Parte C: DOCUMENTO CIENTÍFICO. Máximo 20 páginas.

C.1. PROPUESTA CIENTÍFICA

C.1. 1. Los antecedentes y estado actual de los conocimientos científico-técnicos de la materia específica del proyecto, incluyendo, en su caso, los resultados previos del equipo de investigación y la relación, si la hubiera, entre el grupo solicitante y otros grupos de investigación nacionales y extranjeros

1. INTRODUCTION

The intercontinental transport and the hemispheric pollution by ozone and particulate matter (PM) affect the ecosystems and have a strong impact on climate change (IPCC, 2007; Monks *et al.*, 2009). The effects of air pollution have multifaceted consequences for human wellbeing in areas such as health (WHO, 2013). According to a recent study of the European Environmental Agency (EEA), air pollution is the environmental factor with the greatest impact on health in Europe and responsible for the largest burden of environment-related diseases (EEA, 2014).

Exposure to air pollutants is largely beyond the control of individuals and requires action by public authorities at the national, regional and international levels. In this sense, the current European Directive on ambient air quality and cleaner air for Europe (2008/50/EC) establishes the basic principia of a European common strategy to set the air quality objectives to avoid, prevent or reduce the harmful effect on the health and the environment. One of the topics in which the European Commission has shown a greater concern is the necessity of developing actions that allow increasing the knowledge on transport and dynamics of pollutants to assure the accomplishment of legislation and to inform the population about the levels of pollutants based on the rules for reporting on ambient air quality (2011/850/EU).

In spite of emissions of main air pollutants in Europe have declined significantly in recent decades as a result of several emission reduction measures, the European annual limit values for NO_2 (annual) and PM10 (daily) were exceeded at 42-43% of traffic stations in 2011. The complex links between (precursor) emissions, meteorology factors and atmospheric chemistry means that lower emissions have not always produced a corresponding drop in atmospheric concentrations (Monks *et al.*, 2009). Relatively high levels of pollutants are usually associated to the close proximity of high precursor emissions and as a result of industrial and societal developments. However, the distribution of ambient air pollution is not only dependent on the spread of those emissions, but is also affected by meteorological factors.

To understand the large and widespread problem we that we have in our cities to attain NO_2 AQ standards we have to look at the real-life NO_2 emissions of diesel passenger cars in urban driving condition which are higher than emissions produced for the EURO test driving cycles (Williams and Carslaw, 2011). EURO 4 (2005) and EURO 5 (2009) standards have had a very clear benefits on PM emissions from diesel passenger cars, but not on abating urban ambient PM concentration, neither for reducing NO_2 emissions. Furthermore, the proportion of diesel cars has markedly increased in many European fleets due to the support given to the use of diesel fuel by climate policy.

Recent findings highlight the existence of significant spatial variability in PM levels, both at a regional level and within large urban agglomerations (Eeftens et al., 2012) and thus the issue of spatial scale is of particular importance for the characterization of particle pollution. At a large geographical scale the variability is driven by differences in emission profiles and intensities, climatic characteristics and long range transport processes. On the other hand, within the urban e suburban setting, PM level contrasts are mainly determined by traffic conditions, local sources and topographic characteristics, leading to large intra-urban variations, with severe implications for the characterization of population exposure.

In the Iberian Peninsula a number of studies (e.g. Millán *et al.*, 1997; Querol *et al.*, 2004, 2008; Escudero et al., 2007) shows that the Iberian Peninsula exceeds the limit values of air quality established in the legislation for PM. Additionally, not only the anthropogenic pollution contributes decisively to the failure in the meeting of European directives. In the Iberian

Peninsula, the mineral fraction of suspended particles comes from the local re-suspension and external contributions such as the Saharan/Sahelian dust (Pay *et al.*, 2012a). The latter contributes to the exceedances of the PM10 limit values of Directive 2008/50/EC (Artíñano *et al.*, 2001; Rodríguez *et al.*, 2002).

Under this perspective, ESAP bases on the necessity of understanding the sources contributing to urban air pollution in Spain with the aim of obtaining a precise characterization about their origins that allows to support the design of effective emissions control programs to improve air quality. The quantification of the contribution of various emission sources from specific geographic areas or emissions sources to pollutant levels at particular location is name Source Apportionment (SA). For that purpose, ESAP will develop and apply an *ad hoc* SA toolbox within CALIOPE, which is an air quality modelling system providing forecasts with high spatial and temporal resolution over Spain. The development and application of the CALIOPE for source culpability assessment (CALIOPE-SA) involves a novel to increase the knowledge about the origin of air pollution in main Spanish urban areas, since up to date there are no studies providing information of pollutant formation from predefined geographical regions and/or chemical precursors in the Iberian Peninsula using a mesoscale photochemical model taking into account pollutants with nonlinear responses.

2. SOURCE APPORTIONMENT TECHNIQUES

Application of the SA techniques is targeted for the emerging and scientifically challenging topic of quantifying the impacts of sources in air quality. This task can be accomplished using three main approaches: emission inventories, source-oriented models and receptor models. From the receptor point of view, Belis et al. (2014) define SA as the practice of deriving information about pollution sources and the amount they contribute to observed air pollution levels. From the source point of view, Cohan and Napelenok (2011) describe SA as the practice of quantifying the contributions that different source types (e.g. vehicle exhaust, coal combustions) and different geographic regions (local, regional, etc.) make to pollutant concentrations and depositions.

The source-oriented models (i.e. Chemical Transport Models) are able to provide a more complete and satisfactory analysis of sources contributions evaluation for primary and secondary pollutants as well as taking into consideration complementary phenomena like dry and wet deposition. Moreover, these models can provide detailed resolution of concentrations in terms of space and time. Some of the greatest disadvantages are the high computational burden during simulations and the big storage memory to store the output files as well as skilled professionals required to manage them and to understand the results. On the other hand, the Receptor Models (e.g. chemical mass balance and positive matrix factorization) (Hopke, 1985; Viana et al., 2008), are very versatile tools thanks to their simplicity in terms of input data. They use information about emission fingerprints and so have the advantage of not require detailed emission inventories. Due to the fundamental principle of mass conservation between emission sources and the study site, complex meteorological and chemical processors are not required therefore the computational burden is low. The main disadvantages lie on the domain that has to be limited in size, limited in terms of sources number and type of pollutants investigated. Source-oriented models provides similar, but often complimentary and more specific, type of information about contributors as receptor-oriented SA techniques (Ivey et al., 2015).

SA in photochemical models may be conducted by a brute-force method zeroing out sources one by one, but this may become computationally prohibitive if many emitters are of interest.Thus, a host of tools has been implemented to enable more efficient probing of SA relationship in air quality models (Cohan and Napelenok, 2011). Recently, photochemical models have been instrumented with a variety of extensions allowing for the estimation of source contribution. Approaches to PM source apportionment include Particulate Source Apportionment Technology (PSAT) implemented in CAMx (Wagstrom et al., 2008). Recently, other CTMs have been implemented this tool. The LOTOS-EUROS model has been adapted to contain source apportionment based on PSAT over the Netherlands (Kranenburg et al., 2013). On the other hand, the Integrated Source Apportionment Method (ISAM) has been implemented in the CMAQ model version 5.0.1 (Kwok et al., 2013; 2015).

Current rules for reporting to the EC on source apportionment (2011/850/EU) are based on the method of Lenschow et al. (2001) named as “incremental approach” that uses observed PM10 concentration at stations located at different locations (regional, urban background, and kerbside of a busy street) to estimate source apportionment. Other policy tool is the GAINS integrated assessment model which is employed in the revision of the EU Thematic Strategy on Air Pollution to test the impacts of different pollution control options and calculate least cost solutions for achieving five policy targets. Modelling scheme implemented in the GAINS integrated assessment model to quantifies the source contribution to urban PM in the EU Member States (MS), using a complex station-based modelling approach (Kiesewetter et al., 2014, 2015) relies on a combination of bottom-up modelling of emissions, with a chain of simplified atmospheric chemistry transport models at different scales, EMEP (0.5º x 0.5º) and CHIMERE (7 km x 7 km).

3. SOURCE APPORTIONMENT STUDIES IN SPAIN

There are several source apportionment studies in Spain based on the relationship between air concentrations and Spanish National Emission Inventory (NEI) and policy actions (Querol et al., 2004, 2014; Kassomenos et al., 2014) indicating that in Spain, more than 90% of NO_2 exceedances are attributed to road traffic emissions. The interpretations of the 2001-2012 trends of major air pollutions in Spain based on observational data attributes the declines of SO_2, NO_x and PM2.5 concentrations to the benefits of European directives on power generation and industrial sources together with a sharp 2007-2008 decrease of coal consumption (Querol et al., 2014). However, as for many European MS, there is an inconsistency with the clear downward emission trends and the NO_x reported by the Spanish NEI (MAGRAMA, 2013) and the much less marked trends of observed NO_2 concentrations attributed to the low efficiency of EURO 4 and 5 standards in reducing real life urban driving NO_2 emissions (Williams and Carslaw, 2011). This demonstrates the low impact of the national, regional and local actions on the vehicle related NO_2 emissions. The NEI evidences a marked decreasing trend for primary PM emissions only form the road traffic sector (MAGRAMA, 2013), but the sharp decrease in observed PM2.5 concentration is in agreement with the decrease of the national emissions of PM precursors (SO_2 and NO_2) from power plants caused by the 2008 implementation of the EC Directive on Large Combustion Plants, which contribute to reduce the formation of ammonium sulfate and nitrate (Querol et al., 2014).

Serval source apportionment studies applying receptor modelling at some sites in Spain are focused on PM10 and PM2.5 for identifying sources (Pey et al, 2013). Amato et al. (2009) applied those techniques to data from an urban background site of Barcelona (Spain) to quantify the contribution of road dust resuspension to PM10 and PM2.5 concentrations, which reveals that resuspension was responsible of the 37% of the total traffic emissions in PM10.

Source apportionment studies based on brute force has been applied by the Earth Science Department to analyze the impact of single sector to SO_2 and NO_2 concentrations. For instant, Baldasano et al. (2014) analyzed the impact of the Tenerife’s refinery the urban SO_2 concentration and Valverde et al. (2015a) quantified the contribution of Spanish coal-power plant to NO_2 and SO_2 concentrations under typical synoptic patterns. Recently, in collaboration with the Atmospheric Modeling and Analysis Division (AMAD) at the National Exposure Research laboratory of the Environmental Protection Agency of United States it has been tested for the first time the ISAM to the analysis the origin of ozone pollution in Spain (Pay et al., 2014a). Other applications has been extended to study the contribution of traffic emissions to O_3 concentrations in Madrid and Barcelona (Valverde et al., 2015b).

4. HIGH-RESOLUTION AIR QUALITY MODELLING IN SPAIN: THE CALIOPE SYSTEM

CALIOPE (Pay et al., 2014b) is a complex system that integrates a meteorological model (WRF-ARW), an emission processing model (HERMES, Guevara et al., 2013), a chemical transport model (CMAQ) and a mineral dust dynamic model (BSC-DREAM8b) together coupled in an air quality modelling system. CALIOPE encompasses a high-resolution air quality modelling system which provides 48-h air quality forecasts in Europe (12km x 12km) and Spain (4km x 4km). The system has been widely evaluated during its development over the Iberian Peninsula (Pay et al., 2012a and references there in) and Europe (Pay *et al.*, 2012b and references there in). Furthermore, it has been used for assessing on the contribution of atmospheric processing affecting the dynamic of air pollution and as management tool to study air quality impact of urban management strategies (Soret *et al.*, 2014).

The source separation using CTMs is determined by the level of detail in the emission model. As previously discussed, distinguishing emissions not only by source sector (e.g. road transport exhaust emissions) but also by major fuel type (e.g. diesel) allows identifying with a high degree of detail what is the role that different combustion processes and use of fuels play in the air quality problem. Currently, emissions estimated by HERMESv2.0 are distinguished by source sector level according to the SNAP nomenclature. In the case of road transport (SNAP07), emissions are also differentiated between exhaust, evaporative, wear and resuspended. Splitting the emissions by fuel types will be interesting for residential combustion and transport, because they are main sources of NO_x and PM in urbanized regions.

Furthermore, another basic aspect of an emission model is the representativeness of the activity data and emission factors that characterize the pollutant sectors considered in it. HERMESv2.0 estimates road transport emissions at road stretch level using COPERT IV, an average-speed traffic model that estimates emissions of air pollutants using speed-dependent emission factors that are characteristic of a given vehicle type (EEA, 2009; Ntziachristos et al., 2009). The vehicle average speed data currently used in HERMESv2.0 is constant (not time dependent) and derived from automatic traffic recorders, default free-flow speed information and other traffic survey data. The use of Floating Car Data (FCD) can be used to produce consistent speed at specific roads (Gühnemann et al., 2004; Yu and Peng, 2013) which allow to better characterize speed profiles at each one of the individual road elements that conform the Spanish digitalized road network map.

CALIOPE for source culpability assessment (CALIOPE-SA) will be enhanced in two modules. First, the Community Multiscale Air Quality (CMAQ) will be augmented with a source apportionment algorithm, named ISAM. Second, the HERMES model will be expanded to generate emissions in a consistent multi-year database and provide emissions by socio-economic categories and fuel type. Moreover, the implementation of a new method to calculate traffic emissions based on FCD will improve the emissions characterization in cities. The period of study in the ESAP project will be constraint by the availability of activity data. The HERMES model will be updated to the most recent year with reliable activity data (currently 2013) by means of compiling activity factors from national to local official sources. Activity data for 2004 and 2009 is available for HERMES according to Baldasano et al. (2008) and Guevara et al. (2013), respectively.

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C.1. 2. La hipótesis de partida y los objetivos generales perseguidos

Establishing the origin of air pollution is a complex puzzle as air concentrations are a resultant of heterogeneous emission patterns and complex atmospheric formation routes which interact with prevalent meteorological conditions and the local topography.

The **initial hypotheses** supporting the objectives of the project are:

1. Despite a general improvement expected for the next decade, some urban areas and some regions will still struggle with severe air quality (AQ) problems and related **health effects** in the next two decades. The majority of the European population lives in urban environments where citizens are frequently exposed to levels of air pollutants exceeding the limit values established by the European directives.
2. Urban areas are among the territories where most energy is consumed and most greenhouse gases (GHGs) are emitted. The sources of pollution in cities are mainly linked to **urban activities** such as transport and heating. Other activities such as energy production, industrial activity, agriculture and trans-boundary pollution play an important role.
3. Urban areas are often characterized by specific environmental and anthropogenic factors and will require ***ad hoc*** **additional local actions** to complement medium and long term national and EU-wide strategies to reach EU air quality objectives.
4. There is a necessity **to develop tools** that allow increasing the knowledge on transport, dynamics and origin of pollutants to (i) assure the accomplishment of legislation, (ii) design strategies to fight against air pollution in urban environments and against climate change, ensuring the involvement of the main pollution-generation sectors, and (iii) inform the population about the levels of pollutants.
5. **Numerical air quality models** simulate the complex interactions between pollutant precursor emissions, meteorology, atmospheric chemistry, and deposition. In application for control strategies, they are often useful to quantify the contributions that different source types (e.g., vehicle exhaust, coal combustions) and different geographic regions make to pollutant concentrations and depositions. This practice is referred to as source apportionment.
6. **Air pollution and climate change** are strongly connected and there is therefore a need to consider both environmental and climate considerations when designing emission abatement strategies. Integrated approaches are needed to find long-term, sustainable solutions in the EU.

The **ESAP project aims** at establish a comprehensive and consistent source apportionment analysis of air pollution concentration in urban areas in Spain attributing emission categories and areas to PM and NO_2 concentrations. For that purpose, the project will develop a source apportionment toolbox for Spain based on the CALIOPE system that will be augmented with two extensions developed specifically for the present project. First, with SA algorithm tracking secondary pollutants. Second, with an improved and extended version of the HERMES emission model. Furthermore, the toolbox will be use to assess the changes of emission categories in the period 2004-2009-2013, and to assess the sensitivity of modelled concentration in such approaches.

The ESAP goal is in agreement with the general objectives of several national plans and programs. ESAP contributes to the objectives defined by the ***"Estrategia Española de Ciencia y Tecnología y de Innovación 2013-2020"*** promoting the formation of new research personnel and the stabilization of the staff of BSC-ES. In the last 10 years the group has contribute to the formation of 19 Ph.D. candidates, now working in national and international research centers and universities. The present project aims to continue this important task of formation and will stimulate the mobility of the research staff among national and international research institutions. The promotion of the excellence in the research of the group is one of the key goals defined by BSC. It is worth mentioning that BSC has been selected as one of the Severo-Ochoa awarded centers, by the Ministry of Economy and Competiveness, recognizing its contribution to the excellence in the scientific work developed by the center. The work performed on atmospheric modeling strongly contributes to the development of cutting-edge technologies.

On the other hand, the objectives of the present proposal are in agreement with the research lines defined by the ***"Plan Nacional de Calidad del Aire y Protección de la Atmósfera 2013-2016: Plan aire"*** of the Ministry of Environment. The Plan identifies PM and NO2 as the critical pollutants to monitor and over which further modeling activities are required. One of the targets of the Plan is the emission reduction of precursors of secondary aerosols. Mostly 40% of PM10 is composed of secondary aerosols. In this sense, the modeling tools under development in the present project will provide valuable information about the sources contributing to secondary PM and will allow identifying those mechanisms that may impact on their reduction in the atmosphere. Concerning the actions to promote the research, the Plan identifies air quality modeling as a key topic where the Spanish research community has to further increase its expertise. Models need to be improved with advanced tools that allow to increase the knowledge on air pollution. The ESAP has as first objective the improvement of the current CALIOPE system to perform SA studies which provides to the administration the required information to activate information actions or mitigation strategies to improve the air quality of our urban and rural areas.

Furthermore, the topic of the present proposals responds to the objective defined in the "**HORIZON 2020 Social Challenge on climate action, environment, resource efficiency and raw material"** which is to achieve a resource efficient and climate change resilient economy and society, the protection and sustainable management of natural resources and ecosystems, and a sustainable supply and use of raw materials, in order to meet the needs of a growing global population within the sustainable limits of the planet's natural resources and eco-systems. In this sense, the improvement and evaluation of air quality modeling system and the advancement in the anthropogenic forcing that are enhancing the climate change are key areas of research at the European level. The present project is also in line with the "**HORIZON 2020 challenge of demonstrating the concept of Citizen Observatories"**. Speed data profiles based on Floating Car Data (FCD), which is a type of crowd-sourced data collected from citizen's positioning (GPS) or cellular-based systems, will be used in the present project with the aim to improve the estimation of Spanish road transport emissions.

C.1.3. Los objetivos específicos, enumerándolos brevemente, con claridad, precisión y de manera realista (acorde con la duración prevista del proyecto).

1. Improvement of the HERMES emission model to multi-year studies, support source apportionment application, and to better reproduce traffic emission in urban areas.
2. Development of an efficient SA toolbox within the CALIOPE system that provides consistent contribution of sources and regions to urban pollution in Spain. The quantify the robustness of the SA toolbox will be done within the FAIRMODE intercomparison exercise
3. Quantification of the contribution of emission categories (SNAP) and geographic regions (local, regional, national and long-range) to PM and NO2 concentrations in main Spanish urban areas in 2013
4. Understanding the processes (meteorology or emission) driving urban air pollution changes during the study period 2004, 2009 and 2013 taking into account the model uncertainty for trends analysis.

C.1.4. El detalle de la metodología propuesta, incluyendo la viabilidad metodológica de las tareas. Si fuera necesario, también se incluirá una evaluación crítica de las posibles dificultades de un objetivo específico y un plan de contingencia para resolverlas.

For the present project 5 persons from the research team and 5 persons from the working team are envisaged to achieve the objectives proposed. Three external scientists will be part of the working team, Dr. Claudio Belis (JRC), Dr. Leonor Tarrasón (NILU) and Dr. Sergey Napelenok (US EPA). Two PhD students (Victor Valverde and Lorenzo Fileni) working on air quality modelling in Spain will contribute in the analysis and interpretation of the results. Complementing the team, 1 Junior Informatic Engeneer will be hired to perform the technical activities of implementing new codes and managing the simulations. In order to achieve the proposed objectives, it has been defined the six activities and related tasks. A contingency plan for expected constraints and risks is foreseen.

Activity 1: Project management and monitoring of the project progress

Objective 1: to manage and coordinate the members of the groups and the resources to deliver the activities as scheduled to achieve the project objectives.

Task 1.1. Project management

- To manage and coordinate protocols and resources to deliver the actions as scheduled to achieve the project objectives.
- To report on technical and financial progress to the Ministry.
- To release staff, equipment and final accounts as necessary.

Task 1.2. Monitoring of the project progress | Participants: PI

- Implement a project management software based on a free web-based application (e.g., the Trello free software) to keep informed all the member of the group (reseach and work) about the status of the projects (deadlines, delivelables, new, anouncement, etc.) and to revise the progress of the project according to the approved work plan.
- To evaluate the costs according to the budget.
- To identify and apply corrective actions when required.

Participants: The PI of the project will lead this Activity.

Activity 2. Modelling emissions for source apportionment studies

Objective 2: to improve the HERMES emission model from v2.0 to v3.3 to multi-year studies, support source apportionment, and better reproduce traffic emission in urban areas.

Task 2.1. Development and implementation of a multi-year activity input database (2004 - 2009 - 2013)

- Updating of the activity input database for the most recent year with activity data available (2013 currently). It involves:compiling activity factors from national to local official sources with special focus on: (i) the energy and industrial and (ii) the road transport sector (updating of the vehicle activity data and the vehicle fleet composition, including new Euro vehicle categories currently not considered, e.g. Euro 5 and Euro 6 passenger cars). For the year 2004, the activity database used in the previous version of HERMES model.
- Set-up the HERMESv3.1 to be use for multiyear activity (i.e. 2004, 2009, 2013) which facilitates the integration of any activity data from national, regional and local sources whenever it is available.
- Comparison the emission results estimated with HERMESv2.0 for the years 2004, 2009 and 2013 against the official emissions reported by the Spanish NEI. This action will allow to assess the consistency of the results obtained with the HERMESv2.0 model.

Task 2.2. Categorization of emissions by major fuel type

- The HERMESv3.1 will be extended to v3.2 to output estimated emissions by emission categories not only by sector but also by major fuel type. The classification by fuel types will be performed to residential combustion and road transport sectors, including the following fuel identifiers: (i) gasoline, (ii) diesel, (iii) LPG, (iv) natural gas, (v) fuel-oil, (vi) coal and (vii) biomass.
- The results of emissions distinguished by fuel identifier will be contrasted against the fuel detailed TNO_MACC-III emission inventory. TNO_MACC-III is the updated version of the previous TNO_MACC-II inventory (kuenen et al., 2014) and it is currently used in the source apportionment inter-comparison exercise promoted by the FAIRMODE WG3.

Task 2.3. Improvements of traffic emissions using speed data derived from Floating Car Data

- Collect and process the RACC to produce consistent speed profiles linked to each one of the individual road elements that conform the Spanish digitalized road network map (unique value for hour-of-the-day and day-of-the-week.

- Update the HERMESv3.2 to process time-dependent speed profiles from FCD (HERMESv3.2).
- Sensitivity study for the city of Barcelona to analyze the effect of the speed input parameter on the overall calculation of road transport emissions using COPERT IV. A comparison will be carried out between estimated emissions derived using hourly speed data from FCD with the base case using flat speed data profiles. For this task a visit to Leonor Tarrasón (NILU), who is the current leader of FAIRMODE WG2, is foreseen to supervise actions on the application of best practices techniques (use of speed data derived from Floating Car Data) for the compilation of traffic emissions. Both activities focus on providing emissions data representative for urbanized regions.

Participants: This activity will be led by Marc Guevara, expert on emission models. For Task 2.1, Task 2.2 and Task 2.3 the participation of a hired informatics engineer is foreseen. The support of Oriol Tinto (PhD student in computer science) will be useful for optimization of the codes in the model. The PI will monitor the full activity.

Activity 3. Modelling air quality for source apportionment analysis

Objective 3: to set-up an efficient SA toolbox within the CALIOPE system that provides consistent contribution of sources and regions to urban pollution in Spain.

Task 3.1. Simulation of the meteorological fields

- Set-up of the meteorological model following the CALIOPE system set up described in Pay et al. (2012): EU mother domain at 12-km resolution, and nested domain over Iberian Peninsula at 4-km resolution, 33 vertical levels.
- Simulation of meteorological fields for 2004, 2009 and 2013, which implies 6 simulation 3 for the EU domain and 3 for the nested domain.

Task 3.2. Simulation of the source contributions

- Set-up of the CMAQ-ISAM within the CALIOPE system to be able to generate the contribution from sectors and source to pollutants. Furthermore, the code will be improve to increase it computational efficiency, for that issue this task involves a short collaboration with the model developer (Sergey Napelenok) and the involvement of the hired informatical engineer working together. At some point, the support of Oriol Tinto, PhD student in optimizing sources of High Performance Computing application will be required.
- Generation of chemical boundary condition to the Spanish domain for the year of study (2004, 2009, 2013). Global boundary conditions will be downloaded from the EMEP climatological data. Regional boundary conditions will be estimated ad hoc for every year with the CALIOPE system running at 12-km resolution over Europe (3 annual simulations over Europe).
- Simulations of source apportionment fields for 2004, 2009 and 2013 for sources and regions. These simulation will be done in parallel with the regional simulations. The management of the simulation (control, storage and post-processing) will be performed by the hired IT due to high volume of technical work.

Task 3.3. Model performance evaluation

- Compilation and analysis of meteorological (temperature, wind direction, wind speed, precipitation, etc.) from the METAR network over Spain for the years: 2004, 2009, and 2013.
- Compilation and treatment regulatory pollutants concentration (O3, NO2, SO2, PM10 and PM2.5) from public available data from Spanish monitoring network data (including AIRBASE), background concentration from EMEP (www.emet.int) for the years 2004, 2009, and 2013. At the same time, the IDAEA-CSIC (that acts as "ente promotor observador") will provide measurements of chemical components of PM.
- Model performance evaluation (MPE) will be performed by comparing air quality simulations against observed data of regulatory pollutants and PM chemical components. It is a mandatory step before performing any source apportionment analysis and quantify the model uncertainty. MPE will be performed using the Delta tool, which is a software developed in the framework of FAIRMODE.

Task 3.4. Quantifying the robustness of the source apportionment technique in the context of FAIRMODE

- Set-up the CALIOPE-SA to the prescribe domain and receptors in the model intercomparison exercise for the reference site Lenz in France. Run the simulation for the period of study: summer and winter
- Compared the CALIOPE-SA performance with other Source apportionment techniques and estimate the uncertainty. Claudio Belis from the woking group will be in charge of this task.

Participants: this activity will be led by the PI. The meteorological simulation will be set-up and run by Antonis Gkikas, with high expertise in meteorology over the Mediterranean. Simulation in Task 3.2 and 3.3 will be done by the hired engineer. Oriol Tinto will support on the optimization of the codes for source apportionment. Task 3.3 will be done for the two PhD student in the working group, due to their experiences in managing model outputs.

Activity 4. Quantify the contribution of emission categories and geographic regions to urban air pollution in Spain

Objective 4: Quantify the contribution of emission categories (SNAP) and geographic regions (local, regional and long-range) to PM and NO2 concentrations in main Spanish urban areas in 2013

Task 4.1. Quantify the contribution of emission categories (SNAP)

- Estimation from different categories using the ad hoc extended version of the HERMES model (Activity 1) which allow specific source classification detailing fuels for SNAP 2 and 7. Particularly, emissions due to combustion in the civil sector will be split according to five fossil fuels plus solid biomass. Emissions from road transport sector will be split according to three main fuels (gasoline, diesel and LPG/natural gas), while non-exhaust sources includes evaporation and wear.
- Estimation the contribution of the following emission categories (SNAP): power plants (1), fossil fuels combustion in domestic sector (21-25), biomass burning in domestic sector (26), gasoline road transport (71), diesel road transport (72), other exhaust emissions in road transport (73-74), wear emission and resuspended paved road (75), international shipping (81-82), and agriculture (10).

Task 4.2. Quantify the contribution of regions in urban areas

- Definition of regions in main urban areas in Spain in terms local emissions, regional emission and long-range transport. The criteria will be defined based on population and land-use categories from CORINE Land Cover.
- Analyze the contribution of emission regions over the main urban areas with more than 500.000 inhabitants (i.e., Madrid, Barcelona, Valencia, Sevilla, Málaga y Zaragoza)

Participants: this activity will be led by the PI. The Task 4.1 will be performed by the PI with the support of Antonis Gkikas in the analysis of the dust contribution. Also the participation of Marc Guevara on the emission interpretation is foreseen. Task 4.2 will be will be performed by the PI with the support of Antonis Gkikas and the PhD students in the working group.

Activity 5. Analyze the variability of source contributions to urban air pollution in Spain for the years 2004-2009-2013

Objective 5: to understand the processes (meteorology or emission) driving urban air pollution changes during the study period 2004, 2009 and 2013 taking into account the model uncertainty for trends analysis. Furthermore, the source apportionment practice to the methods suggested by the European Commission.

Task 5.1. Quantifying the increment of emissions in the period of study: 2004-2009-2013.

- Interpretation of the change of major air pollutants emission (NOx, CO, SOx, NMVOCs, NH3, PM10 and PM2.5) by sectors in Spain during the period of study (2004-2009-2013).

- Identification and link of the main drivers of these trends to the results obtained (e.g. major policy actions and financial crisis).

Task 5.2. Sensitivity of modelled trends compared with observation

- Calculate trends over three years for observed and modelled concentrations of regulatory pollutants.
- Evaluate the CALIOPE system's performance to reproduce concentrations of regulatory pollutant a long different years identifying uncertainties in meteorology, emission and physical and chemical processes.

Task 5.3. Trends analysis of the contribution of activity sectors in Spain

- Interpretation of the meteorological change for the years 2004-2009-2013 using the simulation of Activity 3.
- Interpretation of the change of emission category contributions to PM and NO2 concentrations. This results will be linked with the efficiency of the European and regional policies in urban environments in terms of emissions and air quality, meteorological conditions and economic activity.

Task 5.4. Comparison of source apportionment techniques with current method used in the Air Quality Directive.

- Estimation of the contribution of regions based on the rules for reporting on ambient air quality (2011/850/EU), named as "the incremental approach". For this task a visit to Claudio Belis at JRC is foreseen to apply the method of incremental approach in main cities in Spain.
- Estimate the uncertainty of incremental approach and SA based on CTM to reproduce the temporal variability (different emissions and meteorological fields) over main cities in Spain.

Participants: this activity will be led by the PI. The Task 5.1 will be performed by Marc Guevara as expert on emissions. Task 5.2 will be done by the two PhD student who previously have compiled the observations. Task 5.3 will be performed by the PI with the support of Marc Guevara. Task 5.3 will be done in collaboration with Claudio Belis.

<u>Activity 6. Dissemination of the project results</u>

Objective 6: to inform about the development ESAP and its results to scientific communities, stakeholders and specialized audience, for contributing to increasing consciousness about environmental problems and actions that government and civil society need to implement to solve them.

Task 6.1. Communications of project results on conferences and workshops

- Participation in three FAIRMODE technical meetings which are organized on regular basis ones a year dedicated to model experts to develop and agree on common methodologies, carry out actual benchmarking and establishing good procedures and guidance.
- Participation in three international conferences: the Community Model and Analysis System (CMAS) conference, theInternational Technical Meeting on Air Pollution Modelling and its Application (ITM) and the Harmonization within Atmospheric Dispersion Modelling for Regulatory Purposes (HARMO) to present the ongoing work of the project and discuss with the scientific community about its impact.
- Organization of two meetings during the execution of the project. First, a kick-of meeting to present the ESAP objectives, to get feedback and to engage potential participants. Second, final project meeting to disseminate the ESAP results and the lessons learned as a mean to contribute to the return of the investment in the project. Both meetings will be addressed to small and medium enterprises interested in the project, national and regional authorities, specialized audience and scientific communities.
- Five personalized talks addressed to stakeholders are foreseen: MAGRAMA, Catalonia Government, RACC, Barcelona Harbour, and EUROCITIES.

Task 6.2. Publications of project results

- Three publications in international scientific journals.
- A project web page inside the department website.
- Leaflet addressed to general audience.
- A technical report with the project results to stakeholders.

Participants: All the members will be involved in the dissemination task. Organization of meeting, training and diffusion to general audience will be a task of Montserrat Gonzales, who is member of the Training and communication group as BSC.

Risks and contingency plan

Organizational risk

- Member not willing or not able to perform their commitments. In each task the contribution of more than one partner is foreseen. This choice will allow to cover a wider range of situations as well to introduce a higher degree of flexibility in organizing different activities. The PI will be involved in all the tasks monitoring the process, distributing human resource accordingly, and giving support if one member is not able to perform their commitments if no replacement.

Technical risks:

- High volume of technical tasks in the implementation of new codes and algorithms in the SA toolbox, as well as the management of computational demanding simulations. The technical work is foreseen to be done by RG3 together with the two-years hired IT.
- Big data set (~8 TB). The storage at the MareNostrum Supercomputing to each user to 1TB. The acquisition of two external disk is foreseen in the budget.
- Computational resources. The BSC-ES is allowed to use the certain percentage of the MareNostrum supercomputer, this computation hours are shared among their members. The application to more resources to the Spanish Network of Supercomputing will be foreseen.

C.1.5. La descripción de los medios materiales, infraestructuras y equipamientos singulares a disposición del proyecto que permitan abordar la metodología propuesta.

The project application will be run at the MareNostrum Supercomputer. BSC-CNS hosts MareNostrum, the most powerful supercomputer in Spain. In March 2004 the Spanish government and IBM signed an agreement to build one of the fastest computer in Europe. With the last upgrade (2012-2013), MareNostrum has a peak performance of 1,1 Petaflops, with 48,896 Intel Sandy Bridge processors in 3,056 nodes, and 84 Xeon Phi 5110P in 42 nodes, with more than 100.8 TB of main memory and 2 PB of GPFS disk storage. In June 2013, MareNostrum was positioned at the 29th place in the TOP500 list of fastest supercomputers in the world. Marenostrum is also part of the PRACE Research Infrastructure as one of the 6 Tier-0 Systems currently available for European scientists. Marenostrum will be used as main computing facility for the executions required by the project. Different ground-based and satellite observations will be included in the evaluation of the model simulations. Data from EMEP, AIRBASE, and the Spanish Monitoring Network. Air quality observations from the EBAS (http://ebas.nilu.no) database will be used for the evaluation of the aerosol composition over Europe. EBAS is a database hosting observation data of atmospheric chemical composition and physical properties and it is developed and operated by the Norwegian Institute for Air Research (NILU).

C.1.6. Un cronograma claro y preciso de las fases e hitos previstos en relación con los objetivos planteados en la propuesta

Table 1 shows the chronogram of the ESAP project along the 36 months. Deliverables (D) and Milestones (M) are indicated related to the objectives (O) where each member of the group is associated to the different tasks. Furthermore, the following paragraphs list and describe the milestones and deliverables corresponding to project month (PM), and related task (T) as shown in the chronogram.

Table 1. Working plan

Objectives	RRHH	1st year												2nd year												3rd year											
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
Activity 1. Project management and monitoring of the project progress																																					
Task 1.1. Project management	PI												D1						D2						D3												D4
Task 1.2. Monitoring of the project progress	PI	M1																	M2																		
Activity 2. Modelling emissions for source apportionment studies																																					
Task 2.1. Development and implementation of a multi-year activity input database (2004 - 2009 - 2013)	PI, RG1, RG3, IT			M3																																	
Task 2.2. Categorization of emissions by major fuel type	PI, RG1, RG3, IT						M4	D5																													
Task 2.3. Improvements of traffic emissions using speed data derived from Floating Car Data	PI, RG1, WG2, RG3, IT									M5	D6	D7																									
Activity 3. Modelling air quality for source apportionment studies																																					
Task 3.1. Simulation of the meteorological fields	PI, RG2										M6		D8																								
Task 3.2. Set-up of the chemical transport model for source apportionment	PI, WG3, IT												M7				D9				D10				D11												
Task 3.3. Model performance evaluation	PI, WG4, WG5															D12									D13												
Task 3.4. Quantifying the robustness of the source apportionment technique in the context of FAIRMODE	PI, WG1																		D14																		
Activity 4. Contribution of emission categories and regions to urban air pollution in Spain																																					
Task 4.1. Quantify the contribution of emission categories (SNAP)	PI, RG1, RG2																					D15															
Task 4.2. Quantify the contribution of regions in urban areas	PI, RG2, WG4, WG3																								D16												
Activity 5. Variability of source contributions to urban air pollution in Spain for 2004-2009-2013																																					
Task 5.1. Quantifying the increment of emissions in the period of study: 2004-2009-2013.	PI, RG1												D17																								
Task 5.2. Sensitivity of modelled trends compared with observation	PI, WG4, WG5																												D18								
Task 5.3. Trends analysis of the contribution of activity sectors in Spain	PI, RG2																																D19				
Task 5.4. Comparison of CALIOPE-SA with incremental approach	PI, WG1																																			D20	
Activity 6. Dissemination of the project results																																					
Task 6.1. Communications of project progress and results on conferences and workshops	all	M8					D22				D23								D25	M9 D27		D28									D30			D31			M10
Task 6.2. Publications of project results	all		D21										D24							D26					D29											D32 D33	D34

Pincipal Investigator (PI): MT. Pay | Research Group (RG): M. Guevara (RG1), A. Gkikas (RG2), O. Tinto (RG3), M. González (RG4) | Working Group (WG): C. Belis (WG1), L. Tarrasón (WG2), S. Napelenok (WG3), V. Valverde (WG4), L. Fileni (WG5) | Informatic Engeneerier (IT): hired person.

O1: Project management and monitoring of the project progress (Activity 1).
Period (Project Month, PM): PM01-PM26 (total = 36 months)
M01 | PM02 | T1.2 | Web-based application for the management of ESAP Activities (A1-A6).
M02 | PM18 | T1.2 | ESAP progress meeting.
D01 | PM12 | T1.1 | First year annual report.
D02 | PM18 | T1.2 | Minutes of internal meeting on ESAP progress.
D03 | PM24 | T1.1 | Second year annual report.
D04 | PM36 | T1.1 | Final year annual report.

O2: Improvement of the HERMES emission model (Activity 2).
Period (Project Month, PM): PM01-PM11 (total = 11 months)
M03 | PM03 | T2.1 | HERMESv3.1 to multiyear emissions calculation (2004 - 2009 - 2013) .
M04 | PM06 | T2.2 | HERMESv3.2 to estimates emissions by source and fuel type.
M05 | PM09 | T2.3 | HERMESv3.3 to integrate hourly speed profiles based on FCD.
D05 | PM07 | T2.3 | Set of modelled emissions (netCDF) for A4 and A5.
D06 | PM10 | T2.3 | Report on emissions inventories comparison: HERMESv3.3, NEI and TNO_MACC-III.
D07 | PM11 | T2.3 | Report on sensitivity analysis to speed data in traffic emissions calculation.

O3: Set-up an efficient SA toolbox within the CALIOPE system that provides consistent contribution of sources and regions to urban pollution in Spain (Activity 3).
Period (Project Month, PM): PM10-PM24 (total = 15 months)
M06 | PM10 | T3.1 | Set-up of the WRFv3.5 for the European and the Spanish domains.
M07 | PM12 | T3.2 | Set-up of SA toolbox based on CMAQ-ISAM within the CALIOPE system.
D08 | PM12 | T3.1 | Meteorological dataset for SA simulations in T3.2.
D09 | PM16 | T3.2 | SA dataset (sector and regions) for 2013.
D10 | PM20 | T3.2 | SA dataset (sector and regions) for 2009.
D11 | PM24 | T3.2 | SA dataset (sector and regions) for 2004.
D12 | PM15 | T3.3 | Meteorological and air quality dataset for 2004, 2009, and 2013.
D13 | PM24 | T3.3 | Report on MPE using the DELTA tool.
D14 | PM18 | T3.4 | Report on CALIOPE-SA robustness within the FAIRMODE intercomparison.

O4: Quantify the contribution sources (categories and regions) to urban air pollution in 2013 (Activity 4).
Period (Project Month, PM): PM19-PM24 (total = 6 months)
D15 | PM28 | T4.1 | Report on SA by emission categories over main Spanish urban areas.
D16 | PM32 | T4.2 | Report on SA by regions over main Spanish urban areas.

O5: Understand the processes driving urban air pollution changes during the study period 2004, 2009 and 2013 taking into account the model uncertainty for trends analysis (Activity 5).
Period (Project Month, PM): PM11-12, PM25-PM35 (total = 13 months)
D17 | PM12 | T5.1 | Report on emission changes in 2013-2009-2004.
D18 | PM28 | T5.2 | Report on sensitivity of modelled concentration to emission changes.
D19 | PM32 | T5.3 | Report on SA changes in 2013-2009-2004.
D20 | PM35 | T5.4 | Report on SA compared with other methods.

O6: Inform about the development ESAP and its results (Activity 6).
Period (Project Month, PM): PM1-2, PM6, PM10, PM12, PM18-19, PM21, PM24, PM30, PM33, PM35-36 (total = 13 months)
M08 | PM01 | T6.1 | Kick-off meeting and stakeholder consultation.
M09 | PM19 | T6.1 | Stakeholders information: Five personalized presentations to stakeholders.
M10 | PM36 | T6.1 | Final project meeting.

D21 | PM02 | T6.2 | Web-site section on the ESAP desciption inside the BSC-ES website.
D22 | PM06 | T6.1 | Mission report on the FAIRMODE technical meeting.
D23 | PM10 | T6.1 | Mission report on the CMAS conference addressed to WG and SG.
D24 | PM24 | T6.2 | Scientific paper 1.
D25 | PM18 | T6.1 | Mission report on the FAIRMODE technical.
D26 | PM19 | T6.2 | Leaflet on the preliminary results of the project.
D27 | PM19 | T6.1 | Mission report on the meeting with stakeholders.
D28 | PM21 | T6.1 | Mission report on the ITM conference.
D29 | PM24 | T6.2 | Scientific paper 2.
D30 | PM30 | T6.1 | Mission report on the FAIRMODE technical meeting to WG and SG.
D31 | PM33 | T6.1 | Mission report on the HARMO Conference.
D32 | PM35 | T6.2 | Update Web-site section of ESAP project with final results.
D33 | PM35 | T6.2 | Technical report of the project results.
D34 | PM36 | T6.2 | Scientific paper 3.

C.1.7. Si se solicita ayuda para la contratación de personal, justificación de su necesidad y descripción de las tareas que vaya a desarrollar.

The ESAP project plans to apply for one contract devoted to the capacitation of one PhD student, whose research will be an extended analysis of source apportionment studies to ozone pollution, which is another regulatory photochemical pollutant with high number of exceedances in Spain. The PhD thesis will take the advantage the scientific objectives and the precise working plan defined in the proposal, together with its developments. The availability of the PhD student will not be a limitation for the ESAP progress, since this PhD thesis will be an extension of the project results to other regulatory pollutant. The tasks of this PhD thesis will be the same as those planned for ESAP. The capacitation of one PhD student will be on (1) the development and application of sophisticated numerical model, (2) the increase of knowledge on the chemical and physical processes that drive ozone formation, transport, and deposition, and (3) the improve of communication and writing skills by means of publications and presentations. These issues will contribute to (1) expand the knowledge on source apportionment studies to ozone pollution, (2) reinforce the capacity building of the Earth Science Department, and (3) to increase the diffusion of the results. The PhD student will be involved in the framework of the PhD in Environmental Engineering at the Technical University of Catalunya (UPC). This Doctorate programme had the MEC Quality Mention until 2010 (MCD2004-00394) and presently has MEC Excellence Mention from 2011 (MEE2011-0335).

C.2. IMPACTO ESPERADO DE LOS RESULTADOS

C.2.1. Descripción del impacto científico-técnico social y/o económico que se espera de los resultados del proyecto, tanto a nivel nacional como internacional.

The ESAP project will promote the generation of scientific knowledge about the causes of air pollution in urban areas and guide on the mitigation plans, promoting the synergies between different scientific groups, companies and governments. ESAP boosts the I+D+i actions on the efficient use of resources and raw materials related to economic-activity sectors (transport, residential, commercial, energy, agriculture, etc.) will allow a sustainable development of the society. ESAP quantifies the emissions and the contribution of socio-economic activity sectors to the air quality, taking into account the processes that contribute to the generation of secondary pollutants and the influence of climatic and geographical variables. For that purpose, ESAP develops an extended version of the CALIOPE air quality forecast system that allows the identification of socio-economic activities and geographical areas contributing to air pollution in Spanish urban areas. In other words, ESAP fosters the integration of advanced tools for the assessment and modelling air quality with the idea of testing innovative technological options and strategies to improve air quality in urban areas. The BSC-ES, qualified and experienced research group, will design and develop the toolbox architecture, adapt and optimize existing tools and conceive those that are necessary but not yet available.

The scientific and technical impacts will contribute to support to EU air policy at the Spanish level, to guide the societal transformation to a green economy, to improve air quality in Spanish cities in the medium- to long-term, to reduce the negative effects on health together with the cost associated with air pollution in Spain, and to materialize the goals of the Smart Cities and Communities Innovation Partnership.

The small and medium enterprises involved in the project (RACC and Barcelona harbor) will provide new technological concepts and solutions for specific sectors like the on-road traffic and shipping. National (MAGRAMA) and Regional (Generalitat de Cataluña) governments will contribute to the demonstration phase of the project, and to share best practices through peer to peer learning tools. In addition, thanks to the support of the EUROCITIES environment forum, 5 Spanish cities will be indirectly involved in the project by providing feedback to the tools and methodology tested. The modelling activities will be developed in agreement with and with the endorsement of the Forum for Air Quality Modelling (FAIRMODE) which is joint response initiative of the European Environment Agency (EEA) and the European Commission Joint Research Centre (JRC) that sets quality assurance rules for air quality modelling. Communication and information exchange with FAIRMODE is ensured because Marc Guevara (BSC) is currently co-chairing FAIRMODE WG2 on Emissions, and María Teresa Pay (PI) is member of both the WG1 on Assessment and WG3 on Source Apportionment.

A high profile Advisory Board, including, the EC Joint Research Centre, the Atmospheric Modeling and Analysis Division (AMAD) at the National Exposure Research laboratory of the Environmental Protection Agency of United States (US EPA), and the Norwegian Institute for Air Research (NILU), which takes part in the implementation of the future Copernicus Atmosphere services, will externally support the project activities.

C.2.2 El plan de difusión e internacionalización en su caso de los resultados

A specific activity on dissemination of the project results (Activity 6) is introduced in the working plan. This activity will be devoted to disseminate the results of the project. Both during the project duration and after completion, the results suitable for dissemination will be published in peer-reviewed international journals (open-access) and/or presented in international meetings and conferences. In addition, results will be disseminated through specialized audience such as stakeholder, companies and populations through leaflets, technical report and adapted talks. A summary of them will also be posted on the web site of the CALIOPE system. Deliverables of the project progress are defined as reports of Activity 1, but the final goal is the publication of the results in international journals. The report format is preferred to avoid the delays on publication process in the working plan of the project. It is expected that part of the results will be published after the finalization of the project.

Two open meeting during the first and the last year of the project are foreseen. A first workshop will be organized in to present the ESAP objectives, to get feedback and to engage potential participants. The second workshop will be conducted at the end of the project to disseminate the ESAP results and the lessons learned as a mean to contribute to the return of the investment in the project. Both meetings will be addressed to small and medium enterprises interested in the project, national and regional authorities (Spanish Environmental Ministry and Generalitat de Barcelona), specialized audience (e.g. air quality platforms) and scientific communities (e.g., FAIRMODE, RETEMCA which is the Spanish network of air quality modellers). Dedicated talks addressed to main identified stakeholders' are foreseen (MAGRAMA, Catalonia Government, RACC, Barcelona Harbour, and EUROCITIES) in order to identify their requirements that can be faced with ESAP. Furthermore, a website about the model and the project will be created to disseminate the activities and results of the project. News about the project will be placed on the News section of the BSC webpage. The experience of the BSC in the organization of international conferences is considered a valuable point for the dissemination activities described. Claudio Belis and Leonor Tarrasón have been organizing on regular basis the FAIRMODE plenary and technical meetings over the last 6 years which brings together modelling experts and national contact point from European Member States and delegates from the DG Environment.

For the internalization of the project the lessons learn on running source apportionment applications in supercomputing platforms will be included in the program of the specialized training courses organized by the PRACE Advanced Training Center and the CUDA Center of Excellence in which the Earth Science Department takes part.

C.2.3. Si se considera que puede haber transferencia de resultados, se deberán identificar los resultados potencialmente transferibles y detallar el plan previsto para la transferencia de los mismos.

The ESAP project will improve the CALIOPE system with a source apportionment toolbox that can be used to support policy makers for the conception, design, and implementation of air quality policies. The scientific outcomes will be disseminated through presentations in international conferences, workshops and publication in international journals. From this dissemination effort contacts may arise with the scientific community to exchange experience and knowledge about the fields of study. On the other hand, several institutions have expressed interest on the project results through letters of supports (avaible for revision). The institutions and the transferred results are as follows:

- **FAIRMODE** is interested in the ESAP project results because it will develop and test toolbox which supports air quality model users in their policy-related model applications and promote good modeling practice among Member States. Furthermore, the project will contribute to the quantification of the robustness of the source apportionment technique within FAIRMODE (model intercomparison exercise, WG3). In additions, ESAP project will apply best practices techniques for the compilation of urban traffic emissions which is in agreement with WG2. The results will be presented in the FAIRMODE Meetings. This will create a framework of collaborations in the context of FAIRMODE and possible publications.
- The **Consejo Superior de Investigaciones Científicas - Institute of Environmental Assessment and Water Studies** (CSIC-IDAEA), a recognize research team with high expertise on characterizing aerosol in Spain will support the ESAP project by means is expertise on the analysis of the results from the source attributions to PM10 and NO_2 concentrations in urban areas in Spain. They highlight that those results are essential for policy makers giving the information about the contribution of different sources to air pollution in Spain.
- **Barcelona harbour** is interested in the results of the ESAP project to increase the knowledge on the contribution of shipping to air pollution in cities. The results of the projects will provided through technical report.
- **Real Automovil Club de Cataluña** (RACC) is interested in the ESAP project because the results of the project increase the knowledge about the application of Floating Car Data in the calculation of the traffic emission, as well as a better understanding on the contribution of on-road traffic to air pollution in urban areas. The results of the projects will provided through technical report.
- **EUROCITIES** is interested in the results of ESAP because the proposed project and the results derived therefrom are a topic of interest to EUROCITIES, which foster the integration of advanced tools for the assessment and modelling air quality – including source apportionment – with the idea of testing innovative technological options and strategies to improve air quality and reduce the carbon footprint of urban areas. The results of the projects will provided through technical report.
- The **Atmospheric Modeling and Analysis Division** at the Environmental Protection Agency of United States is interested in the project because it will involve the continued development, evaluation, and application of the CMAQ based source apportionment methodology. The improvement of the model accuracy and computational efficiency is desired along with developing new evaluation techniques for increasing confidence in the apportionment results. The result of the ESAP project will be presented in the Community Modeling and Analysis System Conference allowing the model user and development communities to share their experiences with air quality models, modeling, and model development. In addition, it is planned to give a technical talk at AMAD to share experience with the model developers.
- **Ministerio de Agricultura Alimentación y Medio Ambiente** (MAGRAMA) and **Generalitat de Catalunya**, as the national and regional governments, is interested in the project results. The ESAP project will provide a priority list of emission categories that

contribute to air pollution in urban areas in Spain as well as the contribution by geographical area. These results will be a decision support information for authorities focused on investing and implementing air quality abatement strategies. Furthermore, the ESAP project will develop a ready-to-use source apportionment toolbox for PM and NO_2 inside the CALIOPE air quality system for Spain that can be used in testing the impact of air quality abatement strategies. The results of the projects will provided through technical report.

C.3. CAPACIDAD FORMATIVA DEL EQUIPO SOLICITANTE

C.3.1. El plan de formación previsto en el contexto del proyecto solicitado.

The BSC-ES is an experienced research group directly involved in training and education activities at national and international level directed to students as well as scientists. During the last years, the team has offered several editions of the four-day PRACE (Partnership for Advanced Computing in Europe) course *"Earth Sciences Simulation Environments at BSC"*, participated in Severo Ochoa Research Seminars at BSC, co-organized the RES (Spanish Supercomputing Network) Earth Science Seminar, participated in the Industry sessions at FIB Barcelona School of Informatics, organized Summer Schools as the 2nd E2SCMS Second European Earth System and Climate Modeling School and participated in the BSC International Doctoral Symposiums.

Moreover, as part of the BSC team, the Earth Sciences Department gets specialized support from the Education and Training team of the same organization, which is fully dedicated to establish a curricula based on cutting-edge scientific research and development of models, software tools and simulation environments for High-Performance Computing and application areas, targeting research communities and industry with supercomputing needs. This curricula includes: Master's Degree in High Performance Computing, PhD opportunities, Master and bachelor final project placements, Specialized training courses organized by the PRACE Advanced Training Center and the CUDA Center of Excellence, Scientific seminars and training courses organized by the Spanish Supercomputing Network, Severo Ochoa Research Seminar Series, BSC International Doctoral Symposium, and International Workshops (e.g. at ISC and SC conferences).

Additionally, BSC staff counts with a professional development plan that is designed for each member of BSC and tailored according to their profile and objectives. The BSC is also awarded with the HR Excellence in Research seal that gives public recognition to research institutions that have made progress in aligning their human resource policies with the principles set out in the European Charter and Code for Researchers.

C.3.2. Relación de tesis realizadas o en curso (últimos 10 años) con indicación del nombre del doctorando, el título de tesis y la fecha de obtención del grado de doctor o de la fecha prevista de lectura de tesis

The applying group takes part of the Earth Science Department of the Barcelona Supercomputing Center, directed by Dr. Francisco Doblas-Reyes. BSC-ES has published 54 peer-reviewed papers in international journals during the last 5 years (http://www.bsc.es/earth-sciences/publications-and-communications) and has presented 19 PhD thesis during the las 10 years (http://www.bsc.es/earth-sciences/phd-thesis). Currently, two PhD thesis are directed by the IP of the project:

PhD Student: Victor Valverde / PhD title: Characterization of atmospheric pollution dynamics in Spain by means of air quality modelling / Supervisors: Maria Teresa Pay and José María Baldasano / University: Technical University of Catalonia (Spain) / Date: From 2012 to December 2015 (Expected)

PhD Student: Lorenzo Fileni / PhD title: Analysis of particulate matter origins in Spain by means of chemical transport model and source apportionment methodology / Supervisors: Maria Teresa Pay and José María Baldasano / Technical University of Catalonia (Spain) / Date: From 2014 to December 2017 (Expected)

C.3.3. Breve descripción del desarrollo científico o profesional de los doctores egresados del equipo de investigación.

Dr. **Maria Teresa** got her B.S. in Chemical Engineering (University of Murcia, Spain, Juny 2006) and PhD in Environmental Engineering with the Degree of European Doctor and the Special Doctoral Award (Technical University of Catalonia, Spain, November 2011). From 2012 to 2014 she worked as a postdoc researcher at École Polytechnique in the "Laboratoire de Météorologie Dynamique" in Palaisaeu (France). Now, she is a scientific researcher at the Earth Sciences department at the Barcelona Supercomputing Center. Her research interest includes atmospheric chemistry, air quality modelling (forecast, evaluation and improvement) and environmental impact assessment to support policies. Since 2012, she is a Marie Curie fellow under the Beatriu de Pinós programme (BP-DGR 2011). She is a scientific expert on the Forum for Air Quality Modelling (FAIRMODE) and in the Task Force on Measurement and Modelling (TFMM) under the EMEP and the United Nations - Economic Commission for Europe (UNECE). She is a member of the ACCENT/GLOREAM community and EURODELTA. She has participated in 8 national (Severo Ochoa, CALIOPE, CONSOLIDER, CICYT, IBERDROLA, Spain-Portugal integrated actions, CALIOPE-AND, CALIOPE-CAN) and 2 European (FP7, LIFE+) research projects. She has co-authored 3 chapters in books, 2 technical reports, and 17 papers in international scientific journals (with 15 publications within the Q1, an 8 h-index and 190 citations, accoding to SCOPUS). Currently, she is supervising 2 PhD Thesis at the Technical University of Catalonia. She co-authored over 50 communications to International conferences. She has acted as a reviewer of several international journals.

Dr. **Marc Guevara** got his B.S. in Industrial Engineering (Technical University of Catalonia, Spain, October 2010) and PhD in Environmental Engineering (Technical University of Catalonia, Spain, December 2014). In 2010 he was enrolled as research support engineer at the Earth Sciences Department of the Barcelona Supercomputing Center, and in 2014 moved to the emission modelling postdoc researcher position. His research interest includes high resolution emission modelling (development, evaluation and improvement), air quality modelling and environmental impact assessment. He is co-chair of the Emissions Working Group of the FAIRMODE community. He has participated in the Spanish air quality-related CALIOPE-And project and the FP7 Framework programme APPRAISAL, as well as in several national technology transfer projects related with air quality impact assessment. He has coauthored 8 papers in international scientific journals and 8 communications to International conferences. He has acted as a reviewer of several International journals.

Dr. **Antonis Gkikas** received his BSc title in 2004 from the Technological Educational Institute of Crete, Greece, in the field of Natural Resources and Environmental Engineering. In 2007, he got his MSc in the field of Meteorology, Climatology and Atmospheric Physics) [MSc thesis: Aerosol optical properties in the broader area of the Mediterranean basin] from the University of Ioannina. In 2012, he got his PhD at the University of Ioannina. He worked as a Postdoctoral Researcher in the Laboratory of Meteorology (University of Ioannina) collaborating with the National Observatory of Athens, the University of Aegean, the University of Crete and Democritus University of Thrace from 2012 to 2014. In 2014, he was granted with a Marie-Curie scholarship. Through this scholarship he is now working as a Scientific Researcher at the Earth Sciences Department of the Barcelona Supercomputing Center. Since 2006, he has worked in 9 research scientific projects, participated as a coauthor in 13 publications in peer-reviewed scientific journals and 42 scientific conference proceedings (10 National and 32 International). In addition, he has participated as a reviewer in four scientific journals. His main scientific interests lie in the field of aerosol and radiation studies, meteorology and atmospheric modelling.

C.4. IMPLICACIONES ÉTICAS Y/O DE BIOSEGURIDAD