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

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Abstract: Improving air quality is an eminently inter-disciplinary task. The wide variety of sciences and stakeholders 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. This paper presents the current developments in the design and application of an Integrated Assessment Model for the Iberian Peninsula (AERIS). This model is able to provide concentration profiles for NO_2, O_3, SO_2, NH_3 and PM_{10} as a response to percentual changes in the emissions of the most relevant sectors present in the studied domain which include urban and highway road traffic, power generation, domestic heating and agriculture. Such results are obtained from a series of transfer matrices based on an air quality modeling system that relies on the WRF model for meteorology and on the CMAQ model for atmospheric chemical processes. The accuracy of the IAM has been tested by statistically contrasting the obtained results with those yielded by the conventional air quality model, exhibiting in most cases a good agreement level. Although the model has been developed only to describe the emission-concentration link, its structure is versatile enough to provide results for deposition, impacts on ecosystems and abatement costs. The programming structure is MATLAB®-based, allowing great compatibility with typical software such as Microsoft Excel® or ArcGIS®. In conclusion, the main asset that AERIS provides is its accuracy in predicting outcomes for a wide variety of scenarios through a simple yet robust modeling platform, without dealing with complex programming and avoiding long computing times.

Key words: *Integrated Assessment Model, Air quality modeling, Iberian Peninsula, Decision support, Air pollution*

INTRODUCTION

The conception of an Integrated Assessment Model (IAM) for describing an environmental problem goes beyond a modeling exercise: it obeys, in a strict sense, a methodology that is used for gaining insight over the complex linkages that exist between phenomena. To this respect, constructing an air pollution IAM is useful when describing the bonds that exist between the emissions of pollutants, their transport and chemical transformations in the atmosphere as well as the impacts they produce on health and ecosystems, and even estimating their economic and political consequences (Carnevale et al., 2012).

Traditionally, the full description of the air pollution phenomena has been carried out by comprehensive air quality models (AQM) that are able to simulate a wide variety of complex reactions and physical interactions (Amann et al., 2011). These are also susceptible of being coupled with health and ecosystem impacts models (e.g. Boldo et al., 2011; de Andres et al., 2012), as well as with optimization and economic modules (Cofala et al., 2010). However, AQMs have computer-intensive algorithms and depend on a large volume of data. Their configuration and implementation require a high degree of technical and computing expertise. Since the air pollution problem has deep implications in policymaking, the high complexity of AQMs makes them inefficient for satisfying the needs of stakeholders. To this respect, IAMs are constructed to provide real-time policy support as well as to answer specific environmental management questions under a holistic approach.

The use of IAMs in Europe has been intensive in the recent decades as a consequence of the application of the UNECE Convention on Long Range Transboundary Air Pollution (CLRTAP) (Kaldellis et al., 2007). Of these IAMs, the RAINS/GAINS Integrated Assessment system (Schöpp et al., 1999; Amann et al., 2011) has been the most used and is considered an essential tool for European-level policymaking and negotiations. However, the need of having IAMs at the national or regional level has led to the development of more detailed versions that seek to capture phenomena that occur at a lower scale (i.e. urban areas). In this line, the Technical University of Madrid (UPM) has developed AERIS (Atmospheric Evaluation and Research Integrated model for Spain) as an IAM especially conceived for the Iberian Peninsula (Spain and Portugal) and based on the SIMCA project (Borge et al., 2008a,b). The main objective was creating a reliable tool for air quality prognosis able to provide real-time support needed by policymakers at local and national levels, being useful to many other stakeholders. This is especially relevant for a country like Spain, whose political division (17 autonomous regions) might result in the elaboration of several different regional air quality management plans.

This paper presents the first version of AERIS. It briefly describes its structure and appearance, as well as the methodology followed in its modeling process. Additionally, it presents an evaluation of its performance against the conventional AQM. Finally, a discussion is conducted on the potential capabilities of AERIS to include impact and monetary evaluations, as well as an identification of future research lines.

THE AERIS MODEL

The AERIS model is a multi-pollutant IAM that addresses air quality variations, expressed as policy-relevant indicators, as a function of percentual variations in emissions against a reference scenario. It is currently able to describe the fate of criteria pollutants such as sulfur dioxide (SO_2), nitrogen oxides (NO_x), ammonia (NH_3) and two fractions of particulate matter (PM_{10}, $PM_{2.5}$). AERIS is also able to describe the formation of ground-level ozone (O_3) and secondary aerosols. For the time being, the current version of the model is not able either to quantify health-impacts or link results to any costs and optimization module.

The domain described by AERIS is composed by a grid of 4550 cells of 16×16 km centered in 40°N and 3°W which covers the entire Iberian Peninsula (Spain and Portugal) and the Balearic Islands as well as Andorra, parts of France, Morocco and Algeria. This modeling domain (Fig.1a) corresponds to the national-scale domain developed in Borge et al., (2008).

The structure of AERIS consists of an emission module and an atmospheric dispersion and chemistry module. The emission module has been constructed with emissions coming from the National Emission Inventories of Spain (SNEI) and Portugal (PNEI) (MARM, 2009; APA, 2010) and processed with the SMOKE model (IE, 2009). This module has a reference scenario (RS) of emissions which corresponds to the 2007 version of the SNEI. As a consequence, any change in the emissions should be given as a variation percentage of the RS. The emission module is consistent with the Selected Nomenclature for Air Pollution (SNAP) and the EMEP/CORINAIR methodology used in the SNEI and PNEI.

The atmospheric dispersion module is a reduced-form representation of a full AQM composed by the Weather Research Forecast (WRF) model for the description of meteorology and the Community Multiscale Air Quality model (CMAQ) for atmospheric chemistry and dispersion. WRF is a non-hydrostatic mesoscale model that includes the latest developments for meteorological modeling (Skamarock and Klemp, 2007). CMAQ is a multi-pollutant Eulerian air quality model that is able to describe atmospheric transport, transformation and deposition on regional and urban scales (Byun and Schere, 2006).

The parameterizations and configuration details of the AQM can be found in Borge et al., (2008a, b). In general, the AQM allowed the construction of a set of functional relationships for a number of SNAP activities through the use of transfer matrices (TM). The TM of AERIS were built by systematically perturbing the emissions (-90%, -50%, +50%, +90%) of each activities around the RS following the methodology published in Bartincki (1999). Through the use of these TM, AERIS is able to quickly predict the ambient concentration represented as policy-indicators maps through a simple calculation.

AERIS has been programmed to run as a MATLAB®-based GUI (Fig. 1b), which can be installed in any market-available PC. It has been constructed to be as user-friendly as possible, with a full compatibility with typical desktop applications such as ArcGIS® or Microsoft Excel®. Moreover, I/O data-flows to and from AERIS are in the form of ordinary text files (.txt) which reduces any tune-up or configuration techniques to a minimum.

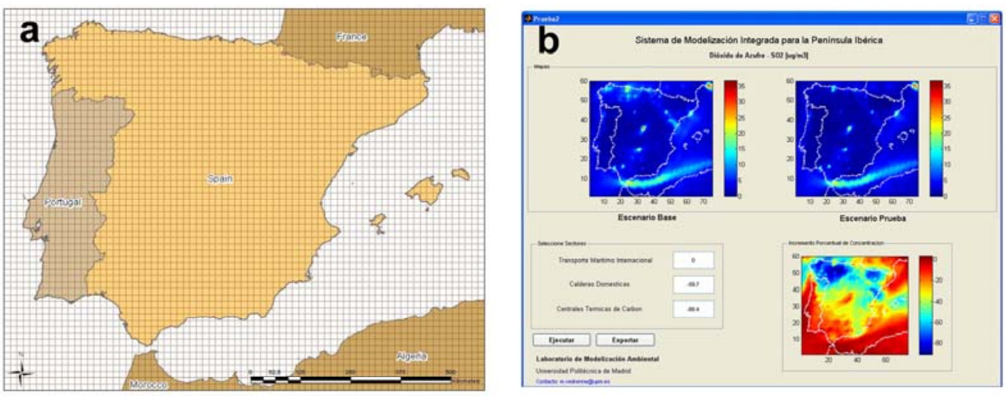

Figure 1. a) Modeled domain of AERIS. b) Aspect of the Graphic User Interface (GUI) of AERIS.

MODEL TESTING AND VALIDATION

In order to test the ability of AERIS in accurately reproducing the air quality levels as a consequence of changes in emissions (E), a hypothetic scenario (HS) was processed by the IAM and its results compared to those produced by the conventional AQM. To this respect, the two models were run for a complete year and the outputs statistically evaluated.

Scenario definition

The HS outlines a range of emissions likely to occur in Spain in year 2014 and is a consequence of the application of technical and non-technical measures to the RS. Both scenarios were created and evaluated according to Lumbreras et al., (2008, 2009). The emissions of four pollutants were followed: SO_2, NO_x, PM_{10}, and NH_3. Table 1 describes the emissions of the hypothetic scenario (HS) as a variation percentage of the emissions of the RS.

Table 1. Emissions at the hypothetic scenario (HS) as a variation percentage of the reference scenario (RS).

SNAP Code	Activity name	SO_2		NO_x		PM_{10}		NH_3	
		E_{RS} [a]	$\%_{HS}$	E_{RS}	$\%_{HS}$	E_{RS}	$\%_{HS}$	E_{RS}	$\%_{HS}$
010101	Combustion plants ≥300MW	805700	-88.6%	235331	-58.8%	17632	0.0 %	0	0.0 %
020202	Residential plants <50MW	12544	-59.7%	24648	15.5%	23461	-5.74%	0	0.0 %
030000	Combustion in manufacturing	83069	-33.0%	225942	-58.8%	27676	0.0 %	0	0.0 %
070101	Passenger cars: highway driving	599	0.0 %	135466	-62.1%	5387	-48.2%	5225	0.0 %
070103	Passenger cars: urban driving	571	0.0 %	75670	-17.3%	8052	-67.5%	473	0.0 %
070301	HDV >3.5 t: highway driving	605	0.0 %	111414	-9.9%	4564	-69.1%	339	0.0 %
070303	HDV >3.5 t: urban driving	324	0.0 %	72325	-65.0%	4049	-88.6%	226	0.0 %
0707/08	Road, tire and break abrasion	0	0.0 %	0	0.0 %	11621	-17.5%	0	0.0 %
100102	Cult. with fertilizers: arable lands	0	0.0 %	8361	0.0 %	736	0.0%	110927	-20.4%
-	Portugal (total)	22918	0.0 %	145250	0.0 %	80563	0.0%	48970	0.0%

[a] Emissions are presented in annual metric tons ($t \cdot yr^{-1}$)

Evaluation criteria

The performance of AERIS against the ordinary AQM for the analyzed pollutants (i.e. SO_2, NO_x, PM_{10}, NH_3, and O_3) was statistically evaluated through the indicators listed in Table 2, which are typically used during model benchmarking (Thunis et al., 2011). These indicators seek to characterize the correlation level as well as the accumulated deviation between both models. In a broader sense, the discussion on the validation of AERIS is developed following its ability to reproduce the results yielded by the usual AQM. At this point we are also assuming that the results provided by the AQM are sufficiently relevant in terms of policymaking due to the fact that these have been contrasted against observations (Borge et al., 2010).

Table 2. Statistic indicators used for model comparisons and benchmarking.

Indicator	Definition	Units	Range
Mean Bias (MB)	$MB = \frac{1}{N} \cdot \sum_{i=1}^{N} (P_i - M_i)$ [b]	μg/m³	-∞ – ∞
Mean Error (ME)	$ME = \frac{1}{N} \cdot \sum_{i=1}^{N} \lvert P_i - M_i \rvert$	μg/m³	0 – ∞
Normalized Mean Bias (NMB)	$NMB = \sum_{i=1}^{N} (P_i - M_i) \Big/ \sum_{i=1}^{N} M_i$	%	-100 – ∞
Normalized Mean Error (NME)	$NME = \sum_{i=1}^{N} \lvert P_i - M_i \rvert \Big/ \sum_{i=1}^{N} M_i$	%	0 – ∞
Correlation coefficient (r)	$r = \left(\sum_{i=1}^{N} P_i \cdot M_i - N \cdot \overline{P} \cdot \overline{M} \right) \Big/ (N-1) \cdot s_P \cdot s_M$	dimensionless	0 – 1

[b] *P*-AERIS results, *M*-AQM results, *N*-number of cells of the domain, *s*-standard deviation of the dataset.

RESULTS

The validation of AERIS against the conventional AQM is presented in Fig. 2, along with the model benchmarking indicators (Table 3). It shows that, in most cases, the correspondence between the results of AERIS and the AQM is good. The positive values of MB and MNB 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 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.

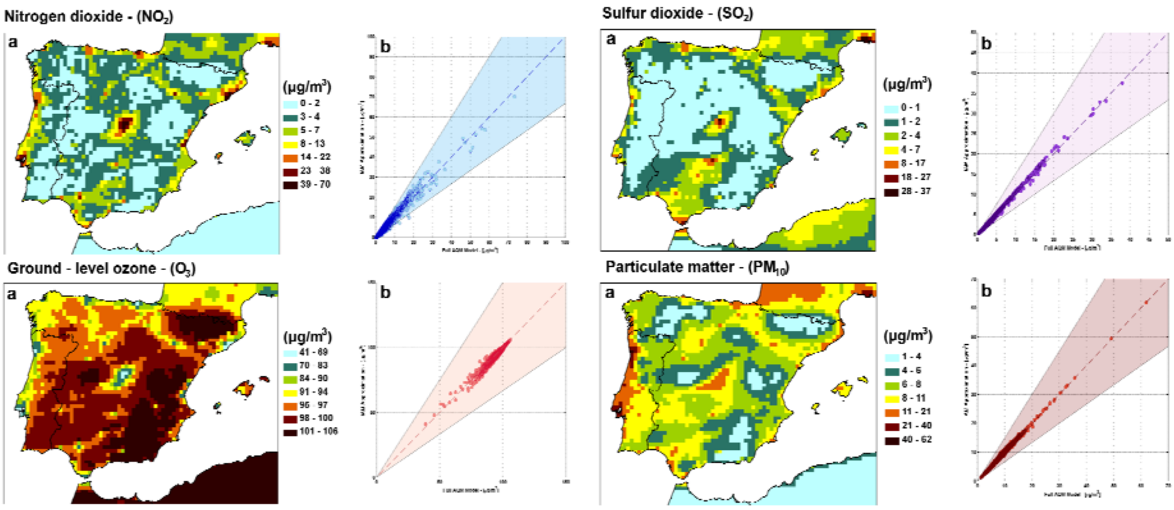

Figure 2. a) Mean annual concentration results yielded by AERIS. b) Comparison of the results of AERIS against AQM.

Table 3. Statistic indicators used after comparing AERIS and the conventional AQM.

Pollutant	MB ($\mu g/m^3$)	ME ($\mu g/m^3$)	MNB (%)	MNE (%)	R
NO_2	0.9548	0.4892	4.15	13.11	0.9841
SO_2	0.0944	0.1400	3.35	4.97	0.9986
PM_{10}	0.0854	0.2243	1.04	2.73	0.9966
NH_3	-0.0406	-0.0877	-6.42	13.85	0.9654
O_3	-0.5892	0.8275	-0.61	0.86	0.9810

A qualitative inspection of the maps presented in Fig. 2 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 BS. Additionally, a limitation that AERIS presents is the fact that any simulation must be referred to the specific BS, which impedes using any custom baseline scenario directly.

In a broader sense, it is crucial to keep in mind that constructing IAMs from sophisticated AQMs through statistical simplifications involves an important amount of uncertainty that is likely to be originated by methodological aspects. IAM-related uncertainties have been extensively studied and deemed difficult to reliably quantify (Schöpp et al., 2005). As a result, any user should be able to interpret the results provided by the model in terms of its limitations and particularities. Currently, efforts are being done to provide reliable results to a broader audience of stakeholders. Additionally, it should be stressed that AERIS is still under development and is open to improvements and further modifications.

CONCLUSIONS.

The development of an Integrated Assessment Model such as AERIS has been addressed in this paper in terms of its structure and methodological issues. It has been shown that, although simplifying full AQM processes, it performs in a similar way when describing the same hypothetic emission scenario for a variety of pollutants. This performance similarity is evidenced by good correspondence levels of model benchmarking indicators. Additionally, small-scale phenomena such as concentration hotspots from cities and industrial clusters are reproduced by AERIS due to its fine scale and high-quality emission inventories. Although difficult to determine, the uncertainty levels associated with the model predictions as well as its inherent limitations are being evaluated. The correct identification of these uncertainties and limitations will serve as guidance for further improvements on the model. Simultaneously, a more complete and accurate version of AERIS is currently under construction, which will incorporate ecosystem and health impact modules with the associated cost-benefit module as well as transfer matrices for new emission sectors.

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