Uncertainties in atmospheric emission projections

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ABSTRACT

Emission projections are important for environmental policy, both to evaluate the effectiveness of abatement strategies and to determine legislation compliance in the future. Moreover, including uncertainty is an essential added value for decision makers. In this work, projection values and their associated uncertainty are computed for emissions (both air pollutants and greenhouse gases) in Spain following two different approaches.

The first one consists of the application of advanced statistical techniques to the most significant activities in terms of emissions. Uncertainty bands have been derived for the Business As Usual (or without measures) scenario through autoregressive integrated moving average (ARIMA) models. As for the baseline scenario resampling techniques (bootstrap) were applied as an additional nonparametric tool, which does not rely on distributional assumptions and is thus more general.

The second approach is based on a sensitivity analysis of emission projections to key inputs on a sectoral basis (both activity rate and emission factor-related parameters). Results from the baseline (or with measures) scenario have been compared with re-computed emission trends in a low economic growth perspective, providing a good test of the method.

INTRODUCTION

The development of effective environmental policies is needed in order to meet regulatory standards, international legislation and agreements in the future. The design, assessment and comparison of control strategies require the support of an integrated modeling system. The Technical University of Madrid (UPM) is currently developing and implementing such a modeling system for Spain. The system is based on three major components, which should be considered as a work in progress, since they are currently being upgraded and improved. These components are as follows:

1) Spain's Emission Projections (SEP)[1] model as a result of the application of the Consistent Emission Projection (CEP) model to Spain[2]. Emissions for the main atmospheric pollutants and greenhouse gases are available up to 2020. These emissions are based on individual, highly-detailed projections for nearly 300 emission categories according to the Selected Nomenclature for Air Pollution (SNAP) classification. National figures are obtained through an integration methodology that guarantee full consistency among individual projections and complete agreement with the National Atmospheric Emission Inventory (SNAEI)[3] estimates for past years. A piece of software called EmiPro[1] has been developed to implement the SEP's methods and support the QA/QC process in emission projections. This tool also assists

report generation, including mapping to other nomenclatures relevant in the framework of the Clean Air For Europe (CAFE) program and comparison with other European models (RAINS, PRIMES, etc.)

2) An air quality modeling system for the Iberian Peninsula based on WRF, SMOKE and CMAQ models. It includes the adaptation of the SMOKE system to European conditions and the integration of the SNAEI and SEP's databases as inputs to the emission preparation for modeling process.
3) Impact-oriented modules. Complementary to the regulatory view of air pollution, the system includes a series of ancillary modules to evaluate the impact of air pollution on human health and ecosystems in a consistent way.

This paper is focused on the first component and specifically on the development of different methods to estimate emission projection uncertainties. As many experts expose, these uncertainties are inevitable[4]. Moreover, they play a major role in environmental decision-making as atmospheric emission estimates from all sectors must be accompanied by uncertainty estimations[5]. However, due to the complexity of emission projection systems, an appropriate treatment of uncertainties is far from trivial[6]. Most of worldwide emission projections include a sensitivity analysis as a first step to show possible uncertainties. This approach is useful to identify the main parameters that influence model results. Nevertheless, it does not permit to obtain uncertainty bands to help decision making. The aim of this paper is to present several methods to obtain these bands.

The first approach is applicable to scenarios based on past trends that show how emissions would grow in the absence of any technical or non-technical control measure implemented, adopted or planned after the base year. This scenario is called "without measures" or "business as usual". The method relies on the ARIMA time series modeling[7] as presented in Lumbreras et al. (2009)[8]. This modeling assumes that the value of the series for a given time point is a linear combination of previous values (lags) with decreasing weights and a constant conditional variance. The linear behavior results from the assumption of multivariate normality for the joint distribution of the series. The ARIMA methodology has been applied for decades with great success (especially on air quality forecasting[9, 10]), although other models that allow, for example, for conditional heteroscedasticity[11, 12] have been derived later.

The second approach[8] uses a non-parametric technique called bootstrap that was developed by Efron[13]. It is used for building forecast intervals in a "with measures" scenario (i.e. including implemented policies and measures for reducing emissions through technology improvements and dissemination, demand-side efficiency gains, more efficient regulatory procedures, and shifts to cleaner fuels). In this case, the intervals are derived from the original projections including the past (inventory) values.

The third method has been developed by the authors to use sensitivity analysis as a source of information to derive uncertainty bands. This methodology simplifies uncertainty assessment and allows other teams/regions to take advantage of their sensitivity analyses (rather than uncertainty computation).

Uncertainty computations value integrated assessment modeling because they:

- Allow a more accurate estimation of commitments compliance in future years (such as Kyoto Protocol or EU Directives)
- Offer a wider range of future emissions usable for negotiations
- Include uncertainty estimations of the effect of policies and measures to reduce emissions

METHODOLOGY

ARIMA method applied to "without measures" scenarios (WoM)

The analysis is done for each pollutant at activity level (i.e. the third hierarchical level of the EU Selected Nomenclature for Air Pollution – SNAP) applying univariate time series analysis[8]. These models are capable of explaining the structure and predicting the evolution of a variable which is observed over time. It is assumed that data are available for regular time intervals, in such way that the inertia of the series is used for projecting.

The integrated autoregressive moving-average process of orders p and q, which is referred to as the ARIMA (p,d,q) process, is a process defined by equation (1):

$$(1-B)^d(1 - \Phi_1 B - \Phi_2 B^2 - \Phi_3 B^3 - \ldots - \Phi_p B^p)z_t = (1 - \theta_1 B - \theta_2 B^2 - \ldots - \theta_q B^q)\, a_t, \qquad (1)$$

where B is the backshift operator such that $By_t = y_{t-1}$, the roots of $\Phi(B)=(1-\Phi_1 B\ldots)=0$ are on or outside the unit circle, and the roots of $\theta(B)=(1-\theta_1 B\ldots)$ are outside the unit circle and a_t are the innovations which are serially uncorrelated; *p* is the order of the autoregressive component; *q* is the order of the moving average component and *d* is the order of the integration.

To project emissions for WoM scenario using this method, the model of emissions should be obtained. To do this, in a first step, the series were transformed to achieve stationarity in mean and variance. After this, parameter estimation was done by means of maximum likelihood. Subsequently, the hypotheses of the model must be validated. The hypotheses assumed on the errors are:

1) Zero mean
2) Constant variance
3) Uncorrelated for all lags
4) Normally distributed

Additionally, diagnosis should include the detection of any deterministic terms, whenever present. If the hypotheses are validated, the model could be used to forecast, otherwise the model must be redefined.

Finally, forecasts are obtained from the estimated model assuming that the parameter estimates in eq. 1 are the true values. Thus, the uncertainty intervals are computed assuming that the parameters are known, only taking into account the uncertainty of future innovations (i.e. a_t in eq. 1).

Bootstrap method applied to "with measures" scenarios (WM)

Other techniques (resampling, i.e. bootstrap) have been applied to compute the uncertainty associated to the WM scenario emission projections[8].

They consist of the evaluation of statistics through resampling or subsampling of the original data (i.e. WM scenario[2]). The most popular resampling techniques in the literature are the jackknife[14, 15] and the bootstrap[13]. The jacknife consists of, for a sample of size *n*, obtaining n new artificial samples of size *n-1* by deleting in turn each of the observations and computing the n estimates corresponding to each artificial sample; we thus obtain a sample of size *n* of the estimator, which can be used to estimate variances and compute confidence intervals. The bootstrap is a more sophisticated version of artificial sampling: given the original sample of size n, we obtain new artificial samples by selecting at random with replacement n elements of the sample. We could obtain n^n different possible artificial samples with this procedure, in practice we are restricted to more reasonable size e.g. 10000. A new value of the estimator can now be obtained for each of the 10000 samples and, by means of a procedure equivalent to the one applied in the jacknife, this sample of estimator values can be used to estimate variances and compute confidence intervals.

Simplified method based on Sensitivity Analysis applied to "with measures" scenarios

As an alternative to obtain uncertainty bands for WM scenario, a method based on sensitivity analysis has been developed. It easies the procedure since it does not need any advanced statistical tool. However, it is not as accurate and well established as the previous option.

The method consists of six steps:

1. Selection of the most relevant sectors from the emissions point of view
2. List the key factors driving emissions for each selected sector
3. Analysis of the influence of each factor on emission both at sectoral and national level
4. Definition of the most probable range of variation for each factor based on statistical analyses (standard deviation of values from past years) and expected evolution of drivers in the future (GDP, population, Policies and Measures, etc.)
5. Computation of the variation effect on national total emissions using factor values within the abovementioned ranges
6. To derivate uncertainty bands from results on a national scale

RESULTS AND DISCUSSION

WoM scenario using ARIMA method

The methodology has been applied to the 20 key emission sources in Spain for the period

2001-2020, using historical data from 1990-2000. For the inventory data up to 2006 these activities coverages (proportion of real values inside bootstrap forecasting intervals) are, in most of the cases, reasonably close to the theoretical ones (50, 70 , 90 and 95%).

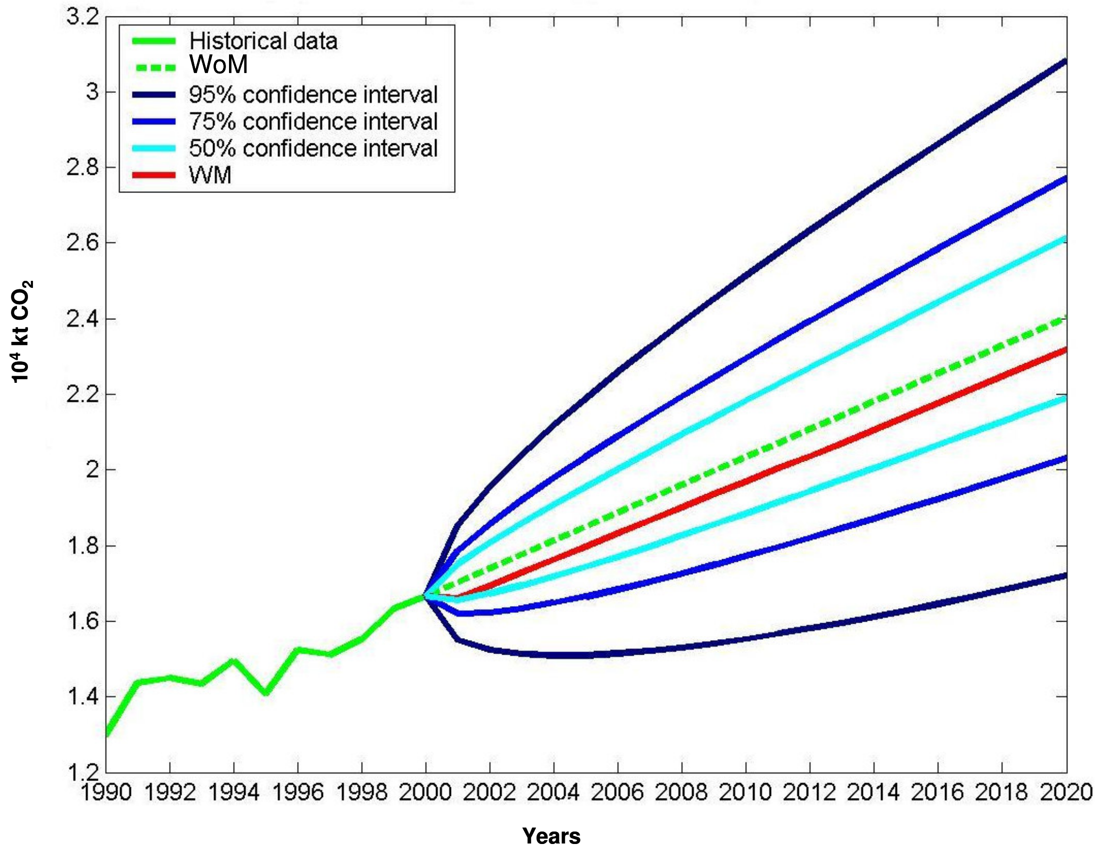

Figure 1. Uncertainty bands for WoM scenario for CO_2 from combustion plants in the residential sector

As an example, Figure 1 presents the result for combustion plants < 50 MW (boilers) in the residential sector. The historical emission series for the period 1990-2000 is shown, along with the projection intervals for 2001-2020. It also includes the "With Measures" (WM) scenario figures, with the purpose of observing if they fall in the intervals of the WoM scenario. If this is not the case it could be interpreted that the measures to be taken to reach the WM scenario constitute a significant improvement versus the WM scenario falling inside the WoM bands. In this example, CO_2 emissions under the WM scenario fall in the 50% projection interval. This situation means that the measures included in the WM scenario may not imply future emission reductions with respect to the WoM scenario, so the expected measures do not significantly alter the past trend.

WM scenario using bootstrap method

The bootstrap techniques were also applied to the 20 key sources for Spain. This application allows the computation of WM scenario uncertainty bands and, therefore, it is possible to assess the effect of P&M on the fulfillment of emission objectives included in Protocols and Directives.

As an example, uncertainty bands for CO_2 from combustion plants in the residential sector[8] are shown. We have selected the same activity as for the first method to compare results. Figure 2 provides the original and differenced series as well as the value of the Bayesian Information Criterion (BIC) used to select the order of the AR(p) model. It can be seen that the minimum for the BIC is obtained for an autoregressive model of order 8, thus an AR(8) is fitted and the residuals for this model are obtained. Figure 3 shows 1000 bootstrap replications of the process (historical data, 1990-2000) and WM scenario 2001-2020 (in bold) while Figure 4 shows the resulting bootstrap forecast intervals. A small degree of uncertainty can be expected in the effects of the measures included in this scenario. For this particular case, this is related to the low potential effect of the measures

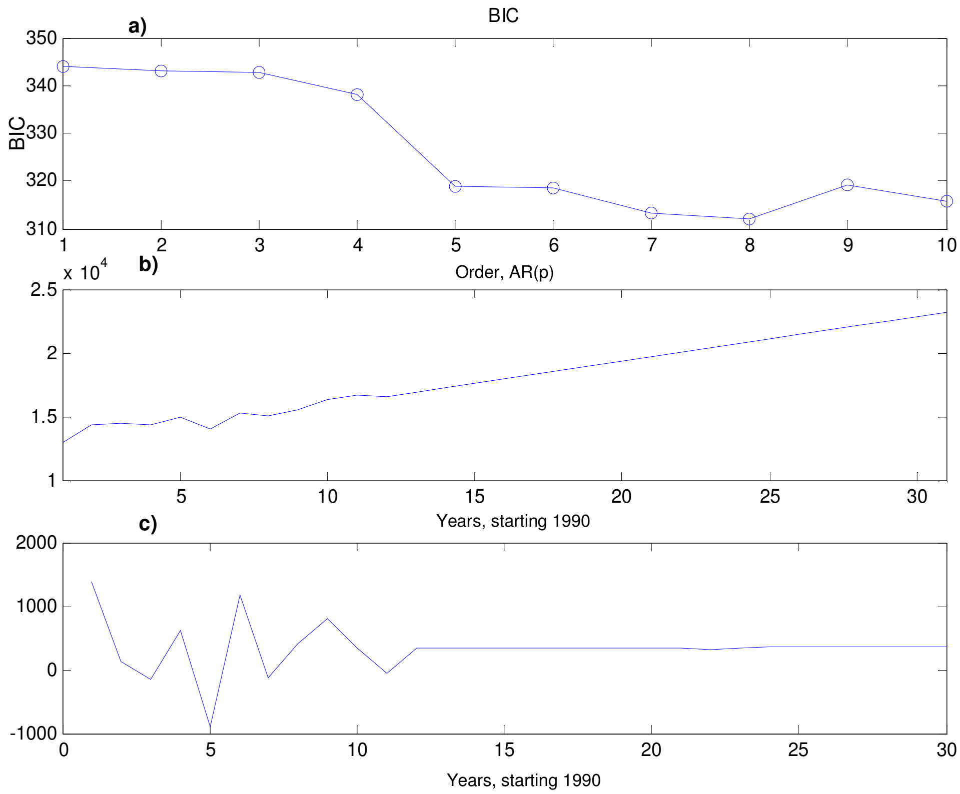

Figure 2. a) BIC for different orders of autoregressive models, AR(p), fitted for differenced series. b) Original, and c) differenced series CO_2 from combustion plants in residential sector

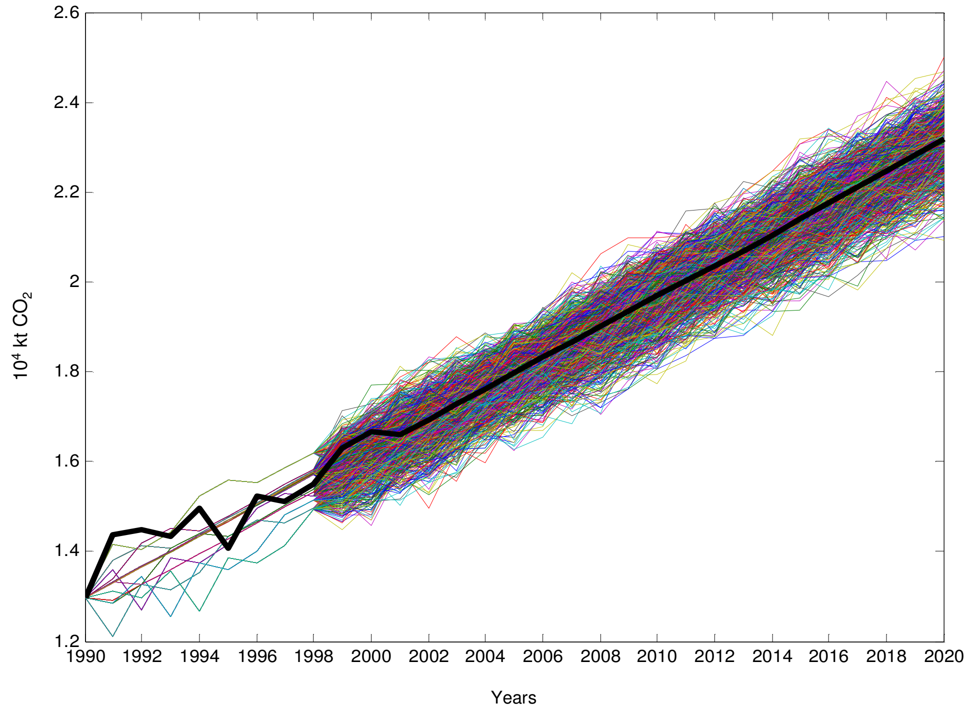

Figure 3. Bootstrap replicas for CO_2 from combustion plants in residential sector

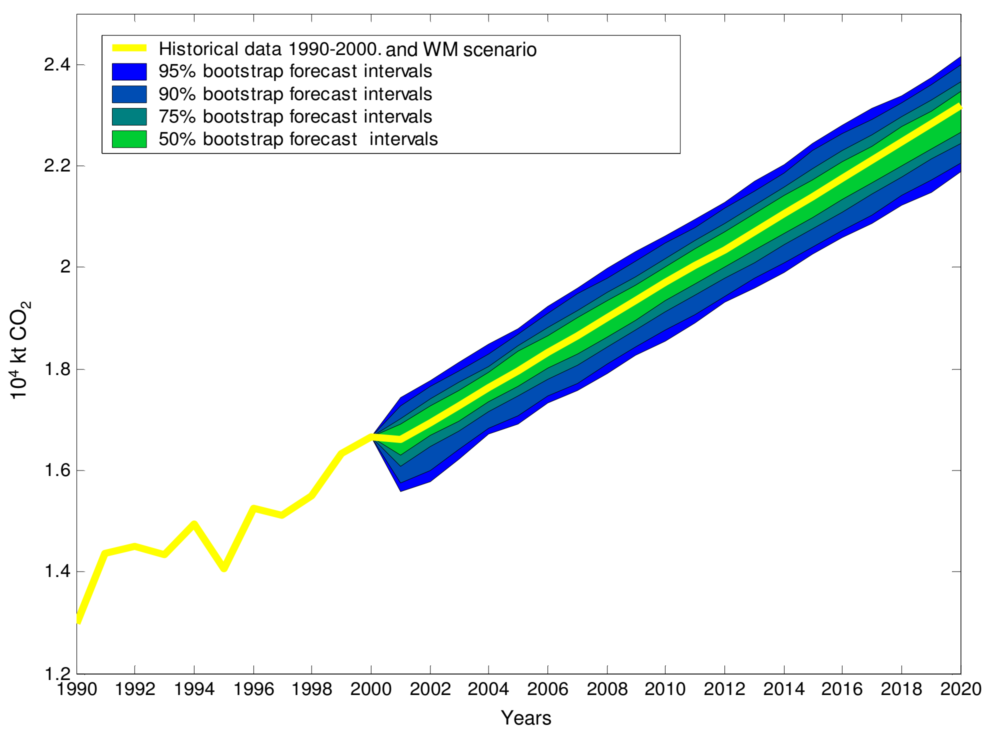

Figure 4. Emission projections for CO_2 from combustion plants in residential sector under "With Measures" scenario.

A comparison of the results from both methods for this activity shows that uncertainties under "with measures" scenario are lower due to the dispersed evolution of past values along with the smooth trend expected for the future. In other cases, especially where effective policies and measures are likely to be applied in the future, uncertainties are greater and the contrary situation is observed.

WM scenario derived from Sensitivity Analysis

Uncertainty bands for total national projections were calculated following the steps presented in section 2. The sectors selected for Sensitivity Analysis are shown in Table 1.

Afterwards, the driving factors were identified. An analysis of their influence on emissions was done by varying their values and calculating associated emissions. Finally, the most probable range of variation was determined for the calculation of emission bands. Table 2 and Figure 5 show these steps for the agricultural sector (cultures, enteric fermentation from animals, manure management and use of pesticides and limestone).

Table 1. Sectors selection including their contribution to national emissions

Sector	SO_2	NOx	NMVOC	NH_3	CO_2	N_2O	CH_4	SF_6	HFC	PFC	$PM_{2.5}$
Power Plants	70,6%	19,4%	0,8%	0,0%	28,0%	1,8%	0,2%	0,0%	0,0%	0,0%	7,1%
Residential sector	1,1%	1,2%	4,0%	0,0%	5,0%	0,7%	1,5%	0,0%	0,0%	0,0%	16,3%
Combustion in industry (except cement)	8,5%	15,3%	2,8%	0,0%	15,2%	1,6%	0,4%	0,0%	0,0%	0,0%	3,4%
Cement sector	1,5%	3,4%	0,2%	0,0%	7,9%	0,3%	0,0%	0,0%	0,0%	0,0%	0,5%
Aluminium	0,3%	0,1%	0,0%	0,0%	0,2%	0,0%	0,0%	0,0%	0,0%	55,5%	0,4%
Solvent and painting use	0,0%	0,0%	37,3%	0,0%	0,2%	0,0%	0,0%	0,0%	0,0%	0,0%	0,0%
Refrigeration equipments	0,0%	0,0%	0,0%	0,0%	0,0%	0,0%	0,0%	0,0%	76,1%	43,0%	0,0%
Electric equipments	0,0%	0,0%	0,0%	0,0%	0,0%	0,0%	0,0%	100,0%	0,0%	0,0%	0,0%
Road transport	0,2%	31,7%	17,5%	1,8%	26,5%	8,9%	0,4%	0,0%	0,0%	0,0%	24,6%
Rail transport	0,0%	0,25%	0,05%	0,0%	0,1%	0,1%	0,0%	0,0%	0,0%	0,0%	0,2%
Waste management	0,0%	0,1%	0,0%	1,7%	0,2%	0,2%	18,2%	0,0%	0,0%	0,0%	0,0%
Agriculture (including livestock)	1,2%	8,7%	11,5%	94,6%	2,1%	56,9%	59,7%	0,0%	0,0%	0,0%	0,0%
TOTAL	**83%**	**80%**	**74%**	**98%**	**85%**	**71%**	**81%**	**100%**	**76%**	**98%**	**52%**

Table 2. Most probable range for agricultural factors

Factor	Upper limit	Lower limit
Agricultural surface	+ 4 %	- 4 %
Inorganic fertilization rate	+10	-10
Number of dairy cows	+ 4 %	- 4 %
Number of other cattle	+ 4 %	- 4 %
Number of fattening pigs	+ 4 %	- 2 %
Number of sows	+ 4 %	- 2 %
Number of ovine	+ 4 %	- 4 %
Number of laying hens	+ 4 %	- 4 %
% of urea use	+ 2 %	- 4 %

Results are shown in Figure 6. They have been compared with re-computed emission trends under a low economic growth situation (LEG scenario). This scenario was calculated applying also the CEP model to Spain but considering new economic forecasts for 2009-2011 that considered the financial and economic crisis. These forecasts provide new activity rates (electricity consumption, industrial production, mobility, etc.) and macroeconomic values (GDP, population, prices, etc.). Results for LEG scenario are within uncertainty bands but very close to the lower values. This shows that bands are able to reflect possible variation on activity rates due to external conditions such as the current crisis.

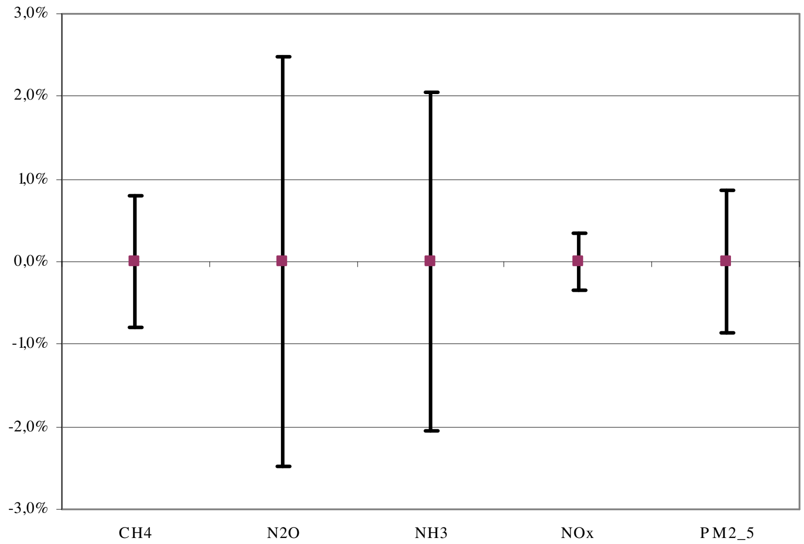

Figure 5. Emission projections sensitivity analysis for agricultural sector (factors changes effect on national emissions).

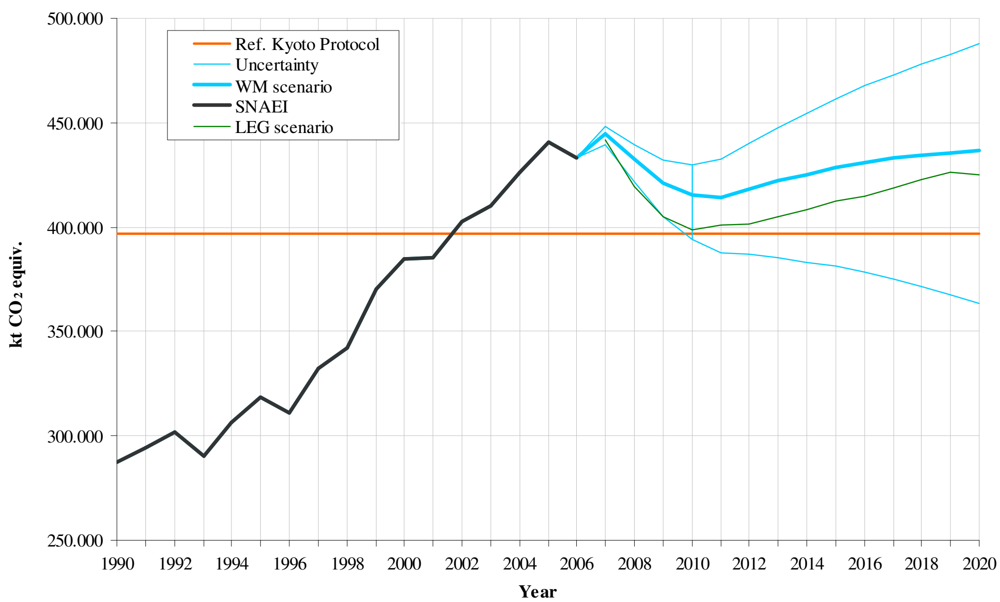

Figure 6. Uncertainty bands for CO_2 eq emissions under WM scenario

CONCLUSIONS

Uncertainty bands for Spain’s emission projections were obtained using three different methods; each applied to different emission projection scenario.

1) For the “without measures” (business as usual) scenario, the ARIMA methodology has produced forecast intervals, which quantify uncertainty. The intervals have been computed assuming gaussianity for the residuals. ARIMA models are an important sophistication with respect to

regression models.

2) For the “with measures” (baseline) scenario, where the starting point were the annual projected values computed by means of the CEP methodology applied to Spain, two contributions are included in this paper:

a) the incorporation of stochastic modeling to produce forecast intervals by means of non parametric bootstrap methods. The essential added value of non parametric techniques is that they are not restricted to distributional assumptions, thus being of more general application.

b) the calculation of uncertainty bands based on sensitivity analyses carried out for the most pollutant sectors

From the application of the first method for the most important activities in Spain in terms of emissions it was found (although not shown) that in most of the cases WM projections fall within the WoM uncertainty bands. However, when effective policies and measures are expected for the future, the trend has inflection points and the values of future emissions are close to the boundaries of the bands. Intervention analysis can be applied in future research to quantify the effect of these policy changes.

The second method allows the calculation of uncertainty bands for the scenario used to evaluate compliance of international commitments. It provides a better estimate of future situation. However, it would be necessary to carry out the uncertainty analyses for the total national emission projections, i.e. for the sum of individual emissions over all activities. This raises the problem of how uncertainties are added up, which is highly dependent on the correlation between emissions for different activities. This would provide a means of computing the total uncertainty when evaluating compliance.

The third method quantifies this total uncertainty in a more simple way. It has been applied for Spanish projections showing a very good performance. Moreover, it has been compared with re-computed emission trends in a low economic growth perspective, providing a good test of the method. It appears as a good possibility to carry out uncertainty assessments for countries that are currently developing sensitivity analyses.

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KEY WORDS

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