in the United States (Adams et al., 1986). In general lines, air pollution-damage to plants is caused by the entrance of gases (particularly $O_3$) through the opening of the stomata or through the direct contact of leaves with acid rain. Once inside the plant tissue, gases react to product by-products that provoke crop losses via the reduction in the photosynthetic activity because of stomatal closure or in the waste of carbohydrates to produce detoxification systems (Andersen and Rygiewicz, 1991;
The most common effects of this damage include chlorotic and necrotic lesions on the surface of the leaves of sensitive species, reductions in photosynthesis and reductions in both the quantity and quality of crop yield (figure 8.1) (Gimeno et al., 1999; Benton et al., 2000; Piikki et al., 2003). When air pollution damages plant species that are destined for human consumption (crops), this results in direct and indirect economic losses that are issue of political and scientific concern in order to take action. This is relevant when analyzing food-safety issues; for example, a recent study in the United States quantified that a 25% decrease in surface O₃ would provide benefits to agriculture of almost 2,000 billion dollars per year. In Europe, it was estimated that crop losses for 23 horticultural and agricultural crops for year 2000 were equivalent to €6.7 billion in economic damage (Tong et al., 2007; Van Dingeren et al., 2009). In less critical cases, pollution-affected crops may be rejected from the food market due to the fact that the resulting visible injuries make the products unlikely to be saleable (Vlachokostas et al., 2010; Humblot et al., 2013).

Particularly, the Iberian Peninsula and its surrounding Mediterranean region are ozone-sensitive areas due to intense photochemical reactions in the atmosphere that are especially favorable under the regional meteorological conditions (González-Fernández et al., 2014). There are enough studies that indicate that air pollution is responsible for considerable crop losses of ozone-sensitive species in the region such as wheat (20-27%), tomatoes (17-24%) and watermelon (19-39%) due to air pollution (Fumagalli et al., 2001). Other pollution-related phenomena such as acid rain (produced basically as a consequence of sulfur-related compounds) may intensify the degree of the damage produced by O₃ or directly affect plants destined for human consumption (Baker et al., 1986). It is of interest therefore, to quantify the possible damage caused by both pollutants simultaneously to have a broader perspective of the potential crop losses under relevant emission scenarios. It is worth noting that so far, no synergies in the generation of impacts due to other effects (i.e. deposition) are being considered.
Air pollution also affects the vegetation of forests and other ecosystems. In particular, forest are crucial since they store more than 80% of the aboveground carbon and more than 70% of all soil organic, acting as global carbon sinks. Additionally, forests generally protect soils against erosion as well as settlement areas and infrastructures against natural hazards such as avalanches, mudflows, floods and rockfall (Smidt and Herman, 2004). Although forests are affected by several other processes like atmospheric deposition, aerosol formation, climate warming and acidification, this section focuses only on the damages associated with exposure to air pollutants, namely $O_3$ and $SO_2$ (Matyssek et al., 2012).

Aiming to complement the diagnostic capabilities of AERIS, a module that is able to quantify the air quality impacts associated to vegetation (crops and forests) has been constructed. This module addresses impacts that are related to exposure to gaseous pollutants and does not refer in any case to damage associated to atmospheric deposition since this has been already included in the impacts to ecosystems module. The main motivation for the construction of this module is to be able to estimate the potential burdens that are associated with the exposure of vegetation to air pollutants under different scenarios in the Iberian Peninsula. Impacts are presented in this chapter in two different sections, impacts on crops and impacts on forests respectively, where specific details on the general methodology can be found.

### 8.2 Modeling approach for impacts on crops

The assessment of air pollution impacts on crops focuses on the damage produced by tropospheric ozone ($O_3$) and sulfur dioxide ($SO_2$). The quantification of these impacts is carried out through the use of quantitative methods that describe the relationship between concentration of pollutants and a given variable that is a measure of the risk or the resulting damage called exposure-response (E-R) functions (Alonso et al., 2008). These E-R functions require the definition of a set of indicators which express the crop relative yield ($RY_i$) as a function of the impacting agent for each crop. E-R functions are usually pooled from a series of cultivars in America and Europe and are assumed representative of the average response of the commonly-grown crop in those regions without the need to use individual cultivar distributions (Van Dingenen et al., 2009). Some examples of E-R functions for different types of crops are available in scientific literature, yet the most efficient and easy-to-use models are those published in Mills et al., (2007). These models correlate a relevant policy - indicator for ozone which is $AOT_{40}$ with the relative yield through a linear model for 19 agricultural and horticultural crops (equation 8.1).

\[
RY_i = a \cdot AOT_{40} + b
\]
To this respect, using $AOT_{40}$ as indicator is very relevant considering that it is a critical indicator in establishing ozone target values and long-term objectives for the protection of vegetation in the European Union (de Andrés et al., 2012). For the concrete case of sulfur dioxide, a similar model than the one proposed by Mills et al., (2007) has been adopted, according to what has been published in Mirasgedis et al., (2008). The general approach for the evaluation of crop losses is an adaptation of the one outlined by Holland et al., (2006), which involves the calculation of the crop production loss ($CPL_i$) as a function of the relative yield ($RY_i$) and the actual crop production ($CP_i$) for the baseline scenario in each cell and for a given plant species.

$$CPL_i = \frac{RY_i}{1 - RY_i} \times CP_i$$

(8.2)

From equation 8.2 it can be seen that actual crop production values in gridded format are needed for the crops of interest. The election of the crops to be assessed will depend on the availability of the gridded datasets, on the reliability of the E-R function and on the importance of this crop to the national or regional agricultural markets.

### 8.2.1 Modeled crop species

The current version of AERIS considers 9 different crop species, of which 5 are agricultural crops (maize, potato, rice, sunflower and wheat) and 4 are horticultural crops (grape, tobacco, tomato and watermelon). These crops were selected due to the fact that there is an E-R function for each of them published in either Mills et al., (2007) or Mirasgedis et al., (2008). Furthermore, some of them are of incontestable economic importance for Spain and Portugal, a fact that can be witnessed in table 8.1 where the total production of the respective crops in year 2007 as well as the international production ranking are shown (FAOSTAT, 2013).

Agricultural crop species such as wheat (*Triticum aestivum*) and maize (*Zea mays*) are very important in the agricultural picture of the Iberian Peninsula, concentrating 8.6% of the total agricultural activities in Spain and 14% of the total vegetal production. The cultivation of wheat in the region has an important historical and cultural character, being particularly intensive in the autonomous communities of Castilla y León, Castilla-La Mancha and Andalucía. In the case of maize, cultivation is basically localized in the communities of Aragón, Cataluña and Extremadura (MAGRAMA, 2012). The case of rice (*Oryza sativa*) is of great importance in Spain, due to the fact that it concentrates 20% of the total agricultural surface in the EU destined to its cultivation, which has a share of 0.73% of the total national agricultural activity (Tornos et al., 2015). Most of the rice that is produced in the country is quantified as “paddy”, and its cultivation is concentrated in the communities of Andalucía, Cataluña, Comunidad Valenciana and Extremadura. Another agricultural crop that is of tremendous importance in...
Table 8.1: Crop production and world rankings in 2007 for Spain and Portugal.

<table>
<thead>
<tr>
<th>Crop specie</th>
<th>Spain</th>
<th>Portugal</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Prod. [kt/yr]</td>
<td>Ranking</td>
</tr>
<tr>
<td>Grape</td>
<td>5,962,643</td>
<td>5°</td>
</tr>
<tr>
<td>Maize</td>
<td>3,610,937</td>
<td>24°</td>
</tr>
<tr>
<td>Potato</td>
<td>2,479,582</td>
<td>25°</td>
</tr>
<tr>
<td>Rice</td>
<td>723,426</td>
<td>36°</td>
</tr>
<tr>
<td>Sunflower</td>
<td>733,154</td>
<td>10°</td>
</tr>
<tr>
<td>Tobacco</td>
<td>29,248</td>
<td>26°</td>
</tr>
<tr>
<td>Tomato</td>
<td>4,081,477</td>
<td>8°</td>
</tr>
<tr>
<td>Watermelon</td>
<td>790,947</td>
<td>12°</td>
</tr>
<tr>
<td>Wheat</td>
<td>6,436,359</td>
<td>19°</td>
</tr>
</tbody>
</table>

Spain and Portugal is potato (*Solanum tuberosum*), which is widely cultivated throughout the Iberian Peninsula and Southern France, concentrating its activity in the autonomous communities of Galicia, Castilla y León and Aragón. Finally, the case of sunflower (*Helianthus annuus*) is also considerable in the Iberian Peninsula, but much more noticeable for the regions of North Africa (namely Algeria). Its cultivation is quite simple and versatile, being its seeds highly appreciated for the production of oil (Gómez-Arnau, 1989).

The selected horticultural crops are also of relevance within the regional modeling context. The most popular and representative specie is tomato (*Solanum lycopersicum*), which also has a considerable economic value along with an ever-increasing demand. In Spain, production is concentrated in Andalucía, Murcia, Extremadura and Aragón (Gázquez-Garrido, 2007). In the same line, the cultivation of grapes is of paramount importance for the Spanish economy, since it is strictly related to the production of wine. The vast majority of the production of grape corresponds to the community of Castilla-La Mancha, followed by Murcia, Comunidad Valenciana and Cataluña (García and Mudarra, 2007). The case of tobacco (*Nicotiana tabacum*) is relevant not in terms of production but in terms of market value and the regional importance in the areas where it is cultivated: Extremadura, Castilla-La Mancha, Navarra and País Vasco. Finally, the cultivation of watermelon (*Citrullus lanatus*) was considered important due to the fact that Spain is one of the most competitive producing countries within the European Union of this fruit. It is cultivated throughout the Spanish territory, but the centers of production are Andalucía and Islas Baleares (Reche-Mármol, 1994).

8.2.2 Crop-specific agricultural covers

As it was already stated, actual crop production values are necessary in gridded format in order to locate the specific areas within the modeling domain in which the cultivation of a certain crop is being carried out. To this respect, crop-specific agricultural covers were provided by
8.2. Modeling approach for impacts on crops

The EarthStat project, which is a collaborative effort between the University of Minnesota’s Institute on the Environment and the McGill University’s Land Use and Global Environment laboratory. This project focuses on analyzing agricultural issues at a global scale and provides detailed datasets for 175 crops (Monfreda et al., 2008; Ramankutty et al., 2008)....Two specific type of datasets were used for obtaining crop-specific agricultural covers: (i) harvested areas and (ii) unitary yields for the crop species of interest. Therefore, the actual crop production ($C_P_i$) can be quantified as the multiplication of the harvested areas ($A_{h,i}$) usually indicating the fraction of grid cell that is destined to the cultivation of a crop, and the respective yields ($Y_i$) (equation 8.3).

$$C_P_i = A_{h,i} \times Y_i$$ (8.3)

The before mentioned datasets are obtained directly from the project’s repository in GeoTIFF format on a global scale for year 2000. While the harvested areas datasets have a pretty acceptable resolution for the modeling domain of AERIS, the resolution of the yields posed a problem since it presents data on a NUTS-2 statistical level for Spain (Autonomous community). To produce a finer result, the actual crop production values were processed in a Geographic Information System software (ArcGIS®) to create the associated Thiessen polygons that were further clipped with the agricultural land uses of the Level 2 CORINE Land Cover database.
The resulting spatial cover for the actual crop production (yield per hectare) is shown in figure 8.3 for wheat. In this figure, one can see the actual zones where wheat is actually being harvested, such as Castilla y León, Castilla-La Mancha, Aragón or southern France. The rest of the modeled crops can be found in figures 8.4 and 8.5. It should be noted that the colors of every polygon in this figure correspond to mean values, being thus likely to have smaller extents with either higher or lower values than the ones presented. These datasets were finally adapted to the modeling domain of AERIS in order to estimate crop losses.

### 8.2.3 Exposure-response functions

As already explained in section 8.2, the exposure-response functions (E-R) that were chosen for its application in AERIS are those specified by Mills et al., (2007) and Mirasgedis et al., (2008), which are linear relationships between $AOT_{40}$ and the relative yield ($R_Y$) as shown in equation 8.1. The quantification of $AOT_{40}$ in AERIS is carried out through a secondary parameterization which depends on air quality observations according to what has been presented in section 4.6.8.

To this respect, it is worth noting that $AOT_{40}$ is a concentration-based descriptor of ozone effects on vegetation that is used to inform air pollution abatement policies and is calculated
8.2. Modeling approach for impacts on crops

Figure 8.4: Actual crop production (yield per hectare) of a) grapes b) maize c) potato and d) rice.
Figure 8.5: Actual crop production (yield per hectare) of a) sunflower b) tobacco c) tomato and d) watermelon.
8.2. Modeling approach for impacts on crops

according to equation 8.4 for the period in which the plant is photosynthetically-active (Denby et al., 2010).

\[ AOT_{40} = \int_0^t \max(O_3 - 40 \text{ppb, } 0) \cdot dt \] (8.4)

The coefficients of the E-R functions that were effectively applied in AERIS that correlate \( AOT_{40} \) (ppm \( \cdot \) h) are shown in table 8.2 as well as their equivalents for exposure to \( \text{SO}_2 \), which are a function of the mean annual concentration of sulfur dioxide (\( C_{\text{SO}_2} \) – ppb) according to Mills et al., (2007) and Mirasgedis et al., (2008). It should be noted that these functions are being directly applied to the mathematical structure of the model, despite the fact that they may be limited by its representativeness in terms of the quality of the statistical parameterization that originated them (measured by their respective Pearson correlation coefficient).

Table 8.2: Exposure - response functions for \( O_3 \) and \( \text{SO}_2 \) based damage for crops.

<table>
<thead>
<tr>
<th>Crop specie</th>
<th>Pollutant</th>
<th>E-R function</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grape</td>
<td>( O_3 )</td>
<td>( RY = 0.003 \cdot AOT_{40} + 0.99 )</td>
<td>Soja et al., (1997)</td>
</tr>
<tr>
<td>Maize</td>
<td>( O_3 )</td>
<td>( RY = -0.0036 \cdot AOT_{40} + 1.02 )</td>
<td>Rudorff et al., (1996)</td>
</tr>
<tr>
<td>Potato</td>
<td>( O_3 )</td>
<td>( RY = -0.0057 \cdot AOT_{40} + 0.99 )</td>
<td>Pleijel et al., (2004)</td>
</tr>
<tr>
<td>Rice</td>
<td>( O_3 )</td>
<td>( RY = -0.0039 \cdot AOT_{40} + 0.94 )</td>
<td>Maggs and Ashmore (1998)</td>
</tr>
<tr>
<td>Sunflower</td>
<td>( \text{SO}_2 )</td>
<td>( RY = 0.0074 \cdot C_{\text{SO}<em>2} - 0.0055 \cdot C</em>{\text{SO}_2}^2 )</td>
<td>Baker et al., (1986)</td>
</tr>
<tr>
<td>Tobacco</td>
<td>( O_3 )</td>
<td>( RY = -0.0055 \cdot AOT_{40} + 1.04 )</td>
<td>Heagle et al., (1987)</td>
</tr>
<tr>
<td>Tomato</td>
<td>( O_3 )</td>
<td>( RY = -0.0083 \cdot AOT_{40} + 1 )</td>
<td>Calvo (2003)</td>
</tr>
<tr>
<td>Watermelon</td>
<td>( O_3 )</td>
<td>( RY = -0.0321 \cdot AOT_{40} + 0.97 )</td>
<td>Gimeno et al., (1999)</td>
</tr>
<tr>
<td>Wheat</td>
<td>( \text{SO}_2 )</td>
<td>( RY = -0.0161 \cdot AOT_{40} + 0.99 )</td>
<td>Gelang et al., (2000)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( RY = -0.0069 \cdot C_{\text{SO}_2} + 0.09 )</td>
<td>Baker et al., (1986)</td>
</tr>
</tbody>
</table>

Through the exposure-response functions that are listed in table 8.2 along with equation 8.2, it is possible to quantify the total crop losses attributable to tropospheric ozone and acid rain. The application of the methodology explained in this section to the 2007 baseline scenario allowed quantifying crop losses as an example. It is worth noting that unlike concentration and deposition estimates that are computed on an emission-variation basis (and therefore involve a baseline scenario) crops and forest impact estimates are computed directly from a given concentration scenario. Figure 8.6 illustrates the losses of wheat produced by the air quality situation resulting of the emissions of the baseline scenario. Analogous calculations were made for the rest of modeled crop species and are presented in figures 8.7 and 8.8. From these figures it can be seen that losses are concentrated only in those cells that present production
of the crop specie of interest, being particularly dramatic for the Mediterranean coast of Spain and North Africa. The favorable nature of the south-western regions of the Iberian Peninsula for the formation of $O_3$ makes that crop losses in these zones especially evident. The crop losses associated to exposure to $SO_2$ for sunflower and wheat can be found in annex 8.7.

### 8.2.4 Final remarks on crop impact evaluation

It becomes evident from the explanation of the methodology that the approach that was selected for the description of impacts on crops is of a statistical nature. This means that the results it provides cannot be taken as absolute truth due to the fact that they rely on a series of generalizations that despite their quality and representativeness, also have a significant amount of limitations associated. It is therefore of the greatest importance to keep in mind that results might be affected by a substantial degree of uncertainty that is a consequence of the numerous parameterizations and assumptions and that, for the time being, has not been quantified. Yet in general lines, the modeling approach that was followed for the characterization of impacts on crops seems to provide reasonable estimates within acceptable orders of magnitude. More importantly, the presented developments opens the door to the implementation of more scientifically sound methodologies for impact assessments such as those based on fluxes (de Andrés et al., 2012).
Figure 8.7: Total $O_3$ crop loss of a) grapes b) maize c) potato and d) rice for the baseline scenario [kg/ha yr].
Figure 8.8: Total $O_3$ crop loss of a) sunflower b) tobacco c) tomato and d) watermelon for the baseline scenario [kg/ha yr].
8.3 Modeling approach for impacts on forests

The assessment of air pollution impacts on forests focuses only on the exceedance of critical levels of nitrogen dioxide \((NO_2)\) and sulfur dioxide \((SO_2)\). This means that AERIS is able to quantify the absolute exceedance of the actual concentration of pollutants and the respective critical levels for those cells in which forests are present. Critical levels for forests are described in different manners according to the pollutant of interest, including mean concentrations, cumulative exposures and fluxes through plant stomata. The expected effects may be significant and vary between receptor and pollutant, including growth changes, visible injuries and reduced seed production (Ashmore et al., 2004).

To this respect, it is important to remind the concept of critical level \((C\ell)\) as an instrument in the evaluation of environmental risk for forest ecosystems on a national and European level. The use of this critical threshold within the LRTAP convention is characterized by an emission-oriented approach whose goal is to reduce the risk by acting at the source (Ardö et al., 2000). This approach is also in line with the concept of emission ceilings’ targets contemplated in the National Emissions Ceilings Directive and the Gothenburg protocol (Barros et al., 2015).
Chapter 8. Crops & vegetation impacts module

The critical levels for sulfur dioxide ($SO_2$) and nitrogen dioxide ($NO_2$) are usually concentration-based. These values have been set, reviewed and revised in a series of UNECE Workshops and are commonly accepted throughout Europe. The critical levels for $SO_2$ were defined in Ashmore and Wilson, (1993) and defines exceedance for forests when either the annual mean concentration or the winter half-year mean concentration is greater than the critical level, which in this case equals 20 $\mu g/m^3$. The critical level for $NO_2$ is actually defined for $NO_x$ in terms of the annual mean and equals 30 $\mu g/m^3$ (Mills et al., 2011).

In general, annual means are used due to the greater reliability for representing long-term effects associated to these pollutants. Although lower concentrations might also be indicative of short-term effects, there is presently insufficient evidence to evaluate on this matter. To this respect, the definition of critical level exceedance ($\mu g/m^3$) can be written as in equation 8.5 for a relevant pollutant $i$.

\[
EXC_i = \max\{C_i - C\ell_i, 0\} \quad (8.5)
\]

According to equation 8.5, it is necessary to identify the cells of the modeling domain on which forests are present. Following an analogous process to the one followed for estimating impacts on crops, a reliable link between detailed spatial forest covers and the respective indicators of air pollution had to be established.

8.3.1 Forest covers

The approach that was followed for identifying cells in which forests are present relied on the use of the CORINE Land Cover 2000 database (CLC 2000) (figure 8.2). This database is a European land cover map produced by photo-interpretation of Landsat ETM+ images, whose land cover component contains geographical information on biophysical land cover (Heymann et al., 1994). CORINE is the only pan-European land cover map that has a spatial resolution of less than 100 m that consistently describes forest land use with a high degree of reliability and allows compatibility between European-scale studies (Pekkarinen et al., 2009). For the purposes of this study, the term forest corresponds to a land use macro-category composed of broadleaved deciduous forests, broadleaved evergreen forests, mixed leaf type forests, needle-leaved evergreen forests and regularly flooded forests (saline) according to the suggestions presented in Feranec et al., (2010) and Pilli, (2012). The resulting cover is shown in figure 8.9 which was then overlapped to the modeling domain grid. Including new land use covers in AERIS is possible as soon as versions are updated, by relying on GIS techniques that allow updating the model's databases and thus its predictive capabilities.
8.3. Modeling approach for impacts on forests

Figure 8.10: Exceedance of critical levels \( (E_{\text{critical}}) \) for (a) \( NO_2 \) and (b) \( SO_2 \) for the \( BS \) (annual mean concentration) for all forest categories.

An example of the skills of the modeling approach in estimating the exceedance of critical levels for \( NO_2 \) and \( SO_2 \) is given in figure 8.10. From this figure one can see that exceedances occur only in cells that actually have forest in them, being these exceedances in the case of \( NO_2 \) as high as 60% of the critical level \( (C^*\)\. In general, it can be seen that the most affected forest areas are those located in areas of Castilla-La Mancha that border the province of Madrid, which is reputed of being an important pollution hotspot in the Iberian Peninsula. Other cities like Zaragoza and Toulouse seem to be responsible for the exceedances that are being observed in the surrounding forests, while the ship transit would be imputable for generating the exceedances shown in the Mediterranean coast of Algeria.

8.3.2 Final remarks on forest impact evaluation

The methodology for the estimation of indicators that allow quantifying impacts on forests due to air pollution, reflected as an exceedance of the so-called critical levels \( (C^*) \) does not exhibit any additional uncertainties associated to the modeling process other than the reliability of the CORINE Land Cover proper. Unlike the modeling process of impacts on crops, the estimation of impacts on forests has been carried out through concentration-based indicators that are directly obtained from the air quality system, that has been thoroughly validated and whose limitations have been discussed in chapter 5.
9 Health impacts module

Public health protection is one of the strongest motivations for developing a consistent air pollution policy and is one of the most powerful driving forces for the development of modeling tools, including those produced under an integrated assessment framework (Peled, 2011). It is generally accepted that the air pollution problem has deep implications in public health and is therefore desirable to estimate to what extent does it affect human well-being. Trying to provide answers to these issues, a health impacts module was constructed in AERIS which is based on the air quality system that was formulated and validated in sections 4 and 5. The objective of this chapter is the explanation of the modeling methodology that allowed the construction of the module, which only focuses on fine particulate matter ($PM_{2.5}$) and tropospheric ozone ($O_3$). Although other pollutants might bring about health damage, only these two were considered due to the extensive epidemiologic studies and references that support translating concentrations into health impacts.

9.1 Theoretical background

It is incontestable that air pollutants cause adverse effects on human health. From a human perspective, air pollutants may produce serious illnesses or may pose a present or potential hazard to human health. The determination of whether a pollutant poses a health risk to human populations is based on clinical, epidemiological or animal studies which demonstrate the relationship between exposure to this pollutant and adverse health effects (Giechaskiel et al., 2009). Under this framework, the term risk to human health should be defined as the probability that an adverse health effect may happen.

According to their nature, pollutants exhibit different impacts whether they are gaseous or particulate matter, but there is enough consensus in that airborne pollutants enter the human body through the respiratory tract via inhalation or ingestion. To this respect, fine particulate matter of less than $2.5 \mu m$ is associated with severe health effects because it is propense to deposit in the upper respiratory tract and even reach the lung alveoli (Boldo et al.,
9.1. Theoretical background

Moreover, particulate matter can absorb and transfer multitude of pollutants which can include metals, organic compounds, material of biologic origin, ions, reactive gases as well as carbon (Kampa and Castanas, 2008). Tropospheric ozone on its behalf, is reputed of being highly oxidant and high-concentration episodes are related with an increased number of hospital admissions for respiratory and cardiovascular disease (Anderson et al., 2004).

Particularly in Europe, air pollution is reputed for being the most important environmental factor that contributes in a non-negligible manner to the total burden of mortality in urban areas (Künzli et al., 2000). As a consequence, and taking into consideration the before mentioned health damages, stakeholders at all levels are interested in controlling the causes of air pollution in order to minimize its effects on the public health systems. For this particular purpose, IAMs are useful tools for estimating long-term population exposures to air pollution because they have the ability to reflect the spatial variability of the concentration of pollutants in the long term (Aguilera et al., 2013).

In this line, a health impacts module was configured for AERIS in order to have an estimate of the potential burdens that are associated with air pollution under different emission scenarios in the Iberian Peninsula. As it was already stated, this module is able to estimate health impacts related to fine particulate matter ($PM_{2.5}$) and tropospheric ozone ($O_3$). The following sections are devoted to the explanation of the methodological approach that was followed to formulate and construct the present module.
9.2 Modeling approach for $PM_{2.5}$-related impacts

The estimation of the impacts related to fine particulate matter is based on three different related indicators: the change in statistical life expectancy per person ($\Delta e_c$), the total amount of life years lost ($YOLL$), and the disability adjusted life years ($DALY$). These indicators provide information on health impacts under different perspectives and are especially useful for determining the degree of the burdens to health that particles produce in the long term. The general conceptual framework that has been followed is the one applied to IIASA’s GAINS model and published in Mechler et al., (2002). This framework consists in the following steps:

1. Investigate from relevant databases information on current and future mortality rates for the six countries that are present in the modeling domain of AERIS: Spain, Portugal, Andorra, France, Morocco and Algeria.

2. Estimate the exposure of the population of the before mentioned countries to particulate matter pollution for an initial year of the time series (in this case 1990) and assume a validity analysis period of 10 years.

3. Through the use of relationships between particulate matter pollution and mortality found by epidemiological studies, determine the change in mortality rates due to exposure.

4. Compute and compare modifications in the health indicators for the baseline scenario of AERIS and for a comparable (reference) scenario.

As stated in Mechler et al., (2002), a study of such proportions is very appropriate under an integrated assessment perspective because it combines information about results from different epidemiological studies that quantify the impacts of air pollution on mortality with geographically explicit estimates of air pollution and demographic structures in the countries present in the model. For the concrete case of AERIS, the estimates of fine particulate matter are the result of the complex interplay between primary $PM$ emissions as well as precursor gases such as $NO_x$, $SO_2$ and $NH_3$ that form secondary aerosols. In the following sections, a complete explanation of the modeling hypotheses that were selected for the description of health impacts is given in terms of the ancillary databases and epidemiologic studies.

9.2.1 Epidemiological studies for $PM_{2.5}$

Under an air quality management point of view, the objective of epidemiological studies is the establishment of a relationship between pollutant concentrations and the possible sanitary risks (Makri and Stilianakis, 2008). These epidemiological analyses provide concentration-response functions (CRFs) that describe in mathematical language the relationship between impacts and environmental stressors. Its application allows determining the number of disease or death cases as well as the generic loss in life expectancy of a population that are
9.2. Modeling approach for $PM_{2.5}$-related impacts

Figure 9.2: Estimated survival functions for the countries located within the AERIS modeling domain.

In general, epidemiological studies state that longer exposures provoke more severe health impacts. The most useful epidemiological studies for carrying out particulate matter evaluations are the so-called cohort studies (and their re-analyses) of annual average $PM$ exposure and age-specific death rates in a given city and region (Dockery et al., 1993; Krewski et al., 2000; Pope et al., 2002). Conducting cohort studies is a very complex activity so only a limited number of analyses are available. Among these studies, the work of Pope et al. (2002) is the most used since it examined during 16 years the possible associations of mortality in a given population with a wide range of variables such as age, sex, race, body mass, occupational exposure and diet, among others. This study allowed quantifying a relative risk of mortality ($RR$) for exposure to air pollution. This cohort study was applied to the modeling process of AERIS due to the fact that for the time being, there is no European equivalent (Pilling et al., 2005). This factor will be essential for determining health impacts expressed as indicators which are explained in the following sections.

9.2.2 Change in statistical life expectancy per person

The change in statistical life expectancy per person ($\Delta e_c$) refers to the period of time (expressed in years, months or days) that is subtracted from the life expectancy of an individual
as a consequence of the exposure to air pollution or any other environmental stressor. The methodology for the calculation of this indicator relies on country-specific mortality rate values and on the methodological approach followed in (Vaupel and Yashin, 1985; Mechler et al., 2002; Amann et al., 2011). The basis for the calculation of this indicator is the survival function \( l(t) \) which indicates the percentage of a cohort alive after time \( t \) has transcurred since starting time \( s \). This survival function is the exponential of the sum of the mortality rates \( \mu_{a,b} \) that are taken from life tables where \( a \) is the age and \( b \) is the calendar years since the beginning of the time series. Due to the fact that in Pope et al., (2002) only cohorts with at least 30 years old were considered, this analysis did not include any younger age groups. To this respect, the survival function for a given cohort \( c \) can be estimated as in equation 9.1. As it can be seen from this equation, the survival function only depends on statistical mortality data that need to come from reliable databases. In the case of AERIS, mortality rates were taken from the World Health Organization (WHO) mortality data and statistics database.

\[
    l_c(t) = \exp \left( - \sum_{z=c}^{r} \mu_{z,z-c+s} \right)
\]  

(9.1)

The survival functions derived from WHO mortality statistics for Spain, Portugal, France, Morocco and Algeria between ages 30 and 60 are shown in figure 9.2. The survival function of Spain was used for Andorra due to the lack of information for this country. The estimation of these survival functions allows estimating life expectancy values of which the remaining life

![Figure 9.3: Evolution of the Spanish population per age groups from 1990 to 2010.](image)
9.2. Modeling approach for PM$_{2.5}$-related impacts

Figure 9.4: Estimated loss of statistical life expectancy (months) for the baseline scenario.

Life expectancy is necessary. To this respect, the remaining life expectancy ($e_c$) for cohort $c$ can be estimated as the total survival rates starting at age $c$ and ending at age $w_1$ and modeled as the integral between these values as in equation 9.2.

$$e_c = \int_c^{w_1} RR_{PM} \cdot l_c(t) \cdot dt$$

On its behalf, the relative risk is defined as a function of the change in particulate matter concentrations and a proportionality coefficient $\beta$, namely $RR_{PM} = \beta \cdot PM + 1$. When this function is introduced in equation 9.2, the relationship between life expectancy and concentrations of pollutants becomes very complex. An approximation based on a first-degree Taylor approximation yields equation 9.3 which allows quantifying the absolute change in life expectancy per person (Amann et al., 2011). The value of the proportionality constant $\beta$ for premature mortality risk is $\beta = 0.006$ according to Pope et al., (2002).

$$\Delta e_c = \beta \cdot PM \cdot \int_c^{w_1} l_c(t) \cdot \log l_c \cdot dt$$

\[175\]
Changes in life expectancy need to be calculated for each of the cells consistently with airborne concentration estimates. However since changes in life expectancy are usually \textit{age-specific}, the estimation of this indicator requires apportioning the population of a given cell in \textit{age groups}. As a consequence, the respective national age-group apportionment in 2007 (baseline scenario) was supposed constant for each of the countries present in the modeling domain.

As an example of this practice, the evolution of the Spanish population per age groups from 1990 to 2010 is shown in figure 9.3. This health indicator was calculated with the $PM_{2.5}$ concentration values of the baseline scenario and the results are presented in figure 9.4. From this picture, it can be seen that the highest life expectancy losses are associated with urban agglomerations (Madrid, Lisbon, Barcelona and Porto) where up to 5 additional months of life expectancy can be subtracted from the normal population patterns of mortality in the respective countries.

### 9.2.3 Total amount of life years lost - $YOLL$

The \textit{total amount of life years lost} ($YOLL$) is an indicator that is derived from life expectancy metrics and is basically the \textit{sum} of the number of years of life that are lost due to \textit{premature mortality}. In summary, the total amount of life years lost corresponds to the number of deaths
9.2. Modeling approach for $PM_{2.5}$-related impacts

multiplied by the standard life expectancy at the age at which death occurs. In general terms, this indicator can be calculated with equation 9.4 for a given cause and specific sexes and age ranges (Murray et al., 2002).

$$YOLL = Deaths_c \cdot l_c(t)$$ (9.4)

The estimation of $YOLL$ varies from a simple comparison of the age of death of a person related to the expected life expectancy to multidimensional life table models that calculate this indicator. The main advantage of $YOLL$ in comparison to direct mortality indicators is that it takes into account the age of victims in a simpler way than considering life-table models (Bouland et al., 2013). According to equation 9.4, the estimation of $YOLL$ is related to the determination of the loss of statistical life expectancy per person. However, it also depends on population data and on the so-called age-apportionment that was carried out in section 9.2.2. In this sense, $YOLL$ can be quantified according to the adaptation of equation 9.4 as presented in Mechler et al., (2002) and Amann et al., (2011).

$$YOLL = \beta \cdot PM \cdot Pop_j \cdot f_c \cdot \int_l^{u_l} l_c(t) \cdot \log l_c \cdot dt \tag{9.5}$$

Where $Pop_j$ is the population count in cell $j$ and $f_c$ is the age-apportionment factor for cohort $c$. Being this so, in order to provide estimates with equation 9.5, population counts for the modeling domain of AERIS had to be investigated. To this effect, population covers for Spain, Portugal, Andorra and France were obtained from the Gridded Population of the World project (GPW) hosted by NASA and the University of Columbia. The equivalents for Morocco and Algeria were taken from the Africa Population Distribution Database of the UNEP/GRID - Sioux Falls Clearinghouse. Both population counts are referred to year 2000 due to the lack of more recent versions. The resulting population count in the modeling domain is shown in figure 9.5. Additionally, due to the lack of concise and relevant information on the matter, the applied age-apportionment criteria were national-scaled according to the distribution percentages estimated from WHO mortality statistics. The $\beta$ coefficient that is derived from the relative risk obtained with epidemiological studies equals $\beta = 0.006$ as it was obtained from Pope et al., (2002).

In order to illustrate the skill of AERIS in estimating the total amount of years of life lost, this indicator was computed for the 2007 baseline scenario and is shown in figure 9.6. From this picture, it is evident that the number of life years that are lost due to exposure to $PM_{2.5}$ pollution are basically concentrated in cities. This fact is especially relevant in two main ways; first, cities are reputed for being pollution hotspots (mainly related to road-traffic which
is an important $PM_{2.5}$ emitter) and for concentrating a large number of inhabitants. The combination of these two factors produces high values for cities such as Madrid, Lisbon, Porto and Barcelona. The loss of years is also evident for less-populated cities such as A Coruña, Bilbao, Palma de Mallorca, Coimbra and Oran. As it was already stated, due to the fact that this indicator takes into consideration population counts, it can be somehow a good complement for the change in life expectancy per person estimated in the previous section.

### 9.2.4 Disability adjusted life years - $DALY$

The disability adjusted life years or $DALY$ is a health gap measure that extends the concept of potential years of life lost due to premature death to include years of healthy life lost by virtue of being in states of poor health or disability (Murray et al., 2002). In other words, one $DALY$ combines in one measure the concept of living with disability and the time lost due to premature mortality. In this sense, this indicator can be considered as one lost year of healthy life and the burden of disease as a measurement of the gap between current health status and an ideal situation where everybody lives into old age free of disease and disability (Murray and López, 1996). The general methodology that allowed estimating the $DALY$ indicator was the one explicated in Rao et al., (2012, 2013) that quantifies the risk associated to $PM_{2.5}$ exposure for men and women above 30 years old. This methodology is based on an approach that defines the population-attributable fraction ($PAF$) as a key parameter for
9.2. Modeling approach for PM$_{2.5}$-related impacts

determining the degree of exposure to pollutants. It takes into consideration the gradient of risk between the theoretical minimum level of air pollution and the estimated observed exposure (WHO, 2002). To this respect, the population-attributable fraction to exposure (PAF) can be calculated as in equation 9.6.

$$PAF = \frac{PM \times (RR - 1)}{PM \times (RR - 1) + 1}$$ (9.6)

Where $RR$ is the relative risk for exposed versus non-exposed populations. In a broader sense, the PAF quantity is the fraction of a disease that is attributed to a risk factor. After this value is determined, the DALY estimates can be computed by a simple multiplication of PAF with the raw values of DALY that are usually found in health databases (Rao et al., 2012). The so-called DALY raw values were obtained from the Mortality and Burden of Disease Estimates for WHO Member States in 2004 which reports such values under egalitarian principles (Mathers et al., 2006). For the concrete case of AERIS, DALY estimates were quantified only for cardiopulmonary health outcomes which have been listed for the countries present in the AERIS domain in table 9.1.

Table 9.1: Raw DALY values per country for PM related health outcomes ($\times 10^{-3}$).

<table>
<thead>
<tr>
<th>Health outcome</th>
<th>GBD</th>
<th>Spain</th>
<th>Portugal</th>
<th>Andorra</th>
<th>France</th>
<th>Morocco</th>
<th>Algeria</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lower respiratory infections</td>
<td>39</td>
<td>32</td>
<td>19</td>
<td>0</td>
<td>45</td>
<td>169</td>
<td>232</td>
</tr>
<tr>
<td>Upper respiratory infections</td>
<td>40</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>Hypertensive heart disease</td>
<td>106</td>
<td>22</td>
<td>6</td>
<td>1</td>
<td>33</td>
<td>63</td>
<td>28</td>
</tr>
<tr>
<td>Ischaemic heart disease</td>
<td>107</td>
<td>271</td>
<td>82</td>
<td>0</td>
<td>265</td>
<td>301</td>
<td>120</td>
</tr>
<tr>
<td>Cerebrovascular disease</td>
<td>108</td>
<td>190</td>
<td>116</td>
<td>0</td>
<td>221</td>
<td>112</td>
<td>160</td>
</tr>
<tr>
<td>Inflammatory heart disease</td>
<td>109</td>
<td>34</td>
<td>6</td>
<td>0</td>
<td>39</td>
<td>24</td>
<td>31</td>
</tr>
<tr>
<td>Respiratory diseases</td>
<td>111</td>
<td>349</td>
<td>88</td>
<td>1</td>
<td>327</td>
<td>154</td>
<td>179</td>
</tr>
</tbody>
</table>

An example of the cardiopulmonary disability adjusted life years produced by exposure to PM$_{2.5}$ is computed for the 2007 baseline scenario and is shown in figure 9.7. The most striking issue that can be observed from this figure is the fact that DALY estimates in Portugal are perfectly differentiated from those of the rest of the model. This behavior is explained by the fact that raw values of DALY are given in a nation-wide scale that are not exclusively related to air pollution exposure. Although PM$_{2.5}$ concentration patterns are more or less evident in this figure, for those areas with low PM$_{2.5}$ levels, DALY values with a poor representative value are obtained due to the fact that the raw value tends to be greater than the PAF component. In figure 9.7, cities are not very clearly represented yet high impact zones are evidenced in the central area of Spain (Madrid) and in the north-eastern Mediterranean coast (Barcelona).
9.3 Modeling approach for $O_3$-related impacts

The estimation of health impacts produced by tropospheric ozone ($O_3$) relies only in one indicator: the cases of premature mortality per year produced by exposure to ozone. The general conceptual framework that was followed is the one applied to IIASA’s GAINS model and published in Amann et al., (2011). This methodology is basically related to concentration profiles expressed as a relevant policy-indicator, which are already reputed for correlating with health impacts. For instance, the World Health Organization highlighted the need to quantify lower ozone concentrations that occur throughout the year and not only peak episodes. As a consequence, the UNECE/WHO Task Force on Health has recommended that health impacts are made through the use of $SOMO_{35}$ as the most relevant ozone indicator (UNECE/WHO, 2004; Amann et al., 2011).

9.3.1 Epidemiological studies for $O_3$

Epidemiological studies on the relationship between tropospheric ozone concentrations and potential impacts on human health are scarcer than those available for particulate matter. Most of these studies focus on the short-term exposure to ozone peaks and analyze the effects of these peaks on minor restricted activity days, hospitalizations for respiratory symptoms, use of bronchodilators, cough days and days with problems of the lower respiratory tract (Bouland...
9.3. Modeling approach for $O_3$-related impacts

Table 9.2: All-cause annual mortality values for the countries considered in AERIS.

<table>
<thead>
<tr>
<th>Country</th>
<th>Mortality</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spain</td>
<td>385,361</td>
</tr>
<tr>
<td>Portugal</td>
<td>103,512</td>
</tr>
<tr>
<td>Andorra</td>
<td>600</td>
</tr>
<tr>
<td>France</td>
<td>546,476</td>
</tr>
<tr>
<td>Algeria</td>
<td>172,000</td>
</tr>
<tr>
<td>Morocco</td>
<td>166,500</td>
</tr>
</tbody>
</table>

et al., 2013). For the purposes of this study, the considered epidemiological studies are the few that focus on the long-term effects and mortality, namely the studies of Anderson et al., (2004) and Jerrett et al., (2009).

9.3.2 Cases of premature mortality per year

The cases of premature mortality per year refer to the number of persons who die before an expected age (i.e. statistical life expectancy). As it was already stated, the methodology that was followed is the one presented in the GAINS model and which relies on national baseline mortality data. According to Amann et al., (2011), the annual cases of premature mortality can be calculated as shown in equation 9.7.

$$\text{Mort}_j = \text{Deaths}_{Nat} \cdot RR_{O3} \cdot \frac{O_{3,j}}{365}$$ (9.7)

Where $\text{Deaths}_{Nat}$ is the national baseline mortality in number of deaths per year (table 9.2), $RR_{O3}$ the relative risk for one percent increase in daily mortality per ppb of 8–h maximum ozone concentration per day and $O_{3,j}$ is the population-weighted $SOMO_{35}$ in cell $j$. In this case, the value of the relative risk equals $RR_{O3} = 5.25 \times 10^{-5}$ (Anderson et al., 2004). The population-weighting procedure was carried out by following equation 9.8 according to Horálek et al., (2013).

$$\overline{O_{3,j}} = \frac{O_{3,j} \cdot Pop_j}{\sum_{j=1}^{N} Pop_j}$$ (9.8)

Where $Pop_j$ is the population count in cell $j$ and $N$ is the total number of cells in a particular country. For determining this indicator, it is necessary to have the values of the national...
baseline mortality in number of deaths per year for each of the countries that are present in the domain. This values were obtained from the Mortality and Burden of Disease Estimates for WHO Member States in 2004 (Mathers et al., 2006) and are listed in table 9.2. The correct estimation of this health impact indicator relies on a secondary parameterization that allows quantifying $SOMO_{35}$ (section 4.6.8). With the before mentioned elements, the quantification of the premature mortality cases per year was made for the 2007 baseline scenario and the results are shown in figure 9.8.

In a similar way, the total years of life lost ($YOLL$), a higher number of premature mortality cases due to exposure to $O_3$ are evident for urban agglomerations such as Madrid, Lisbon, Toulouse or Algiers and their surroundings. Due to the fact that this indicator takes into consideration a population-weighted concentration value ($\overline{O}_3$), premature mortality cases are marginal in rural areas that are reputed for presenting high levels of tropospheric ozone. It is also true that the average concentration of $O_3$ in rural locations is high but peaks are relatively low and short-term high $O_3$ concentrations seem to be the main concern under a health-impact quantification point of view. Although limited, the available information allowed modeling an estimation routine that would provide guidance on the potential impacts of tropospheric ozone on human health and presenting them in maps with high representative value which, for the time being, cannot be obtained with IIASA’s GAINS.
9.4 Final remarks on health impact evaluation

Health impacts are quantified in AERIS for fine particulate matter \((PM_{2.5})\) and for tropospheric ozone \((O_3)\), for which epidemiological studies are available and have been widely contrasted by the scientific community. For both pollutants, the estimated indicators are intimately related to changes in mortality or life expectancy yet it would be very suitable to conduct a similar modeling approach to evaluate effects on morbidity. For the time being, this has not been made due to the lack of methodological frameworks that support these estimations like the GAINS methodology, which only quantifies mortality impacts as they are the dominant factor when carrying out economic benefit assessments. At this point it is very necessary to make notice that the before mentioned estimates should not be taken as absolute truth or of “binding nature” since they are meaningful only in statistical terms. Yet this does not mean at all that they lack interpretative value, but rather good care should be taken in extrapolating them arbitrarily. Up to now, no strict validation procedures for the health impacts module has been whatsoever made. However, a performance comparison against the GAINS model for health impact evaluations has been carried out and is presented in chapter 10.
A crucial step in the development of AERIS as well as on the dissemination of its abilities and skills as a diagnostic tool with a high representative value is the analysis of the credibility and reliability of its estimates. Usually this analysis is based on quantitative or qualitative comparisons that seek to find model acceptance. For models such as AERIS, ranges of accuracy are usually defined through sensitivity analysis, considering that inaccuracy is a consequence of uncertainty in the values of model parameters (Confalonieri et al., 2010). To this respect, carrying out sensitivity analyses is a complex and time-consuming task that is unnecessary under the specific modeling framework of AERIS. As it has been stated in chapters 4 and 5, the potential estimates of AERIS have been assessed within the range of emission variation percentages of $-90\% \leq p_i \leq 90\%$. However, it should be noted that part of the validation involved using the same data for development and testing, in a process which is called re-substitution and in which performance is likely to be conditioned by the fact that AERIS was designed to mimic the results of an AQM (Bennett et al., 2013). In other sections, validation was discussed in terms of qualitative comparisons that rely on often subjective considerations which in many cases provide better quality-statements than a conventional statistical evaluation (Carberry et al., 2002). Additionally in the previous chapters most of the evaluations focused in comparing the outputs of AERIS to those of its parent AQM, while in this chapter a more conventional evaluation of the skills of the model will be made by comparing its outputs against other models.

However, reliability and credibility cannot be assumed only through the application of numerical analysis when model outputs are to be used with and for stakeholders. Numerical analysis provide credibility within the techno-scientific research community which could sometimes be insufficient for decision-makers. When models are to be used for policy making, validity is defined by the fact that stakeholders have sufficient confidence in the model to use as the basis for making management decisions (Alexandrov et al., 2011). As a consequence, the analysis of model credibility will be based on a comparison of the performance of AERIS against that of a reference model for stakeholders. Although operating at a different scale, the selected
model of reference was the GAINS (Greenhouse gas - Air pollution Interactions and Synergies) model, which has been extensively used during time negotiations under the Convention on Long Range Transboundary Air Pollution (CLRTAP) framework and during the revision of the Gothenburg Protocol. This model benefits from a good level of trust among stakeholders since it is the successor of the RAINS model, incorporating latest scientific understanding on the impacts of air pollution (Amann et al., 2011).

10.1 Analysis rationale

If the model comparison between the outputs of AERIS and GAINS reveals a similar degree of performance, it is acceptable to say that AERIS imitates the results of GAINS. However, unlike the evaluation procedures carried out for validating the estimates of AERIS against those of its parent-AQM, the present analysis is not based on a direct quantitative (statistical) comparison. Up to this point, it has been made clear that AERIS and GAINS describe different scales, were derived from different air quality models (AQM) and incorporate information from diverse ancillary sources.

It is therefore misleading to carry out a point-to-point comparison in which model outputs are expected to be different. Yet both models are able to provide information on the same geographic domain and estimate some variables described under similar methodologies. As a result, the comparisons between AERIS and GAINS were conducted qualitatively and by examining the similarity of the probabilistic distributions between the two datasets through the Kolmogorov-Smirnov (K-S) test. For complementary purposes, the value of the Pearson correlation coefficient \( r \) is included in order to obtain possible explanatory relationships between variables (i.e. outputs from AERIS against outputs from GAINS). The quantification procedure for this correlation coefficient has already been introduced in chapter 5. This comparison will be obviously undertaken for the same emission scenario in order to approximate as much as possible the initial conditions of analysis between both models.

10.1.1 Kolmogorov - Smirnov test

The Kolmogorov-Smirnov test (K-S) for a sample is a non-parametric procedure intended to examine the “goodness-of-fit” between the distribution of a given dataset and a specific theoretical distribution. Its objective is to define if the data of the sample are representative of the “population” that has the specified theoretical distribution. In other words, it contrasts whether the observations could reasonably come from a population that follows the specified distribution (Justel et al., 1997). To this respect, we are interested in analyzing whether the distribution of the estimates that AERIS produces for the impacts described in the previous chapters are representative of the original distribution of GAINS (used here as reference). The K-S test relies on an indicator called the K-S statistic which can be directly related to the statistical confidence level \( \alpha \). If this value approaches one \( (p_{KS} = 1.0) \), it can be assumed
Chapter 10. Credibility of AERIS: an analysis

that the degree of correspondence is substantial between samples. In general, analysis should rely on the hypothesis that the fitted curve (in this case the AERIS samples) is different to the empirical curve according to the specifications of the software routine of MATLAB ® (kstest2). In other words, the problem should be formulated assuming that the two samples are from different continuous distributions, an hypothesis that will have to be rejected in order to hint on the credibility of AERIS estimates.

The analysis of the goodness-of-fit between the two samples will be complemented by the use of cumulative distribution function (CDF) plots. These plots are especially relevant for describing the probability that a real-valued random variable \( X \) with a given probability distribution will be found at a value less than or equal to \( x \) and are constructed from individual values (in this case, model outputs) arranged in increasing order. For the K-S test, these plots clearly identify the location of values along the distribution and whenever two datasets are being compared, the relative position of the tested sample against the reference sample is an indicative of such goodness-of-fit (Xue and Titterington, 2011). This approach was selected instead of a traditional point-to-point correspondence analysis due to the fact that substantial differences between the two models are expected, as explained in section 10.1.

10.2 Emission scenario for comparison

In order to have a common basis for comparison, a relevant emission scenario that can be quantified by AERIS and GAINS was selected. Due to the fact that GAINS was actively involved in its elaboration and discussion, the selected emission scenario corresponds to the Gothenburg Protocol Revision in 2011 quantified by the 2010 National Projections under Current Policies for Spain and Portugal. This scenario can be described in terms of the activities and control strategies updated according to the PRIMES 2009 scenario quantified by IIASA. Concerning the emission activities, energy and process activity rate pathways from national submissions were used. As for control strategies, current policies were assumed, including international and national policies (if stricter) (IIASA, 2013). This emission scenario is completely described in GAINS in terms of the emission activities that this IAM considers so these activities need to be “mapped” so that AERIS can reproduce the emission variation percentages \( p_i \) needed to run the model and quantifying the related impacts. The correspondence between GAINS and SNAP categories was based on the nomenclature developed within the SEP project (Lumbreras et al., 2008).

This mapping process involves finding emission sectors in AERIS that are equivalent to the emission sectors of GAINS in order to assign a reduction percentage derived from the baseline scenario of 2007. It should be noted that GAINS considers some other sectors that are currently not being described by AERIS, so a certain degree of statistical mismatch might be expected as a consequence. The sectors of GAINS that have a potential match with a sector described
### Table 10.1: Emissions of the GAINS sectors for the 2011 Gothenburg Protocol Revision for Spain - [kt/yr].

<table>
<thead>
<tr>
<th>GAINS</th>
<th>Activity name</th>
<th>NO(_x)</th>
<th>SO(_x)</th>
<th>PM(_{10})</th>
<th>PM(_{2.5})</th>
<th>NH(_x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PP_ES_L</td>
<td>Power &amp; district heat plants, existing; coal</td>
<td>38.38</td>
<td>22.86</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DOM</td>
<td>Residential, commercial, services, agriculture, etc.</td>
<td>38.13</td>
<td>15.34</td>
<td>2.71</td>
<td>2.21</td>
<td>0</td>
</tr>
<tr>
<td>IS_RO_CO</td>
<td>Industry: transformation sector, combustion in boilers</td>
<td>4.45</td>
<td>5.02</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IS_RO_CR</td>
<td>Industry: combustion of fossil fuels other than coal</td>
<td>19.52</td>
<td>8.91</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IS_RO_ORE</td>
<td>Industry: combustion of coal in large boilers</td>
<td>0.06</td>
<td>0.11</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IS_RO_S</td>
<td>Industry: combustion of coal in small boilers</td>
<td>0.01</td>
<td>0.03</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IS_RO_PAP</td>
<td>Industry: paper and pulp production</td>
<td>9.32</td>
<td>7.82</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IS_RO_CHM</td>
<td>Industry: chemical industry</td>
<td>3.51</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IS_OC</td>
<td>Industry: Other combustion (used in emission tables)</td>
<td>56.56</td>
<td>12.88</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_CEN</td>
<td>Ind. Process: Cement production</td>
<td>0</td>
<td>37.93</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_LIME</td>
<td>Ind. Process: Lime production</td>
<td>0</td>
<td>5.17</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_COKE</td>
<td>Ind. Process: Coke oven</td>
<td>0</td>
<td>1.92</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_GLASS</td>
<td>Ind. Process: Glass production (flat, blown, container glass)</td>
<td>0</td>
<td>3.57</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_OB</td>
<td>Ind. Process: Other non-ferrous metals prod.</td>
<td>0</td>
<td>36.05</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_PULP</td>
<td>Ind. Process: Paper pulp mills</td>
<td>0</td>
<td>19.22</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_REF</td>
<td>Ind. Process: Crude oil &amp; other products</td>
<td>0</td>
<td>43.77</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_SINT</td>
<td>Ind. Process: Agglomeration plant - sinter</td>
<td>0</td>
<td>6.15</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PB_SUAC</td>
<td>Ind. Process: Sulfuric acid</td>
<td>0</td>
<td>13.23</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TRA_RD_LD4C</td>
<td>Light duty vehicles: cars and small buses</td>
<td>91.02</td>
<td>0</td>
<td>3.04</td>
<td>3.04</td>
<td>0</td>
</tr>
<tr>
<td>TRA_RD_LD4T</td>
<td>Light duty vehicles: light commercial trucks</td>
<td>30.17</td>
<td>0</td>
<td>1.17</td>
<td>1.17</td>
<td>0</td>
</tr>
<tr>
<td>TRA_RD_HDB</td>
<td>Heavy duty vehicles - buses</td>
<td>12.39</td>
<td>0</td>
<td>0.17</td>
<td>0.17</td>
<td>0</td>
</tr>
<tr>
<td>TRA_RD_HDT</td>
<td>Heavy duty vehicles - trucks</td>
<td>76.46</td>
<td>0</td>
<td>0.81</td>
<td>0.81</td>
<td>0</td>
</tr>
<tr>
<td>TRA_RD_NEX</td>
<td>Non-exhaust PM emissions</td>
<td>0</td>
<td>0</td>
<td>11.40</td>
<td>4.69</td>
<td>0</td>
</tr>
<tr>
<td>TRA_OU_AIR</td>
<td>Other transport: air traffic - civil aviation</td>
<td>13.76</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TRA_OU_AGR</td>
<td>Other transport: agriculture and forestry</td>
<td>42.25</td>
<td>0.05</td>
<td>3.15</td>
<td>2.98</td>
<td>0</td>
</tr>
<tr>
<td>TRA_OU_CNS</td>
<td>Other transport: construction and industry</td>
<td>17.76</td>
<td>0.03</td>
<td>1.05</td>
<td>0.99</td>
<td>0</td>
</tr>
<tr>
<td>FCON_OG</td>
<td>Fertilizer use - other N fertilizers</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>37.54</td>
<td>0</td>
</tr>
<tr>
<td>FCON_UREA</td>
<td>Fertilizer use - urea</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>4.04</td>
<td>0</td>
</tr>
<tr>
<td>AGR_ARABLE</td>
<td>Agriculture: Ploughing, tilling, harvesting</td>
<td>0</td>
<td>0</td>
<td>8.06</td>
<td>1.79</td>
<td>0</td>
</tr>
<tr>
<td>AGR_BEEF</td>
<td>Agriculture: Livestock - other cattle</td>
<td>0</td>
<td>0</td>
<td>1.26</td>
<td>0.28</td>
<td>0.32</td>
</tr>
<tr>
<td>AGR_COWS</td>
<td>Agriculture: Livestock - dairy cattle</td>
<td>0</td>
<td>0</td>
<td>0.23</td>
<td>0.05</td>
<td>19.18</td>
</tr>
<tr>
<td>AGR_PIGS</td>
<td>Agriculture: Livestock - other animals (sheep, horses)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>AGR_PIGS</td>
<td>Agriculture: Livestock - pigs</td>
<td>0</td>
<td>0</td>
<td>12.41</td>
<td>2.21</td>
<td>101.9</td>
</tr>
<tr>
<td>AGR_PIGS</td>
<td>Agriculture: Livestock - poultry</td>
<td>0</td>
<td>0</td>
<td>10.77</td>
<td>2.39</td>
<td>32.35</td>
</tr>
<tr>
<td>COWS_3000_MILK</td>
<td>Milk yield over 3000 kg/animal treshold</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PORTUGAL</td>
<td>Portugal</td>
<td>115.7</td>
<td>67.26</td>
<td>91.15</td>
<td>62.35</td>
<td>69.62</td>
</tr>
</tbody>
</table>

In AERIS are shown in Table 10.1, along with the emissions for the 2011 Gothenburg Protocol Revision. Due to the fact that AERIS does not actually consider specific control strategies, but rather uses variation percentages directly introduced by the user, it was assumed that...
the reductions quantified for GAINS are completely valid for AERIS too. It should be noted that some sectors in GAINS “lump” together activities that are considered with more detail in AERIS. Such is the case of road traffic with passenger cars, light-duty and heavy-duty vehicles, for which AERIS distinguishes three driving situations. The gross estimates of GAINS were allocated according to the relative contribution of each of these driving situations to the total emissions of the sector. The resulting emissions for the sectors considered by AERIS are shown in table 10.2. Once the emissions quantified by the GAINS model have been grouped in the relevant sectors of AERIS, the variation percentages \( (p_i) \) can be calculated as the relative percentual difference of these emissions with the baseline scenario of 2007 (table 4.8). These variation percentages will be directly introduced into the AERIS tool so that estimates for the relevant impacts can be obtained in order to continue with the comparison. The numerical value of these variation percentages is shown in table 10.2. The emissions of other countries inside AERIS domain (France, Andorra, Morocco and Algeria) are kept constant for all purposes.

Table 10.2: \( p_i \) of GAINS sectors translated to AERIS - 2011 Gothenburg Protocol Revision.

<table>
<thead>
<tr>
<th>SNAP code</th>
<th>Activity name</th>
<th>( NO_x )</th>
<th>( SO_2 )</th>
<th>( PM_{10} )</th>
<th>( PM_{2.5} )</th>
<th>( NH_3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>010000</td>
<td>Coal - fire power plants ≥ 300MW</td>
<td>-81.2</td>
<td>-96.9</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>020202</td>
<td>Residential plants &lt; 50MW</td>
<td>98.4</td>
<td>23.4</td>
<td>-84.7</td>
<td>-85.6</td>
<td>0</td>
</tr>
<tr>
<td>030000</td>
<td>Combustion in manufacturing</td>
<td>-66.0</td>
<td>-69.3</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>040000</td>
<td>Production processes</td>
<td>0</td>
<td>-50.4</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>070101</td>
<td>Passenger cars - highway driving</td>
<td>-52.2</td>
<td>0</td>
<td>-75.3</td>
<td>-75.3</td>
<td>0</td>
</tr>
<tr>
<td>070103</td>
<td>Passenger cars - urban driving</td>
<td>-52.2</td>
<td>0</td>
<td>-75.3</td>
<td>-75.3</td>
<td>0</td>
</tr>
<tr>
<td>070201</td>
<td>Light - duty vehicles - highway driving</td>
<td>-49.1</td>
<td>0</td>
<td>-76.2</td>
<td>-76.2</td>
<td>0</td>
</tr>
<tr>
<td>070203</td>
<td>Light - duty vehicles - urban driving</td>
<td>-49.0</td>
<td>0</td>
<td>-76.2</td>
<td>-76.2</td>
<td>0</td>
</tr>
<tr>
<td>070301</td>
<td>Heavy - duty vehicles - highway driving</td>
<td>-43.6</td>
<td>0</td>
<td>-95.1</td>
<td>-95.1</td>
<td>0</td>
</tr>
<tr>
<td>070303</td>
<td>Heavy - duty vehicles - urban driving</td>
<td>-43.6</td>
<td>0</td>
<td>-71.2</td>
<td>-71.2</td>
<td>0</td>
</tr>
<tr>
<td>0707/08</td>
<td>Break, tire and road abrasion</td>
<td>0</td>
<td>0</td>
<td>-1.1</td>
<td>-26.0</td>
<td>0</td>
</tr>
<tr>
<td>080500</td>
<td>Airports (air traffic)</td>
<td>70.7</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>080600</td>
<td>Agriculture (machinery)</td>
<td>-65.7</td>
<td>-99.5</td>
<td>-96.7</td>
<td>-96.9</td>
<td>0</td>
</tr>
<tr>
<td>080800</td>
<td>Industry (machinery)</td>
<td>-75.3</td>
<td>-82.3</td>
<td>-93.1</td>
<td>-93.5</td>
<td>0</td>
</tr>
<tr>
<td>100101</td>
<td>Culture w/ fertilizers - permanent crops</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-38.5</td>
</tr>
<tr>
<td>100102</td>
<td>Culture w/ fertilizers - arable land crops</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-38.5</td>
</tr>
<tr>
<td>100500</td>
<td>Other agricultural activities</td>
<td>0</td>
<td>0</td>
<td>97.8</td>
<td>138.1</td>
<td>84.5</td>
</tr>
<tr>
<td>110000</td>
<td>Other sources and sinks</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-92.9</td>
</tr>
<tr>
<td></td>
<td>Portugal</td>
<td>-20.2</td>
<td>-21.0</td>
<td>13.1</td>
<td>-3.8</td>
<td>42.1</td>
</tr>
</tbody>
</table>
10.3 Analyzed magnitudes and impacts

The “goodness-of-fit” between the outputs of AERIS and its GAINS counterpart is different according to the relevant magnitude or impact that is being quantified. Not all the impacts quantified by GAINS are reproduced by AERIS and vice versa, so those with a more independent nature were preferred for comparison. In other words, comparisons between datasets that were derived from a common methodological approach (i.e. GAINS, EMEP UBA, etc.) were also included but handled more carefully. To this respect, the following magnitudes and impacts were quantified with both models and analyzed according to the aforementioned.

- **Accumulated annual depositions per unit of area** of oxidized and reduced nitrogen ($N_{ox}$, $N_{red}$) and sulfur ($S$) - $[mg/m^2 yr]$.
- **Mean annual concentration** of fine particles ($PM_{2.5}$) - $[\mu g/m^3]$.
- **Change in life expectancy per person** due to exposure to fine particles ($PM_{2.5}$) - $[months]$.
- **Average accumulated exceedance** ($AAE$) of critical loads of nutrient nitrogen, $CL_{nut}(N)$, for ecosystems - $[eq/ha yr]$.
- **Exceedance percentage** ($Ex_{AC}$) of sulfur critical loads (acidification), $CL_{max}(S)$, for ecosystems - $(%)$.

In order to consistently carry out this **comparison** of the two models, it must be referred to the **same grid** in line with what has been already introduced in **chapter 6**. In summary, the outputs of AERIS (16 km) were aggregated to the scale of GAINS, which corresponds to that of the EMEP model (50 km). The cell-aggregation procedure was carried out according to what is published in Boulton et al., (2002). The spatial extension of the GAINS outputs was limited to that of the **AERIS modeling domain** by the application of GIS-based techniques.

10.4 Credibility analysis

The results of the comparison are summarized in table 10.3. The first impression that the analysis suggests is the fact that performance is (as with other analyses throughout this work) magnitude-specific. This means that the performance of AERIS is “more similar” to GAINS for some quantities, while for some others this similarity tends to decrease. The performance differences can be seen in table 10.3, where the **mean scores** of both models ($\mu_i$) have been included along with the **K-S statistic** ($p_{K-S}$) and the **Pearson correlation coefficient** ($r$). To this respect, the mean score is defined as the domain-averaged result from individual grid cells and including it is useful for having an idea of the **order of magnitude** that is being given by both models, and is a concept that will be useful later in this chapter for further analysis-refining. The $p_{K-S}$ parameter is a measure of the correspondence between the probabilistic...
Figure 10.1: Spatial distribution of deposition and CDFs according to AERIS and GAINS.
10.4. Credibility analysis

Table 10.3: Resulting comparison indicators between AERIS and GAINS.

<table>
<thead>
<tr>
<th>Magnitude</th>
<th>( \mu_{\text{GAINS}} )</th>
<th>( \mu_{\text{AERIS}} )</th>
<th>( p_{K-S} )</th>
<th>( r )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_{\text{Nox}} ) [mg/m(^2) yr]</td>
<td>217.21</td>
<td>58.64</td>
<td>0.8997</td>
<td>0.4041</td>
</tr>
<tr>
<td>( D_{\text{Nred}} ) [mg/m(^2) yr]</td>
<td>323.80</td>
<td>159.69</td>
<td>0.6391</td>
<td>0.5382</td>
</tr>
<tr>
<td>( D_{S} ) [mg/m(^2) yr]</td>
<td>223.62</td>
<td>109.13</td>
<td>0.5063</td>
<td>0.2504</td>
</tr>
<tr>
<td>( C_{P&gt;M2.5} ) [(\mu g/\text{m}^3)]</td>
<td>6.27</td>
<td>5.87</td>
<td>0.3910</td>
<td>0.5350</td>
</tr>
<tr>
<td>( \Delta e_c ) [months]</td>
<td>2.03</td>
<td>1.06</td>
<td>0.8145</td>
<td>0.5821</td>
</tr>
<tr>
<td>( AAE ) [eq/ha yr]</td>
<td>145.75</td>
<td>17.54</td>
<td>0.4838</td>
<td>0.2689</td>
</tr>
<tr>
<td>( E_{\text{AC}} ) [%]</td>
<td>16.92</td>
<td>15.81</td>
<td>0.4291</td>
<td>0.3283</td>
</tr>
</tbody>
</table>

The analysis of the \( PM_{2.5} \)-related magnitudes, namely the mean annual concentration and the change in life expectancy per person is also likely of being described in terms of the indicators of table 10.3 and by the spatial profiles in figure 10.2. Unlike the deposition estimates, the two magnitudes under analysis have similar mean scores, a fact that is further
Figure 10.2: $PM_{2.5}$-related magnitude profiles and CDFs according to AERIS and GAINS.
10.4. Credibility analysis

confirmed by the maps in which a greater variety of values can be observed, although not very dramatic in the case of GAINS. The displacement in the CDF curves of GAINS against those of AERIS is not as considerable as in the past case, but again no zero values are present in the GAINS distribution and this fact could be directly related to the concentration values of $PM_{2.5}$ that GAINS estimate for the regions of North Africa that are present in the domain. It is worth noting that the correspondence between models is higher for the mean annual concentration than for the change in life expectancy. This fact might be attributed to the use of external methodologies and datasets (i.e. epidemiologic studies, population counts, etc.) whose application procedure might have affected the quality of the estimates. To this respect, it can be said that the mean annual concentration of $PM_{2.5}$ is perhaps the output that allows a more straightforward comparison since it is not affected by the health impact computation methodology applied. As a result, the fact that the mean scores are somehow similar endows AERIS with credibility whenever GAINS is taken as a reference. To a lesser extent, the loss in life expectancy predicted by AERIS can also be taken as a comparable indicator with GAINS.

In the case of the probabilistic distributions, the highest similarities among the complete set of analyzed magnitudes are encountered for life expectancy losses, while the $p_K - S$ for the mean concentrations is sensitively lower. This fact is heavily determined by the presence of values below $2 \mu g/m^3$ yielded by AERIS which displace the CDF function when compared to its GAINS counterpart. Additionally, GAINS does not show a sensitivity to $PM$ hotspots such as cities, producing a dataset with a maximum concentration of approximately $10 \mu g/m^3$. Correlation coefficients are approximately $r \approx 0.5$ in both cases, which are basically a consequence of model formulation criteria and the use of different datasets. This fact is of special importance when considering the type of policy recommendations that could be derived from the use of either model, something that is very relevant for GAINS whose general scope is European. Additionally, systematic errors in the quantification of life expectancy variables might be present as a result of the different approaches used in the quantification of such variables (Vedrenne et al., 2014).

Finally, the analysis of ecosystem protection impacts such as the accumulated average exceedances ($AAE$) for nutrient nitrogen and the exceedance percentage of acidification critical loads (sulfur) can be addressed with the indicators shown in table 10.3 and by the spatial profiles in figure 10.3. In the case of the accumulated average exceedance of nutrient nitrogen, the difference between AERIS and GAINS is noticeable, as evidenced by the departure observed between the two mean scores. When examining the spatial profiles, there is a wide variety of values and not a uniform spatial reproduction is whatsoever observed. A review of the CDF curves of GAINS and AERIS shows two completely different probabilistic distributions, with a wider range of values in the case of GAINS. The before mentioned issues are observed in a more dramatic way when analyzing the exceedance of acidification critical loads. Totally different spatial profiles are contradicted with a purported similarity in the mean scores and a higher statistic correspondence as evidenced by the Pearson correlation coefficient. This behavior is a direct consequence of the distributions’ statistical mode, which equals zero in
Figure 10.3: Ecosystem protection magnitude profiles and CDFs according to AERIS and GAINS.
both cases and lowers the value of the means. The disparity observed in the quantification of these impacts by the two IAMs questions the credibility of the outputs of AERIS when considering GAINS as the sole reference. Moreover, the difference in the magnitude of the obtained results from either model might derive different policy recommendations.

Taking the aforementioned into consideration, it is not possible to provide an incontestable verdict on the credibility of AERIS defined as the similarity in performance when compared to GAINS. It has already been anticipated that due to model formulation issues as well as considered scales, a full correspondence was not expected nor desired as it would certainly be artificial for a model that has been developed independently from the GAINS framework. The numerical analysis above did not seek to find the highest performance indicators, but to explore the degree of correspondence between orders of magnitudes and to address it under a more rigorous perspective than a mere comparison “at a glance”. In the author’s opinion, and always under the condition that GAINS is an uncontestable reference, AERIS is credible because its estimates reproduce those of GAINS reasonably well after considering that two independent models were analyzed. The observed discrepancy between the two models can be assumed as a “model departure cost”, and strongly hints on the limitations that the present model comparison process has associated.

10.5 Limitations of the credibility approach

GAINS has forged itself a reputation of “gold-standard” in air quality integrated assessment due to the intense collaboration that exists between IIASA and stakeholders throughout Europe. Its early appearance in the scene of negotiations and policy making made it a valuable tool that is in constant improvement. However, GAINS is naturally subject to modeling limitations and it has important degrees of associated uncertainty. More importantly, it has been conceived to address the European scale within a continental (UNECE) framework which is certainly not the case of AERIS, which stemmed from modeling activities within the Spanish context. This constitutes precisely the first limitation of the credibility approach: due to the difference in scales, a scale-adaptation process had to be carried out with the outputs of AERIS, with the associated quality loss that comes with spatial interpolation procedures. This issue launches the questions, “up to what extent is the low resolution cell (GAINS) representative of at least one of the high resolution cells (AERIS) contained within?” and “why is a mean spatial interpolation approach adequate for describing impacts produced at an eminently local scale (i.e. cities, vicinities of large point sources, etc.)?” The scale issue is by no means a minor aspect that limits the present credibility analysis. Scale is intimately related with the quality of the essential and ancillary data, such as emission inventories, GIS covers (population, forests, soils, critical loads, etc.) and of course, with the performance of the AQM proper. Traveling from a finer to a coarser scale requires much more than a simple interpolation: it must involve the harmonization of data sources, modeling and validation approaches across scales (Vedrenne et al., 2012). In response to the need for having national-scale IAMs, GAINS has been adapted to national versions such as GAINS-Italy or GAINS-NL (Netherlands). Other
national, independent examples such as UKIAM or SONOX exist in Europe and along with AERIS, constitute a relevant set of assessment tools at the national scale that are independent from the European GAINS approach. This is especially true for AERIS, due to the fact that it incorporates more specific data and methods that are better suited for the peculiarities of the Iberian Peninsula.

An additional limitation that has already been addressed in this chapter constitutes the formulation criteria of each of the parent AQM that produced the IAMs. This is a considerable limitation that must not be overlooked, because it affects critical points that ultimately determine the quality of the entire modeling activity and that question up to what extent such elements have a dire influence on the credibility of the results. Elements such as meteorological parameterizations, aerosol mechanisms, chemical speciation profiles ($VOCs$, $PM$, etc.), boundary conditions or grid resolution heavily condition model performance (Appel et al., 2012).

Since AERIS does not rely on the same modeling characteristics than GAINS, it is unrealistic to expect a full-correspondence or to undertake a rigorous model intercomparison exercise. In the same line, the different criteria for grouping emissions in AERIS and GAINS required the use of apportionment techniques for some emission sectors that do not correspond directly with the SNAP sectors considered by AERIS. The geographic situation of the emission sectors in the modeling domain is also different, introducing a further source of modeling discrepancy between GAINS and AERIS. The before mentioned aspects can be considered the most important and noticeable limitations of the credibility analysis approach through the statistical and numerical comparison of datasets and its probabilistic distributions. As it has already been highlighted, models have been developed independently so there might be other sources that discourage considering such an exercise as an absolute source of modeling reliability. Despite the inherent limitations, the lack of comparability that exists between models calls for the need of comparing outputs against independent datasets such as observations or field measurements.

10.6 Final remarks on the credibility of AERIS

In the previous sections, it has been made clear that credibility is usually attained by the means of model evaluation. However, building credibility is not a “once-and-for-all” activity, but an on-going process to check for model compatibility to current evidence (Alexandrov et al., 2011). To this respect, building credibility requires the existence of a community of modeling groups within the context of interest of AERIS. This also requires period meetings of the modeling groups for the specific geographical contexts as well as reporting obligations and dissemination activities.
11 Conclusions

At the beginning of this work (chapter 1), a number of objectives were formulated in order to evaluate the initial intention of building an air quality Integrated Assessment Model. The following chapter will review these objectives and contrast them with the fulfilled goals that have been presented throughout this work. This section will also encompass any discussion on the complete methodological framework that allowed constructing and having AERIS available in its current state.

The principal objective that was formulated was having a reliable tool for air quality evaluation which is available for real-time policy support needed by policy makers at the relevant scales (i.e. national, regional...). Under the specific context of this work, and following the methodology that is here presented, it can be said that AERIS is useful for two reasons. First, at this time, AERIS is available as a fully-functional integrated assessment model which is able to provide consistent results on a number of interesting magnitudes that are very appropriate under air quality negotiation frameworks. Second, the outputs produced by AERIS have undergone several validation procedures under rigorous model benchmarking criteria, highlighting the similarities in performance when compared to its parent air quality model. Despite all these, AERIS has not been used in situ by policy makers or stakeholders, so it cannot be said with full confidence that the produced results meet the needs and requirements of administrations or that they are useful to a wide number of stakeholders. The nature in which results are produced by the model is a consequence of the modeling experience of the author in air quality-related research and in his impressions from the contact with policy makers during this period. Once the model is passed on to stakeholders and used as a focal point for analysis, further confidence on the fitness of the results will be gained.

It is important to highlight that the basic objective of the present work consisted in parameterizing the air quality model, which consists in a modeling system composed by the WRF, SMOKE and CMAQ models for a baseline scenario of 2007. The description of the emission-concentration link was set as the minimum milestone to achieve because it is essentially, a
Chapter 11. Conclusions

highly limiting and resource-dependent stage in a full air quality evaluation. This resource-
dependency is strictly related with the available hardware for conducting air quality simu-
lations with complex (i.e. Eulerian) air quality models, a fact that is proportionally related
to long computing times that come with simulations on high-resolution domains. Due to
the analysis tool nature of integrated assessment, it is unfeasible to conduct immediate or
short screening exercises without having a reasonable parameterization of the emission-
concentration link. As it has already been shown, this has been successfully achieved and
validated through the demonstration of good statistical correspondence levels among the
predictions of AERIS and the outputs of the full air quality model.

It should be widely credited that the determination of a modeling methodology for the con-
struction of AERIS, and especially of the so-called air quality system stemmed from numerous
works previously tested and published. After special modifications, the methodology was
adapted to the particularities of the air quality model and to the specific needs that AERIS
should cover. This modeling methodology has been presented in a transparent way in this
work, aiming to be analyzed by interested readers and, if valuable, disseminated. Anyway, the
results produced by this methodology have been validated against the air quality model proper
as well as independent observations, yielding good results in every case. The observed good
statistical correspondence endowed the model with the minimum level of confidence that
should be mandatory for an integrated assessment model derived from a conventional air
quality model: that it is able to adequately reproduce its outputs.

The elucidation of a versatile methodological framework for AERIS (based on a compre-
hensive software structure in MATLAB ®) allowed extending its modeling capabilities to the
quantification of other magnitudes and impacts, which are very relevant in order to deliver
a fully-operative integrated assessment model. In a reasonable period of time, the results of
AERIS were combined with different modeling assumptions and methods in order to quan-
tify atmospheric deposition processes as well as impacts on ecosystems, soils, vegetation,
crops, and human health. The inclusion of these modules was certainly useful but not abso-
lutely necessary, since results referring to each of the before mentioned magnitudes can be
directly derived from the outputs of the air quality model outside the modeling framework of
AERIS. The decision of including these impacts certainly strengthened the modeling skills and
predictive value of AERIS, as well as increasing its “fitness-for-purpose” which is the extended
use of its capabilities within a regional (Spanish - Iberian) context. To this respect, the majority
of the specific objectives has been fulfilled. In the author’s opinion, the module extension of
AERIS is not as valuable as the fact that a new methodology for calculating magnitudes and
quantifying impacts has been distilled from more robust frameworks such as GAINS. Doing so
allowed further comparisons of the order of magnitude between the estimates of AERIS and
those of the “high-profile” integrated assessment models, in this case the GAINS model. The
ultimate conclusions that were reached from such an exercise were that the model is indeed
able to produce similar (yet not identical) results for some indicators, while in other cases the
results were different. Such a comparison approach, based not only on qualitative judgements but on numeric evaluations, might increase the perception of reliability among potential stakeholders but it should also be taken into account that the choice of a particular model underpinned by specific data and assumptions may have a direct impact in the delivery of policy recommendations. However, this is an essential step towards successfully legitimating model usage among end users and especially highlighting it as a valuable alternative to GAINS for Spain and Portugal. It was also acknowledged that there are sufficient limitations in this evaluation approach, which in turn calls for the need of relying on observations and field measurements for a complete validation.

The main motivation for the creation of AERIS was an existing knowledge gap on integrated assessment for the particular conditions of Spain. To this respect this study is welcome since, apart from describing the basic methodologies that ultimately produced the model, it also provides the first operational evaluation of a model oriented to integrated assessment for the particular conditions of Spain and with a high resolution level (16 km horizontal resolution). In a more practical perspective, AERIS was designed to be a reliable yet simple screening tool that would provide decision and policy making support for different “what-if” scenarios at a low computing cost. Special emphasis has been made throughout this work in the fact that AERIS has been created under a policy-driven framework and by no means should be considered as a substitute of the ordinary air quality model. It stands clear that AERIS is directed to decision makers in the fashion of “concise, scientifically-supported results” while traditional air quality models, although undoubtedly useful for environmental management, usually follow a science-driven trend that limits its use among non-scientific end users.

In a more general level, AERIS should be valued in terms of its descriptive capability of the interactions between pollutants in the atmosphere, and the complex interplay between emission controls across pollutants and sources. In line with other integrated assessment models (i.e. GAINS), it should be helpful for designing common approaches to obtain environmental benefits in the modeling domain. Readers should notice that AERIS, rather than a product, is itself an integrated assessment modeling framework for the special characteristics of the Iberian Peninsula (Spain and Portugal). As of now, it is susceptible of being improved in different ways and to include new modules. However, it can be said that it has emerged as a new screening tool aimed to provide answers to policymakers that would eventually signify improvements in life quality conditions.

11.1 Future research lines

As it has already been stated, AERIS is an ongoing project that is under constant improvement and revision. As this point, the limitations of the model have been identified and as a consequence, the following future research lines are proposed. The exploration of such future
research lines will endow the model with an additional degree of confidence in the produced results and could increase its diagnostic capabilities.

- **Atmospheric dispersion module.** Future research should be conducted in producing different baseline scenarios (other than the 2007 baseline) which could reflect current abatement techniques and that could be used for extending the assessment capabilities of AERIS beyond 2020. The description of new baseline scenarios should necessarily imply reflecting variations due to meteorology in the formulation of the SRMs.

- **Deposition module.** In order to have a wider picture of the deposition assessment capabilities of AERIS, further investigation on the formulation of atmospheric deposition processes considered by CMAQ and the EMEP model should be carried out. An understanding of the source and nature of the variations between these two models could hint on the fitness of their results in an accurate description of the atmospheric deposition in the Iberian Peninsula.

- **Impacts on ecosystems module.** This module could benefit from the inclusion of a bottom-up localization database for ecosystems, as well as new land covers. New critical levels for forests should be included as an update in the model as soon as they become available. Furthermore, a closer integration of variables estimated by the meteorological model of the AQM (WRF) such as humidity, precipitation and soil temperature could be made in order to increase the resolution of the critical loads cover for soils.

- **Crops & vegetation impacts module.** Further research is needed in extending the capabilities of AERIS to include flux-based evaluation methods, as well as other plant species (crops) and forests. Linkages with the existence vegetation impact estimation framework of the Environmental Modelling Laboratory should be reflected in the module's formulation.

- **Health impacts module.** The current formulation of the module could benefit from the update of new population base data that characterise in a more reliable way the current distribution of age groups, as opposed to the current data that only consider a time span of 10 years from 1990 to 2000. An interesting research line that could stem from the current formulation of the health impacts assessment module is the inclusion of functions from BenMAP, and in general to extend the impact estimation methodology to consider endpoints.

- **Credibility analysis of AERIS.** In order to increase confidence in the fitness of the estimates of AERIS for policy delivery in Spain, future investigation should aim to include observations and field-measurements for comparison.

An almost-mandatory line that should always be open is that of **maintenance routines, bug checks** and **programming-structure optimization.** Although strictly outside the air quality
modeling activities, including an **optimization module** of **abatement costs** in order to produce **cost-effective** solutions to environmental burdens is very recommendable to achieve full analytical capabilities with AERIS. A reasonable starting point for this could be done in collaboration with IIASA under the GAINS framework for this purposes. The current trend calls for moving **environmental models** from **software** to **webware**, aiming to make them widely available through web browsers. This can certainly be applied to AERIS, as soon as the model gains visibility and recognition on behalf of the community of potential end users. Increasing the recognition of AERIS obviously needs involving as many types of stakeholders as possible, particularly those with a strong vinculation on policy making processes.

The author is firmly convinced that modeling requires learning from the experience of others, as it is an excellent and efficient educational approach that ultimately yields interesting alternatives to the current state of science. To this respect, an essential activity that needs to be constantly performed is the **dissemination** of the modeling framework and methodologies, as well as the results of the model. Apart from helping improve the actual state of knowledge, it helps to increase the visibility of the model as the (currently) only high resolution integrated assessment model that allows addressing the air quality problem in the Iberian Peninsula under an holistic approach.
12 Dissemination

12.1 Publications about AERIS


12.2 Other publications


12.3 Presentations and Conferences


• 09/05/2013 Oral Presentation. 15th HARMO Conference, Madrid (Spain). Vedrenne, M., Borge, R., Lumbreras, J., de la Paz, D., Rodríguez, M.E. Development and implementation of an air quality integrated assessment model for the Iberian Peninsula.

• 08/05/2013 Poster. 15th HARMO Conference, Madrid (Spain). Borge, R., Lumbreras, J., Pérez, J., de la Paz, D., Vedrenne, M., Rodríguez, M.E. Modelling activities for the development of air quality plans in Madrid (Spain).


• 24/06/2012 Poster. ANQUE International Congress of Chemical Engineering, Seville (Spain). Vedrenne, M., Borge, R., Lumbreras, J., Rodríguez, M.E. Current developments
on air quality evaluations for Spain under an Integrated Assessment Modeling approach.

13 Credits and Support

13.1 Model Credits

- **Community Modeling & Analysis System (CMAS)**. Provided and supported the SMOKE and CMAQ models.

- **Coordination Centre for Effects (CCE)**. Provided and supported the VSD model.

- **International Institute for Applied Systems Analysis (IIASA)**. Provided access to the GAINS model and its databases.

13.2 Data Credits

- **Agência Portuguesa do Ambiente (APA)**. Provided the 2007 National Emissions Inventory of Portugal (PNEI).

- **Coordination Centre for Effects (CCE)**. Provided the documentation on the impacts on ecosystems and soils.

- **European Environment Agency (EEA)**. Provided access to the AirBase monitoring locations database for validation purposes and the CORINE Land Cover database.

- **European Monitoring and Evaluation Programme (EMEP)**. Provided the atmospheric deposition outputs for contrast purposes.

- **Global Agricultural Land Use Data for Climate Change Analysis (GAT)**. Provided crop-specific geospatial information.

- **International Institute for Applied Systems Analysis (IIASA)**. Provided the documentation on the health impacts module.

- **Joint Research Centre - European Comission (JRC-EC)**. Provided access to the EUSOIL, MEUSIS and SPADE soil databases.
Chapter 13. Credits and Support

- **Ministerio de Agricultura, Alimentación y Medio Ambiente (MAGRAMA)**. Previously provided the 2007 National Emissions Inventory of Spain (SNEI). Currently makes the 2011 National Emissions Inventory available.

- **Socioeconomic Data and Applications Center (SEDAC)**. Provided the population counts of Spain, Portugal, Andorra and France.

- **UNEP-Sioux Falls Global Resource Information Database (GRID)**. Provided the population counts of Morocco and Algeria.


13.3 Support

- **Chemical and Environmental Engineering Department**. Provided material and economic support for the development of this doctoral dissertation (2011-2013).

- **Consejo Nacional de Ciencia y Tecnología - México (CONACYT)**. Provided economic support for the development of this doctoral dissertation (2012-2013).
14 Acronyms and Symbols

14.1 Acronyms

- \textit{ACM2} - Asymmetric global mass-conserving scheme.
- \textit{AERIS} - Atmospheric Evaluation and Research Integrated system for Spain.
- \textit{AQ} - Air Quality.
- \textit{AQM/s} - Air Quality Model (-s).
- \textit{ARW} - Advanced Research Weather research and forecast model.
- \textit{BS} - Baseline Scenario.
- \textit{CAFE} - Clean Air For Europe programme.
- \textit{CB-05} - Carbon Bond 05 gas phase chemical mechanism.
- \textit{CCE} - Coordination Centre for Effects.
- \textit{CDF/s} - Cumulative Distribution Function (-s).
- \textit{CLRTAP} - Convention on Long-Range Transboundary Air Pollution.
- \textit{CMAQ} - Community Multiscale Air Quality model.
- \textit{CORINAIR} - Core Inventory of Air emissions.
- \textit{CORINE} - Coordination of Information on the Environment.
- \textit{CRF/s} - Concentration-Response Function (-s).
- \textit{CTM} - Chemical Transport Model.
Chapter 14. Acronyms and Symbols

- CSV - Comma-Separated Value.
- D1 - European domain with 48 km resolution.
- D2 - Iberian domain with 16 km resolution.
- E-R - Exposure-Response function.
- EBI - Euler Backward Iterative solver.
- EIONET - European Environment Information and Observation Network.
- EMEP - European Monitoring and Evaluation Programme.
- ESM - Earths System Model.
- EU - European Union.
- EUSOIL - European soil database.
- GAINS - Greenhouse gas and air pollution Interactions and synergies model.
- GB - Gigabyte.
- GEIA - Global Emissions Inventory Activity.
- GeoTIFF - Geographical Tagged Image File Format.
- GFDL - Geophysical Fluid Dynamics Laboratory.
- GIS - Geographic Information System.
- GNU - “GNU’ s not UNIX”.
- GPW - Gridded Population of the World project.
- GUI - Graphical User Interface.
- HS - Hypothetic Scenario.
- I/O API - Input/Output Applications Programming Interface.
- IA - Integrated Assessment.
- IAM - Integrated Assessment Model (-ing).
- IIASA - International Institute for Applied Systems Analysis.
- JRC - Joint Research Centre.
- K-S - Kolmogorov-Smirnov probability test.
- LPG - Liquefied Petroleum Gas.
14.1. Acronyms

- **MARM** - Ministerio de Medio Ambiente, Medio Rural y Marino.
- **MB** - Megabyte.
- **MCIP** - Meteorology-Chemistry Interface Processor.
- **MEUSIS** - Multiscale European Soil Information System.
- **MPI** - Message Passing Interface paradigm library.
- **MSC-W** - Meteorological Synthesising Centre West.
- **NASA** - National Aeronautics and Space Administration.
- **NEC** - National Emissions Ceilings.
- **NetCDF** - Network Common Data Form.
- **NUTS** - Nomenclature of Territorial Units for Statistics.
- **PC** - Personal Computer.
- **PNEI** - Portuguese National Emissions Inventory.
- **R+D** - Research and Development.
- **RAINS** - Regional Air Pollution Information and Simulation.
- **SEP** - Spain's Emission Projection model.
- **SMB** - Simple Mass Balance.
- **SMOKE** - Sparse Matrix Operator Kernel for Emissions.
- **SNAP** - Selected Nomenclature for sources of Air Pollution.
- **SNEI** - Spanish National Emissions Inventory.
- **SPADE** - Soil Profile Analytical Database of Europe of measured parameters.
- **SRM/s** - Source-Receptor Matrix (-ces).
- **TB** - Terabyte.
- **UBA** - Umweltbundesamt.
- **UN** - United Nations.
- **UNECE** - United Nations Economic Commission for Europe.
- **UNEP** - United Nations Environment Programme.
- **UPM** - Universidad Politécnica de Madrid.
• **USEPA** - United States Environmental Protection Agency.

• **VSD** - Very Simple Dynamic model.

• **WHO** - World Health Organization.

• **WRF** - Weather Research and Forecast model.

• **WSM6** - WRF Single-Moment 6-class microphysics scheme.

• **YU** - Yonsei University.

### 14.2 Chemical Species

• **CO** - carbon monoxide.

• **N** - deposited nitrogen.

• **N_{ox}** - deposited oxidized nitrogen.

• **N_{red}** - deposited reduced nitrogen.

• **NH\textsubscript{3}** - ammonia.

• **NH\textsubscript{4}NO\textsubscript{3}** - ammonium nitrate.

• **(NH\textsubscript{4})\textsubscript{2}SO\textsubscript{4}** - ammonium sulfate.

• **NO** - nitrogen monoxide.

• **NO\textsubscript{x}** - nitrogen oxides.

• **NO\textsubscript{2}** - nitrogen dioxide.

• **PAN** - peroxyacetyl nitrate.

• **PM** - particulate matter.

• **PM\textsubscript{10}** - particles with an aerodynamic diameter \( \leq 10\mu m \).

• **PM\textsubscript{2.5}** - particles with an aerodynamic diameter \( \leq 2.5\mu m \).

• **S** - deposited sulfur.

• **SO\textsubscript{2}** - sulfur dioxide.

• **SVOC** - semi-volatile organic compounds.

• **VOC** - volatile organic compounds.
14.3 Symbols

- \( a \) - proportionality constant of the \( pH \) - \( pAl \) relationship.

- \( a_{Ind,i} \) - regression coefficient for policy indicator calculation.

- \( A_{h,i} \) - harvested area of crop \( i \).

- \( AOT_{40} \) - accumulated dose over a threshold of 40 ppb.

- \( b_{Ind,i} \) - regression coefficient for policy indicator calculation.

- \( BC_{we} \) - weathering rate of base cations.

- \( c \) - any age cohort considered by AERIS.

- \( c_{Ind,i} \) - regression coefficient for policy indicator calculation.

- \( Ca_{we} \) - weathering rate of calcium.

- \( [C_i]_{n \times m} \) - concentration profile for altered scenario of pollutant \( i \).

- \( [C_i]_{n \times m}^0 \) - concentration profile for baseline scenario of pollutant \( i \).

- \( [C_{i,k}]_{n \times m}^0 \) - concentration profile for baseline scenario of pollutant \( i \) for \( k \) region.

- \( C_{\ell,i} \) - critical level of pollutant \( i \).

- \( C_{pool} \) - initial amount of carbon in top layer per unit of area.

- \( CEC \) - average potential cation exchange capacity of the soil.

- \( CL_u \) - critical load of impacting specie \( u \).

- \( CL_{max}(N) \) - maximum acidification critical load for nitrogen.

- \( CL_{max}(S) \) - maximum acidification critical load for sulfur.

- \( CL_{min}(N) \) - minimum acidification critical load for nitrogen.

- \( CL_{nut}(N) \) - critical load for nutrient nitrogen.

- \( CN_i \) - initial carbon-nitrogen ratio in topsoil.

- \( CP_i \) - production of crop \( i \).

- \( CPL_i \) - production loss of crop \( i \).

- \( Deaths_c \) - number of deaths of cohort \( c \).

- \( Deaths_{Nat} \) - national baseline mortality.

- \( D_v \) - hourly deposition per unit of area of deposited specie \( v \).
• $D_{acc}^v$ - annual accumulated deposition per unit of area of deposited specie $v$.
• $D_{h,DRYDEP}$ - hourly deposition per unit of area of deposited specie $v$ in the DRYDEP file.
• $D_{h,WETDEP}$ - hourly deposition per unit of area of deposited specie $v$ in the WETDEP file.
• $DALY$ - disability adjusted life years.
• $e_c$ - remaining life expectancy.
• $E_{BC}$ - Initial base cations saturation.
• $E_i$ - emissions of pollutant $i$.
• $E_{i,BS}$ - emissions of pollutant $i$ in the baseline scenario.
• $E_{i,RP11}$ - emissions of pollutant $i$ in the 2011 real policy scenario.
• $E_{i,RP14}$ - emissions of pollutant $i$ in the 2014 real policy scenario.
• $[E_{i,j}]_{n \times m}$ - altered scenario of emissions of pollutant $i$ and sector $j$.
• $[E_{i,j}]_{0}^{0}$ - baseline scenario of emissions of pollutant $i$ and sector $j$.
• $E_{X,v}$ - exceedance of critical load of specie $v$.
• $E_{XCL,i}$ - exceedance of critical level of pollutant $i$.
• $f_c$ - age-apportionment factor for cohort $c$.
• $[G_{i,j}]_{n \times m}$ - source-receptor matrix of pollutant $i$ and sector $j$.
• $[G_{i}^{PM}]_{n \times m}$ - source-receptor matrix for contribution of pollutant $i$ to $PM$ mass.
• $[G_{O3}^{O3}]_{n \times m}$ - source-receptor matrix for interaction between $NO_x$ and $VOC$ for $O_3$.
• $i$ - any pollutant considered by AERIS.
• $[Ind_{i}]_{n \times m}$ - concentration profile of pollutant $i$ expressed as a policy indicator.
• $j$ - any SNAP sector considered by AERIS.
• $J$ - total SNAP sectors considered by AERIS for pollutant $i$.
• $k$ - any territorial unit considered by AERIS.
• $K$ - total territorial units considered by AERIS.
• $K_{Al}$ - aluminium equilibrium constant.
• $K_{AlBC}$ - aluminium - base cations selectivity constant.
• $K_{HBC}$ - acid - base cations selectivity constant.
• $K_{we}$ - weathering rate of potassium.
• $I_c$ - survival function of cohort $c$.
• $m$ - number of columns of the modeled domain.
• $\overline{M}$ - mean of the modeled data obtained from AERIS.
• $Mg_{we}$ - weathering rate of magnesium.
• $MB$ - mean bias.
• $ME$ - mean error.
• $M_i$ - modeled data obtained from AERIS.
• $n$ - number of rows of the modeled domain.
• $N$ - number of cells in the modeled domain.
• $N_{i,\text{min}}$ - minimum rate of immobilized nitrogen.
• $NMB$ - normalized mean bias.
• $NME$ - normalized mean error.
• $\overline{O}_3$ - population-weighted concentration of $O_3$.
• $p_{CO_2}$ - carbon dioxide pressure in the soil solution.
• $p_{i,j}$ - percentual variation of emissions of pollutant $i$ and sector $j$.
• $p_{K-S}$ - p-value of the Kolmogorov-Smirnov test (K-S statistic).
• $p_{\text{surplus}}$ - precipitation surplus.
• $pAl$ - power of aluminium.
• $pH$ - power of hydrogen.
• $\overline{P}$ - mean of the predictions obtained from the air quality model.
• $P_i$ - predictions obtained from the air quality model.
• $Pop_j$ - population count in cell $j$.
• $PAF$ - population-attributable fraction.
• $q$ - temporal transformation coefficient.
• $[Q_{\text{Dep}}]$ - concentration-transformation deposition matrix.
• $r$ - Pearson correlation coefficient.
Chapter 14. Acronyms and Symbols

- $r_{01}$ - Pearson correlation coefficient for January regressions.
- $r_{08}$ - Pearson correlation coefficient for August regressions.
- $R$ - proportionality constant.
- $RR$ - relative risk.
- $RR_{O3}$ - relative risk for 1% increase in daily mortality per ppb of $8-h$ max. $O_3$ per day.
- $RY_i$ - relative yield of crop $i$.
- $S_i$ - any sector used in the additivity test.
- $SOMO_{35}$ - sum over means of 35 ppb.
- $t$ - additivity test compliance threshold.
- $T_{soil}$ - average soil temperature.
- $X_{AERIS}$ - mean error of AERIS in additivity test.
- $X_{AQM}$ - mean error of AQM in additivity test.
- $WR$ - weathering rate of a non-calcareous soil.
- $YOLL$ - total amount of life years lost.
- $z_{soil}$ - depth of a non-calcareous soil.
- $z_{top}$ - thickness of the soil top layer.

14.4 Greek Symbols

- $\alpha$ - statistical confidence.
- $\beta$ - health impacts proportionality coefficient.
- $\bar{\bar{\gamma}}$ - mean of the intercept matrix.
- $\bar{\gamma}_{01}$ - mean of the intercept matrix for January regressions.
- $\bar{\gamma}_{08}$ - mean of the intercept matrix for August regressions.
- $[\gamma_{i,j}]$ - intercept matrix of pollutant $i$ and sector $j$.
- $\Delta e_c$ - change in statistical life expectancy for cohort $c$.
- $\theta$ - volumetric water content of the soil.
- $\mu_{AERIS}$ - mean score for the AERIS model (Kolmogorov-Smirnov).
14.4. Greek Symbols

- $\mu_{a,b}/\mu_{z,z-c-s}$ - life table mortality rates.
- $\mu_{\text{GAINS}}$ - mean score of the GAINS model (Kolmogorov-Smirnov).
- $\mu_{l}$ - mean score of the Kolmogorov-Smirnov test.
- $\rho_{\text{top}}$ - bulk density of the soil top layer.
- $v$ - any of the deposited species considered by AERIS.
Appendices

AERIS: a general description

Software structure

The primary user interface for AERIS is a graphical user interface designed and programmed in MATLAB®. A key factor for configuring and running AERIS is understanding the directory structure used for reading input files, producing graphical maps and writing output files. It is also essential that users know where to find the run scripts, the graphical configuration files, the SRMs and other files that might be configured for running AERIS at the entire convenience of the users. The AERIS directory structure is the organization of Windows® directories and subdirectories (namely “folders”) that are cross-linked and that allow executing the model. AERIS has been formulated to be as simple as possible, so unlike many environmental models, it does not rely on environment variables. By default, AERIS is provided as a single directory called AERIS. It does not require any installation nor compilation provided that MATLAB® is already installed in the PC. It is up to the user to decide the location or “path” in which this directory will be placed. This path cannot be prescribed to the user because each Windows® user has a different computer and disk names. It is recommendable that the AERIS folder is placed at a simple path, close to the bottom of a directory structure. Using a short directory name will limit the overall directory lengths for some of the subdirectories deeper in the structure of AERIS.

The directory structure of AERIS has a maximum number of three levels, as shown in figure A.1. Within the AERIS upper directory, the user will find 14 files, with 7 different names (AERIS, NH3, NO2, O3, PM10, PM25, SO2) and 2 file extensions (*.fig, *.m). These files constitute the basic programming of AERIS and its GUI. As it is obvious, the name of each of the files makes reference to the given pollutant, while the name AERIS refers to the main menu of the IAM. Files with a *.fig extension include the information of the layout and design of respective windows of AERIS, while those files with a *.m extension are typical MATLAB® code files, which contain the programming routines that allow quantifying the different magnitudes
that AERIS estimates. Any modifications on the code of AERIS should be applied only to these files. The following directories are also found in the main AERIS directory.

**Base directory**

The Base directory contains a series of files that define the initial modeling state that is required before any calculations are carried out in AERIS. It defines the baseline scenario in terms of the different concentration profiles, as well as the regional baseline scenarios for the territorial divisions of Spain that are considered by the model (autonomous communities). These files also allow drawing political divisions and locating emission sources in the modeling domain. In a newly-installed copy of AERIS, the user should count 17 files with a *.csv extension: Base-01, Base-08, Base-AN, Continente, Europa, X-Regional-01,-08, Regions, and Sources, where X is each of the considered pollutants. Each of these files, as with most of the files included in the AERIS directory are presented as arrays of numbers in columns that can be easily opened in a Microsoft Excel @spreadsheet. The baseline scenario can be changed by modifying the first three files according to the modeling methodology of AERIS. The user should not tamper with the rest of the files.

**Exchange directory**

The Exchange directory is destined to contain the intermediate files that are generated during screening exercises in AERIS. When conducting a complete analysis for each of the pollutants,
Appendix A. Appendices

this directory should contain files that allow quantifying the contribution of precursor gases
to the different sizes of particulate matter and the contribution of nitrogen oxides (\(NO_x\)) to

tropospheric ozone (\(O_3\)). Intermediate files are fully accessible to the user through the use of a

* .csv extension. In a newly-installed version of AERIS, this directory should be empty.

Inputs directory

The Inputs directory should be used for placing the files that will allow AERIS to conduct

the screening exercises that are of relevant under a policymaking point of view. Two files are

essential for running the model and should be provided by the user: Emissions.csv and Variations.csv. The first file should contain the emission values of the baseline scenario in annual metric tons [t/yr] for each of the sectors and macrosectors considered by AERIS and for

all the studied pollutants. The second file must have the variation percentages expressed as a
deviation from the baseline scenario for each of the before mentioned sectors (\(p_i\)). Whenever

the user does not have information on a given sector considered by AERIS or just wants to focus

on one sector, zeros can be assigned to those sectors that are to be ignored. These two files
do not have a comprehensive structure and must be produced with the help of an auxiliary

stand-alone file called AERIS-Input.xls. This Microsoft Excel @spreadsheet allows placing

in a fully comprehensive and easy-to-use table, the emissions and variation percentages. After

the table is populated, the user should only save the “Emissions” and “Variations” spreadsheets

within as * .csv files separately. In a newly-installed version of AERIS, this directory should be

empty but in order to initiate a simulation, the before mentioned files are necessary.

Parameters directory

The Parameters directory contains the essential parameterizations, regression coefficients,

and particularities of the modeling domain that allow the user to move the screening exercise

throughout the modules that compose AERIS. In other words, this file contains the necessary
data that allow transforming the variation percentages into policy-relevant indicators, at-
mospheric deposition rates, health and ecosystem impacts, etc. Each of these files contains
the most valuable and innovative part of AERIS, so in order to protect the author's know-how
and the model's novelty, the description of each of the parameters files is not provided. In a
freshly-installed version of AERIS, this directory should contain 34 files with a * .csv exten-
sion, preceded by the Coef* abbreviation. In order to guarantee an adequate functioning of
the IAM, the user should not tamper with any of these files.

Results directory

The Results directory has been created for containing files with a series of modeling results

that have been written under request of the user. In a new version of AERIS, this directory

should contain 6 files with an *.xls extension. The name of each of these files has the form
A.1. AERIS: a general description

X-Results.xls, where X is each of the pollutants considered by AERIS. Moreover, these files should also be empty (without any results written) and with a total size of 578 KB. Each of this files contains columns with an identification number that allows joining the modeling results with the database file (*.dbf) of an ArcGIS ®shapefile (*.shp). Whenever a new simulation is carried out and results are desired, the user must make sure that the columns with the results (Baseline scenario and Tested scenario) are empty because AERIS is not able to overwrite these files.

Temporal directory

The Temporal directory contains the files that allow transforming the temporal scale of the outputs predicted by AERIS. It contains parameterizations for every pollutant and for every month of the year, as well as parameterizations for annual values. This directory contains 6 subdirectories that correspond to each pollutant: NH3, NO2, O3, PM10, PM25 and SO2. Each of these subdirectories contains 13 files with a *.csv extension and a Coef-Temp-X-Y structure, in which X is one of the before mentioned pollutants and Y is the month of the year. These files should not be modified by the user at any time.

Transfer-Matrices directory

The directory called Transfer-Matrices contains the essential databases that allow carrying out the core calculations of AERIS, which correspond to the source-receptor matrices (SRMs). The directory contains at first sight two subdirectories: 01-January and 08-August. Each of these subdirectories contains a total number of 53 files which correspond to the total number of sectors and pollutants that are considered by AERIS. The third and last level of directories in AERIS corresponds to that of 5 pollutants: NH3, NO2, O3, PM10, PM25 and SO2, each of them with a number of SRMs equal to the number of SNAP sectors considered. Within each of these folders, SRM files can be found as simple *.csv files. The naming structure of the SRMs is the following: TM-X-SNAP, where X is the pollutant and SNAP is the code of the parameterized sector or macrosector. Since this files are absolutely essential for the correct functioning of AERIS, the user should refrain from tampering with them.

A.1.2 Running AERIS

AERIS is run in a very simple and straightforward manner. The first step requires opening MATLAB ®and focusing on the command window. According to the path on which the user placed the AERIS folder, it might be necessary to navigate from the default home directory of MATLAB ®using the cd command. The user should then check for the presence of the subdirectories and files that have already been explained with the previous sections. In this first level, the author should clearly identify the AERIS.m file and invoke it by typing its name on the command window. For example:
After this command is invoked, the main menu of AERIS should open after a few seconds. This main menu has been designed to appear as a “checklist” in which individual and separate pollutants are analyzed, as shown in figure A.2. For a given pollutant, the user should check the corresponding square by clicking on top of it, after which the typical interface of AERIS will open. For example, after checking the square of the Nitrogen dioxide - NO\textsubscript{2} option, the GUI that allows carrying out a screening exercise for nitrogen dioxide (NO\textsubscript{2}) should open as shown in figure A.3.

The user should then click on top of the emissions table in order to load the Emissions.csv and Variations.csv files onto the system. Then, the user should define the period of time of reference (annual or monthly) for the outputs, the sources (either national or subnational) and the indicators or impacts by scrolling down the pop-up menus located on the right of the window. Please notice that every pop-up menu should be scrolled down and an option selected. Once this is properly done, the user should click on top of the Run button. After a short period of time, the red map on the Tested Scenario window should change. If the user wants to export the data presented as a colormap in order to use it for reports or pictures, it
can be done so by clicking on the Export button, which will automatically write result files as Excel spreadsheets in the Results folder. In figure A.4, the aspect of the GUI after analyzing the mean annual concentration of NO$_2$ for a given emission scenario can be seen. On the lower right side of the GUI, there is a section of buttons called Secondary pollutants. If the user wants to simulate tropospheric ozone (O$_3$) or particulate matter (PM$_{10}$, PM$_{2.5}$), these buttons should be pressed in order to generate intermediate files (which would then appear at the Exchange directory) that allow quantifying the contributions of the pollutant under analysis to these secondary pollutants. In this case, when pressing the oxidized nitrogen-related secondary particles button, the contribution of NO$_2$ is quantified. In a similar way, the concentrations of NO$_2$ that generate O$_3$ levels are provided.

In general, this is the mechanics that need to be followed to carry out simulations with AERIS. It is very simple and straightforward for any kind of user. Whenever AERIS is formally licensed to a user, the complete documentation of the model is provided in the form of a user’s manual. Due to limitations on text, time and effort, it was not possible to include in this chapter a complete manual and tutorial of the AERIS manual. However, the author strongly believes that an experienced user of complex air quality models will have to invest little time to become a proficient user of AERIS.
A.2 Air quality model & processing tools

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### A.2. Air quality model & processing tools

NUTS - 3 Subdivisions for Spain.

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### Appendix A. Appendices

NUTS - 3 Subdivisions for Portugal.

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### A.3 Emissions & air quality system

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### A.3. Emissions & air quality system

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## Appendix A. Appendices

List of EIONET AirBase stations.

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### E.3. Emissions & air quality system

List of EIONET AirBase stations.

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Appendix A. Appendices

List of EIONET AirBase stations.

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Regression plots for estimating the 19th highest hourly value of NO₂ from mean annual concentrations.
Regression plots for estimating the 25th highest daily value of $SO_2$ from mean annual concentrations.
Regression plots for estimating the 4\(^{th}\) highest hourly value of SO\(_2\) from mean annual concentrations.
Regression plots for estimating the $36^{th}$ highest daily value of $PM_{10}$ from mean annual concentrations.
Regression plots for estimating the 26th highest 8-hour value of $O_3$ from mean annual concentrations.
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Regression plots for estimating SOMO$_{35}$ of $O_3$ from mean annual concentrations.
A.3. Emissions & air quality system

Regression plots for estimating daylight $AOT_{40}$ of $O_3$ from mean annual concentrations.
Regional scenarios for Andalucía (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
Regional scenarios for Aragón (2007). a) NO$_2$ b) SO$_2$ c) PM$_{2.5}$ d) NH$_3$. 
Regional scenarios for Asturias (Principado de) (2007). a) NO$_2$ b) SO$_2$ c) PM$_{2.5}$ d) NH$_3$. 
Regional scenarios for Cantabria (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
Regional scenarios for Castilla - La Mancha (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 

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Regional scenarios for Castilla y León (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
Regional scenarios for Catalunya - Catalunya (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
Regional scenarios for Ceuta y Melilla (Ciudades Autónomas de) (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
Regional scenarios for Comunidad Foral de Navarra - Nafarroako Foru Komunitatea (2007). a) \( NO_2 \) b) \( SO_2 \) c) \( PM_{2.5} \) d) \( NH_3 \).

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A.3. Emissions & air quality system

Regional scenarios for Comunidad de Madrid (2007). a) NO$_2$ b) SO$_2$ c) PM$_{2.5}$ d) NH$_3$. 

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Regional scenarios for Comunidad Valenciana - Comunitat Valenciana (2007). a) $NO_2$ b) $SO_2$

c) $PM_{2.5}$ d) $NH_3$. 

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Regional scenarios for Extremadura (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 

A.3. Emissions & air quality system
Regional scenarios for Galicia (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
Regional scenarios for Islas Baleares - Illes Balears (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 

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Regional scenarios for La Rioja (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
Regional scenarios for Murcia (Región de) (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$.
Regional scenarios for País Vasco - Euskadi (2007). a) $NO_2$ b) $SO_2$ c) $PM_{2.5}$ d) $NH_3$. 
A.4 Air quality system validation

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Appendix A. Appendices

IAM vs. AQM scatterplot for NO$_2$ mean concentrations (SNAP 010000, 020202, 030000).

SNAP 010000

SNAP 020202

SNAP 030000

IAM vs. AQM scatterplot for NO$_2$ mean concentrations (SNAP 010000, 020202, 030000).
A.4. Air quality system validation

IAM vs. AQM scatterplot for NO$_2$ mean concentrations (SNAP 070101, 070201, 070301).

IAM vs. AQM scatterplot for NO$_2$ mean concentrations (SNAP 070101, 070201, 070301).
Appendix A. Appendices

IAM vs. AQM scatterplot for NO$_2$ mean concentrations (SNAP 070301, 070301, 070301).

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A.4. Air quality system validation

IAM vs. AQM scatterplot for $NO_2$ mean concentrations (SNAP 080500, 080600, 080800).

IAM vs. AQM scatterplot for $NO_2$ mean concentrations (SNAP 080500, 080600, 080800).
IAM vs. AQM scatterplot for NO$_2$ mean concentrations (Portugal).
A.4. Air quality system validation

SO$_2$

SNAP 010000

SNAP 020202

SNAP 030000

IAM vs. AQM scatterplot for SO$_2$ mean concentrations (SNAP 010000, 020202, 030000).
Appendix A. Appendices

IAM vs. AQM scatterplot for SO$_2$ mean concentrations (SNAP 040000, 080600, 080800).

IAM vs. AQM scatterplot for SO$_2$ mean concentrations (SNAP 040000, 080600, 080800).
A.4. Air quality system validation

IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (SNAP 020202, 070101, 070103).

IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (SNAP 020202, 070101, 070103).
IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (SNAP 070201, 070203, 070301).
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IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (SNAP 070303, 0707/08, 080600).

IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (SNAP 070303, 0707/08, 080600).
IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (SNAP 080800, 100500, Portugal).
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IAM vs. AQM scatterplot for $PM_{2.5}$ mean concentrations (SNAP 020202, 070101, 070103).

IAM vs. AQM scatterplot for $PM_{2.5}$ mean concentrations (SNAP 020202, 070101, 070103).
IAM vs. AQM scatterplot for $PM_{2.5}$ mean concentrations (SNAP 070201, 070203, 070301).
A.4. Air quality system validation

IAM vs. AQM scatterplot for \( PM_{2.5} \) mean concentrations (SNAP 070303, 0707/08, 080600).

IAM vs. AQM scatterplot for \( PM_{2.5} \) mean concentrations (SNAP 070303, 0707/08, 080600).
Appendix A. Appendices

IAM vs. AQM scatterplot for $PM_{2.5}$ mean concentrations (SNAP 080800, 100500, Portugal).

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A.4. Air quality system validation

IAM vs. AQM scatterplot for $NH_3$ mean concentrations (SNAP 100101, 100102, 100500).

IAM vs. AQM scatterplot for $NH_3$ mean concentrations (SNAP 100101, 100102, 100500).
IAM vs. AQM scatterplot for $NH_3$ mean concentrations (SNAP 110000, Portugal).
A.4. Air quality system validation

Statistical indicators for the monthly-mean parameterizations of nitrogen dioxide ($NO_2$).

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<th>$NME - (%)$</th>
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<td>0.2363</td>
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<td>5.38</td>
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<td>0.1770</td>
<td>0.4096</td>
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<td>12.21</td>
</tr>
<tr>
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<td>-0.0244</td>
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</tr>
<tr>
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<td>5.45</td>
</tr>
<tr>
<td>June</td>
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<td>-0.0611</td>
<td>0.1857</td>
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<td>5.70</td>
</tr>
<tr>
<td>July</td>
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<td>-0.1371</td>
<td>0.3395</td>
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<td>9.98</td>
</tr>
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<td>6.31</td>
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<td>6.36</td>
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<td>0.2400</td>
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Statistical indicators for the monthly-mean parameterizations of sulfur dioxide ($SO_2$).

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<th>$ME - [\mu g/m^3]$</th>
<th>$NMB - (%)$</th>
<th>$NME - (%)$</th>
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</thead>
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</tr>
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<td>0.6425</td>
<td>1.1220</td>
<td>1.1366</td>
<td>39.19</td>
<td>39.70</td>
</tr>
<tr>
<td>March</td>
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<td>0.2041</td>
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<td>6.48</td>
</tr>
<tr>
<td>April</td>
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<td>10.45</td>
</tr>
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<td>6.85</td>
</tr>
<tr>
<td>June</td>
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<td>0.3401</td>
<td>2.96</td>
<td>10.46</td>
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<td>9.15</td>
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Statistical indicators for the monthly-mean parameterizations of particulate matter ($PM_{10}$).

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<th>$ME$ [µg/m$^3$]</th>
<th>NMB (%)</th>
<th>NME (%)</th>
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<td>0.4863</td>
<td>-2.90</td>
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</tr>
<tr>
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<td>0.3793</td>
<td>0.5695</td>
<td>4.09</td>
<td>6.14</td>
</tr>
<tr>
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<td>1.1330</td>
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<td>6.14</td>
</tr>
<tr>
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Statistical indicators for the monthly-mean parameterizations of sulfur dioxide ($PM_{2.5}$).

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<th>$MB$ [µg/m$^3$]</th>
<th>$ME$ [µg/m$^3$]</th>
<th>NMB (%)</th>
<th>NME (%)</th>
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</thead>
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<td>11.41</td>
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<td>4.90</td>
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<td>November</td>
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<tr>
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A.4. Air quality system validation

Statistical indicators for the monthly-mean parameterizations of tropospheric ozone ($O_3$).

<table>
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<th>$ME - \mu g/m^3$</th>
<th>$NMB - (%)$</th>
<th>$NME - (%)$</th>
</tr>
</thead>
<tbody>
<tr>
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Statistical indicators for the monthly-mean parameterizations of sulfur dioxide ($NH_3$).

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<th>$ME - \mu g/m^3$</th>
<th>$NMB - (%)$</th>
<th>$NME - (%)$</th>
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</thead>
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</table>
IAM vs. AQM scatterplot for NO₂ mean concentrations (January to June).
A.4. Air quality system validation

IAM vs. AQM scatterplot for NO$_2$ mean concentrations (July to December).

IAM vs. AQM scatterplot for NO$_2$ mean concentrations (July to December).
IAM vs. AQM scatterplot for SO$_2$ mean concentrations (January to June).
IAM vs. AQM scatterplot for SO$_2$ mean concentrations (July to December).
IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (January to June).
A.4. Air quality system validation

IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (July to December).

IAM vs. AQM scatterplot for $PM_{10}$ mean concentrations (July to December).
IAM vs. AQM scatterplot for $PM_{2.5}$ mean concentrations (January to June).
A.4. Air quality system validation

**PM$_{2.5}$**

IAM vs. AQM scatterplot for $PM_{2.5}$ mean concentrations (July to December).

IAM vs. AQM scatterplot for $PM_{2.5}$ mean concentrations (July to December).
IAM vs. AQM scatterplot for $O_3$ mean concentrations (January to June).
A.4. Air quality system validation

IAM vs. AQM scatterplot for $O_3$ mean concentrations (July to December).
IAM vs. AQM scatterplot for $NH_3$ mean concentrations (January to June).
A.4. Air quality system validation

NH₃

July

October

August

November

September

December

IAM vs. AQM scatterplot for NH₃ mean concentrations (July to December).

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A.5 Protection of ecosystems module

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A.5. Protection of ecosystems module

Critical load functions for acidification drawn with the VSD model.
Critical load functions for acidification drawn with the VSD model.
Critical load functions for acidification drawn with the VSD model.
Critical load functions for acidification drawn with the VSD model.
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Total crop loss of a) sunflower and b) wheat caused by SO₂ for the baseline scenario [kg/ha].
Bibliography


Bibliography


[130] Fuhrer J, 1986. The critical level for effects of ozone on crops and the transfer to mapping, testing and finalizing the concepts. Paper presented at UNECE Workshop, Department of Ecology and Environmental Science, University of Kuopio, Finland.


Bibliography


[152] Heyes, C., Schöpp, W., Amann, M., Unger, S., 1996. A Reduced - Form Model to Predict Long-Term Ozone Concentrations in Europe. International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria.


Bibliography


Bibliography


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About the author

Michel Vedrenne

(b. Mexico City, 1985) Graduated in Chemical Engineering from the Iberoamerican University (Universidad Iberoamericana) of Mexico City. Has worked as a research assistant at the Electrochemistry and Environmental Engineering Laboratory of the same university, where he took part in several investigation projects regarding treatment of wastewaters through non-conventional methods. In 2010 he became part of the Environmental Modelling Laboratory at the Technical University of Madrid (Universidad Politécnica de Madrid), working in different projects related with air quality modelling and monitoring as well as with life cycle analysis. In 2011 he received a Master's Degree in Environmental Engineering from the Technical University of Madrid with a thesis on the analysis and evaluation of emission inventories through air quality simulations. He is in charge of providing, supporting and disseminating the AERIS model, whose development is the subject of this doctoral dissertation. His main interests are related with water and air pollution processes, meteorology and computer modelling. He is a member of the International Environmental Modelling and Software Society (iEMSs), of The Integrated Assessment Society (TIAS) and of the Institute of Air Quality Management of the United Kingdom (IAQM). Since 2014 he works as a Technical Consultant in Ricardo-AEA in London, involved in air quality modelling, national and European policy assessments and local air quality management.

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