Convocatorias 2016
Proyectos EXCELENCIA y Proyectos RETOS
Dirección General de Investigación Científica y Técnica
Subdirección General de Proyectos de Investigación

AVISO IMPORTANTE

En virtud del artículo 16 de la convocatoria **NO SE ACEPTARÁN NI SERÁN SUBSANABLES MEMORIAS CIENTÍFICO-TÉCNICAS** que no se presenten en este formato.

Es obligatorio rellenar los tres apartados (A, B y C). La parte C de la memoria no podrá exceder de 20 páginas.

Lea detenidamente las instrucciones para rellenar correctamente esta memoria, disponibles en la web de la convocatoria.

Parte A: RESUMEN DE LA PROPUESTA/SUMMARY OF THE PROPOSAL

INVESTIGADOR PRINCIPAL 1 (Nombre y apellidos)**:**

Maria Teresa Pay Pérez

INVESTIGADOR PRINCIPAL 2 (Nombre y apellidos)**:**

TÍTULO DEL PROYECTO: Modelización fotoquímica para atribuir fuentes y áreas de emision a altas concentraciones de material particulado en zonas urbanas de España

ACRÓNIMO: PAISA

RESUMEN Máximo 3500 caracteres (incluyendo espacios en blanco):

A pesar de la reducción significativa de emisiones en los últimos años el material particulado (PM) atmosférico es aún una amenaza para la salud humana en zonas urbanas españolas. Futuras estrategias de reducción de emisiones eficientes y focalizadas requerirán un conocimiento preciso del origen de los altos niveles de PM en zonas urbanas. Todavía establecer su origen es un reto complejo porque el PM es resultado de la contribución de diversas fuentes naturales y antropogénicas, complejas vías de formación (procesos físicos y químicos) e interacción con condiciones sinópticas y mesoescalares. En este sentido, las técnicas de contribución de fuentes (SA) pueden permitir evaluar qué actividades económicas determinan la concentración de PM en una localización y cuál es la contribución natural o antropogénica procedente de fuentes locales, regionales y/o de larga distancia. SA es también una información requerida por la Directiva Europea de Calidad del Aire (AQD, 2008/50/CE) sobre zonas que presentan excedencias de los límites de concentración legislados, con el objetivo de definir planes de reducción de emisiones efectivos. El objetivo de PAISA es hacer un salto adelante en nuestra comprensión del origen de las altas concentraciones de PM en las principales zonas urbanas de España y suministrar estimaciones espaciales y temporales de la contribución de diferentes fuentes (actividades y regiones) a los niveles de PM (primario y secundario). Lo relevante de PAISA es desarrollo de un marco de trabajo que incluirá el estado del arte en la emisión de PM, modelización en química de aerosoles, junto con un sistema de atribución de fuentes para basado en el sistema de calidad del aire CALIOPE para España. Los resultados permitirá discriminar la contribución de regiones (urbana, regional, nacional y/o larga distancia), fuentes (naturales y antropogénicas) y de tipo de combustible (diésel o gasolina) para los sectores de tráfico

rodado y combustión residencial, principales fuentes de PM en zonas urbanas. Los resultados de PAISA determinarán en qué medida las concentraciones urbanas de PM están controladas por fuentes antropogénicas específicas y/o por contribuciones regionales o transfronterizas, ofreciendo una mejor información a los políticos en la aplicación y cumplimiento de la AQD.

PALABRAS CLAVE: contribución de fuentes, aerosoles, NO2, SO2, VOC, NH3, aerosoles secundarios, diesel, traffico

TITLE OF THE PROJECT: Photochemical modelling to attribute emission sources and source regions to high particulate matter concentration in urban areas in Spain

ACRONYM: PAISA

SUMMARY Maximum 3500 characters (including spaces):

Despite significant emission reductions in recent years, atmospheric particulate matter (PM) remains as a major health risk factor in Spanish urban areas. Future targeted and efficient reduction strategies will require a precise knowledge of the origin of high PM levels in urban areas. Yet, establishing this origin is a complex challenge because PM results from the contribution from a variety of natural and anthropogenic sources, complex atmospheric formation routes (physical/chemical processes) and interactions with synoptic and mesoscale meteorological conditions. In this sense, source apportionment (SA) methodologies can allow evaluating which economic activities determine the PM concentration at a location and which is the contribution from local, regional, or distant natural and anthropogenic sources. SA is also a mandatory information to report under the European Air Quality Directive (AQD, 2008/50/EC) over non-attainment zones in order to define efficient emission abatement. The aim of PAISA is to make a leap forward in our understanding of the origin of high PM concentrations in main urban areas in Spain and to provide comprehensive spatial and temporal estimates of the contribution from different source classes (activities and regions) to the mixtures of PM components (both primary and secondary). The novelty of PAISA is the development of a framework that includes the state-of-the-art in aerosol emission, modelling and a source attribution system for PM pollution episodes based on the CALIOPE air quality system for Spain. The results will allow discriminating the contribution from regions (urban, regional, national, long-range), sources (natural or anthropogenic) and even further from fuel type (e.i., diesel and gasoline) for on-road traffic and residential combustion activity sectors which are the main sources of PM10 and NOx in urban areas. The outcomes of PAISA will determine to what extent the urban PM concentrations in Spain are controlled by specific anthropogenic sources and/or regional or transboundary contributions, allowing better information to policymakers in the application of the AQD.

KEY WORDS: source apportionment, aerosols, NO2, SO2, VOC, NH3, aerosoles secundarios, diesel, traffic

Parte B: INFORMACIÓN ESPECÍFICA DEL EQUIPO

B.1. RELACIÓN DE LAS PERSONAS NO DOCTORES QUE COMPONEN EL EQUIPO DE TRABAJO (se recuerda que los doctores del equipo de trabajo y los componentes del equipo de investigación no se solicitan aquí porque deberán incluirse en la aplicación informática de solicitud). Repita la siguiente secuencia tantas veces como precise.

1. Nombre y apellidos:
   Titulación: licenciado/ingeniero/graduado/máster/formación profesional/otros (especificar)
   Tipo de contrato: en formación/contratado/técnico/entidad extranjera/otros (especificar)
   Duración del contrato: indefinido/temporal

B.2. FINANCIACIÓN PÚBLICA Y PRIVADA (PROYECTOS Y/O CONTRATOS DE I+D+I) DEL EQUIPO DE INVESTIGACIÓN (repita la secuencia tantas veces como se precise hasta un máximo de 10 proyectos y/o contratos).

1. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay
   Referencia del proyecto: 2011 BP-A 00427, 2011 BP-A2 00015
   Título: Dynamic assessment of atmospheric pollution in the Iberian Peninsula by High-resolution modelling
   Investigador principal (nombre y apellidos): Maria Teresa Pay
   Entidad financiadora: Agència de Gestió d'Ajuts Universitaris i de Recerca
   Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/03/2013 - 29/02/2016
   Financiación recibida (en euros): 111.132,62 €
   Relación con el proyecto que se presenta: mismo tema
   Estado del proyecto o contrato: concedido

2. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay and Marc Guevara
   Referencia del proyecto: 157/PC08/3-12.0, 357/2007/2-12.1, 441/2006/3-12.1
   Título: CALIOPE: Sistema de calidad del aire operativo para España
   Investigador principal (nombre y apellidos): José María Baldasano Recio
   Entidad financiadora: Ministerio de Medio Ambiente. Gobierno de España
   Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/01/2006 - 01/07/2010
   Financiación recibida (en euros): 1.189.285 €
   Relación con el proyecto que se presenta: mismo tema
   Estado del proyecto o contrato: concedido

3. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): María Teresa Pay and Marc Guevara
   Referencia del proyecto: FP7-ENV-2012-one-stage
   Título: APPRAISAL: Air Pollution Policies foR Assesement of Integrated Strategies At regional and Local scales
   Investigador principal (nombre y apellidos): Maria Luisa Volta
   Entidad financiadora: EU
   Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/06/2012-31/05/2015
   Financiación recibida (en euros): 999.989 €
   Relación con el proyecto que se presenta: mismo tema
   Estado del proyecto o contrato: concedido

4. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay and Marc Guevara
   Referencia del proyecto: SEV-2011-00067
   Título: BSC-CNS Severo Ochoa Center of Excellence
   Investigador principal (nombre y apellidos): Mateo Valero Cortés
   Entidad financiadora: MICINN

Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/2012-12/2015
Financiación recibida (en euros): 4.000.000 €
Relación con el proyecto que se presenta: está muy relacionado
Estado del proyecto o contrato: concedido

5. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay
Referencia del proyecto: CSD- REFERENCIA 2007 – 00050
Título: Supercomputación y e-Ciencia, convocatoria CONSOLIDER 2007
Investigador principal (nombre y apellidos): Mateo Valero
Entidad financiadora: MEC-CICYT
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/01/2007 - 31/12/2011
Financiación recibida (en euros): 5.000.000 €
Relación con el proyecto que se presenta: está algo relacionado
Estado del proyecto o contrato: concedido

6. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay and Marc Guevara
Referencia del proyecto: NET838690/1
Título: Development of the air quality forecast system for Andalucía CALIdad del aire OPerativo para ANDalucía
Investigador principal (nombre y apellidos): José María Baldasano Recio
Entidad financiadora: EGMASA S.A. - Agencia de Medio Ambiente y Agua de Andalucía
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/07/2009-31/08/2014
Financiación recibida (en euros): 216.500 €
Relación con el proyecto que se presenta: mismo tema
Estado del proyecto o contrato: concedido

7. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay and Marc Guevara
Referencia del proyecto: CALIOPE_CAN
Título: Development of the air quality forecast system for the Canary Islands CALIdad del aire OPerativo para las Islas CANarias
Investigador principal (nombre y apellidos): José María Baldasano Recio
Entidad financiadora: Consejería de Medio Ambiente y Ordenación Territorial. Gobierno de Canarias
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 22/01/2008-31/12/2010
Financiación recibida (en euros): 198.750 €
Relación con el proyecto que se presenta: mismo tema
Estado del proyecto o contrato: concedido

8. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay
Referencia del proyecto: REPCAN
Título: Determinación del área de representatividad de las estaciones de la red de Control y Vigilancia de la Calidad del aire del Gobierno de Canarias (RVCCAC) utilizando el sistema de calidad del aire CALIOPE
Investigador principal (nombre y apellidos): María Teresa Pay
Entidad financiadora: Consejería de Medio Ambiente y Ordenación Territorial. Gobierno de Canarias
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/09/2015-31/12/2015
Financiación recibida (en euros): 18.000 €
Relación con el proyecto que se presenta: mismo tema
Estado del proyecto o contrato: concedido

9. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Maria Teresa Pay
Referencia del proyecto: REPCAT

Título: Determinación del área de representatividad de las estaciones de la red de vigilancia y previsión de la Contaminación Atmosférica de Cataluña (XVPCA) utilizando el sistema de calidad del aire CALIOPE
Investigador principal (nombre y apellidos): María Teresa Pay
Entidad financiadora: Direcció General de Qualitat Ambiental. Generalitat de Catalunya
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/09/2015-31/12/2015
Financiación recibida (en euros): 18.000 €
Relación con el proyecto que se presenta: mismo tema
Estado del proyecto o contrato: concedido

10. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Marc Guevara
Referencia del proyecto: CPSG/0112A/2015
Título: Desarrollo de un sistema de Pronóstico de calidad el aire
Investigador principal (nombre y apellidos): Marc Guevara
Entidad financiadora: Secretaría de Medioambiente de la Ciudad de México (México)
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/10/2015-31/10/2016
Financiación recibida (en euros): 246.135,19
Relación con el proyecto que se presenta: mismo tema
Estado del proyecto o contrato: concedido

Parte C: DOCUMENTO CIENTÍFICO. Máximo 20 páginas.

C.1. PROPUESTA CIENTÍFICA

1. Introduction and state-of-the-art

The problem of PM: size, chemical composition, and sources

Air pollution by particulate matter (PM) is the environmental factor with the greatest impact on health and responsible for the largest burden of environment-related diseases (EEA, 2015; Lim et al., 2012; WHO, 2014). It is estimated that there were 25,500 premature deaths in 2012 due to exposure to elevated levels of $PM_{2.5}$ in Spain (EEA, 2015). Overall, the health cost of air pollution represents 2.8% of Spanish Gross Domestic Product (GDP) (OCDE, 2015). Not only do PM concentrations determine the effects of particles on human health, but also (1) their size (Pope and Dockery, 2006), (2) their composition (Reiss et al., 2007); and (3) the time of exposure (Pope et al., 2002). Furthermore, the intercontinental transport and the hemispheric pollution by PM affect the ecosystems and have a strong impact on climate change as a function of their chemical nature (IPCC, 2013).

The levels and composition of PM_{10} and $PM_{2.5}$ in the Iberian Peninsula have been widely studied by experimentalists such as Querol et al. (2014 and references therein), Rodríguez et al. (2002) and Viana et al. (2005) and modellers such as Pérez et al. (2006) and Pay et al. (2011, 2012a,b). These studies show the challenge of determining the origin of PM as it results from a variety of local, regional and distant sources, and complex atmospheric formation routes that interact at multiple scales (Millán et al., 1997; Valverde et al., 2014). Figure 1a shows the contributions to PM_{10} from different geographical origins in the Barcelona urban area. At a large geographical scale, the PM variability is driven by differences in emission profiles and intensities, climatic characteristics and long range transport processes. Within urban and suburban settings, PM concentration contrasts are mainly determined by traffic conditions, local sources and topographic characteristics, leading to large intra-urban variations.

Spain is under the influence of natural PM from Saharan dust that contributes to the exceedances of the PM_{10} limit values (Querol et al., 2004; Artíñano et al., 2001; Rodríguez et al., 2002). The Sahara desert is globally the most important dust source (Prospero et al., 2002) and modelling and measurement studies (Querol et al., 2009; Pay et al., 2012a) indicate that its annual contribution to the PM_{10} background concentrations in Spain is around 40% of the PM_{10} in the southeastern Spain. Fugitive dust emissions caused by agricultural activities (i.e. land preparation and harvesting) is also a significant contributor to the primary PM background concentration in Mediterranean countries like Spain, characterised by large agricultural and some semiarid regions and low amounts of precipitation (Schaap et al., 2009).

In Spanish urban areas, on-road transport emissions (exhaust and non-exhaust) and the associated resuspension emissions are unequivocally the most important source of primary PM (Guevara et al., 2014; Amato et al., 2016) together with residential combustion (Figure 1b). Determining the contribution of exhaust and non-exhaust emissions to urban PM level will help designing targeted emission abatement strategies for road traffic, but even further, distinguishing emission contributions to PM by fuel type (e.g. diesel and gas) and exhaust/non-exhaust will contribute to assessing the future of next generation car engines. Improving our knowledge on this distinction is one of the major goals of PAISA.

PM is also formed through gas-to-particle conversion from gaseous precursors (NO_2, SO_2, NH_3 and VOC) or chemical reaction on the primary aerosols. Inorganic gases react in the atmosphere to form ammonium, sulphate and nitrate the so-called secondary inorganic aerosols (SIA). SO_2 and NO_x result from the use of combustion fuels in sectors like energy production, road transport, shipping and industry (Figure 1b). NH_3 is dominantly emitted through agricultural activities as animal husbandry and manure spreading (Figure 1b). Although NH_3 by itself makes a small fraction of the PM mass it plays a decisive role in PM formation chemistry by determining the amount of sulphate and nitrate. SO_x and NO_x declined in Spain by 72% and 32% in the period 2001-2012 and NH_3 emissions have fallen

by only 5% during this period (EEA, 2014). Some studies reveal that the SIA concentrations can only be effectively reduced if all three precursors are reduced to the same extent (Erisman and Schaap, 2014; Pay et al, 2012b; Bessagnet et al., 2014). Because in Spain agriculture is a key sector PAISA will also quantify the role of NH_3 from agriculture in PM levels. Furthermore, a recent study (Bressi et al., 2014) has pointed out that in urban agglomerations like Paris, the long-range transport of SIA is a significant contribution to $PM_{2.5}$ concentrations which suggests that abatement policies implemented at the local or regional level may not be sufficient to notably reduce $PM_{2.5}$ concentrations in this city. Instead, a collaborative work should be conducted between surrounding regions or even countries. Determining the contribution of long-range transport to PM levels in Spanish urban areas is also a key goal of PAISA.

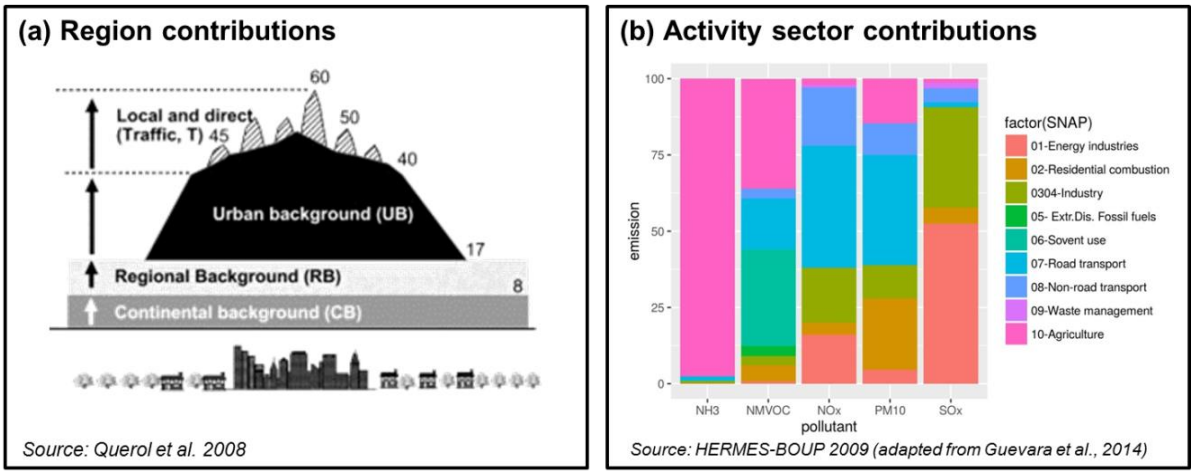


***Figure 1*: The three dimensions of the PM origin: multi-scale, multi-sector and multi-pollutant. (a) Contribution to PM_{10} at different scales. (b) Percentage of annual total emission in 2009 in Spain for main pollutants by SNAP sector.**

Carbonaceous aerosols, consisting of organic and elemental (black) carbon, are emitted by combustion processes and may be formed from natural and anthropogenic non-methane volatile organic carbons (NMVOC) in the atmosphere. Besides fossil fuel combustion, an important contributor to the carbonaceous aerosol burden is biomass burning emanating from residential heating, forest fires and burning of agricultural waste. Recent studies (Amato et al., 2016) have shown that in central and northern Europe biomass burning emissions (mostly linked to wood smoke from fireplace and stoves) present a significant contribution to PM concentrations, meanwhile in northwestern Mediterranean Basin (i.e., Barcelona) this contribution is negligible (< 2%). Overall, the different origin of PM components indicates that different national policies and control strategies might be needed to achieve a reduction of PM on a regional and local scale. The developments within PAISA are designed to contribute to future policies and strategies in Spain.

Management of PM problem in Europe and source apportionment methodologies

Recent studies on trends analysis demonstrate a decrease in PM concentrations in Spain over the last decade, which derive from policy implementations (at European, national and regional scale), the effects of the financial crisis, and meteorological conditions (Querol et al., 2014). Despite tightening of the European emission control legislation, Member States (MS) have been facing severe difficulties to attain PM limit values set by the Air Quality Directive (AQD) in urban areas, and the situation is even more critical with respect to the World Health Organization (WHO) Air Quality Guidelines (AQG). In the period 2011-2013, 87-93% of the urban population was exposed to $PM_{2.5}$ concentration above WHO AQG (i.e. 10 µg$PM_{2.5}$ /m^3 yearly) (EEA, 2015). In the next decades, *ad hoc* additional local actions to complement national and EU-wide strategies will be required in order to reach WHO AQG (EC, 2013).

To define efficient air quality (AQ) plans, source apportionment methodologies are essential to determinate the contribution of main socio-economic activities together with natural sources and the contribution surrounding administrative areas together with the transboundary transport of pollution (Figure 1). Source apportionment (SA) on sources and regions is mandatory to be submitted according to the Implementing Provisions on Reporting

rules (IPR, 2011/850/EU). However, IPR does not precisely guide/recommend about SA methodologies, nor about the list of priority sources. So far, the Source apportionment method widely used among Member States is the incremental approach (Lenschow et al., 2001, also *Lenschow approach*) in which observed PM_{10} at representative stations of regional, urban background, and traffic sites are used to estimate the contribution of different areas and sources (Figure 1a). The Lenschow approach, although valuable, shows several limitations. First, it assumes that rural levels represent the regional background in the cities, which is not always realistic. Second, it cannot be extrapolated everywhere because some sources may have higher contribution in the background area than in the city (e.g. agriculture).

Application of other SA techniques is an emerging field that aims at quantifying the impacts of sources in urban AQ with policy implications. There are two main approaches that are used: the receptor-oriented SA which derives information about pollution sources and the amount they contribute to observed air pollution levels using fingerprints (Belis et al., 2014); and the source-oriented SA which quantifies the contributions that different source types and different geographic regions make to pollutant concentrations and depositions (Cohan and Napelenok, 2011).

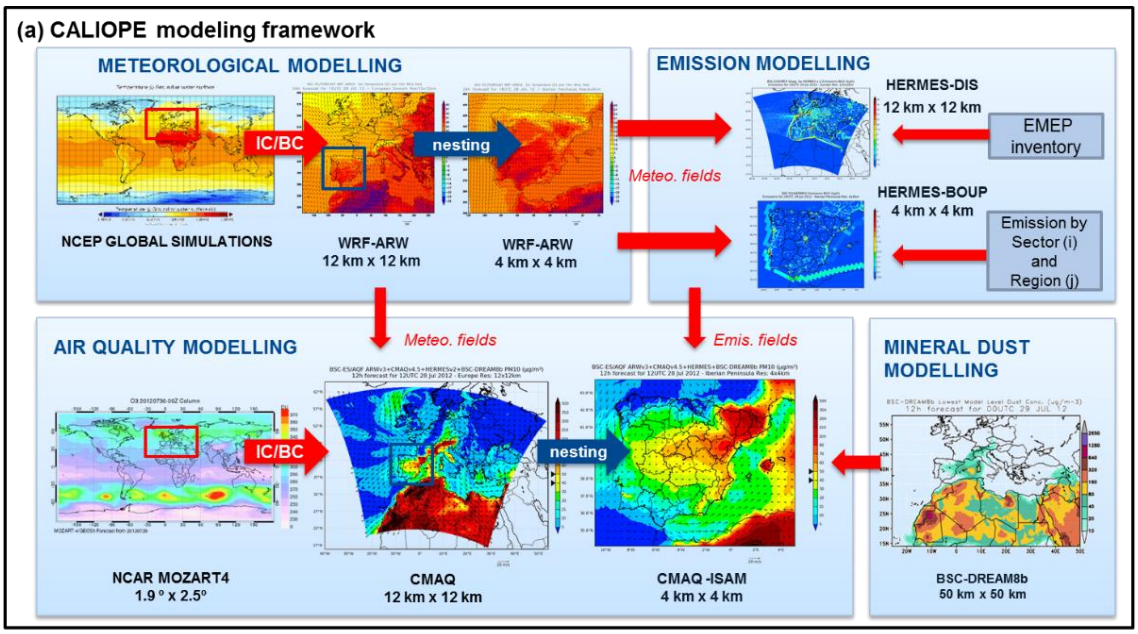
Receptor Models (SA-RM) are versatile tools given their simplicity in terms of input data and atmospheric processes considered. SA-RMs have been applied in Spain to quantify the contribution of specific sector to PM (Viana et al., 2008). Recently, the European AIRUSE project has used SA-RM to characterized PM contribution and sources in urban areas from southern Europe (Amato et al., 2016) and indicates that during high pollution days in Barcelona, the largest sources (i.e. excluding secondary aerosol factors) of PM are vehicle exhaust and non-exhaust (27–22 %). This study reveals that SA-RMs are limited in the domain size (availability of stations), and the sources and type of pollutants, which are critical for tracing the origin of secondary PM species (e.g. sulphate).

Source-oriented models (SA-CTM) provide a more complete analysis of sources contributions in terms of space, time and chemical composition taking into account complementary phenomena like dry/wet deposition and primary/secondary aerosol formation. However, SA-CTMs are based on urban and regional air quality models that include uncertainties in the meteorological, emission and physical and chemical processes (Rouil and Bessagnet, 2013).

SA-RM and SA-CTM provide similar, but often complimentary, type of information about contributors that can be used to establish synergies (Hu et al., 2014; Bove et al., 2014; Ivey et al., 2015). For instance, the SPECIEUROPE (Pernigotti et al., 2016), a new database of PM emission source profiles in Europe, can be used to improve air quality modelling in European applications. There are no direct methods to quantify the uncertainty in the source attribution since there are no measurements quantifying the contributions. In this sense, the Forum for Air quality Modelling (FAIRMODE) has launched an inter-comparison exercise to evaluate the behaviour of both approaches (SA-RM and SA-CTM) in order to assess the European Commission about their performance. The CALIOPE air quality system for Spain, which is the main tool developed and used in PAISA, together with other with other regional model is taking part of this initiative.

Air quality modelling in Spain: state-of-the-art

Several operational air quality forecasting systems exist for Europe (Zhang et al., 2012). In the Spanish context, the Earth Science Department of the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS) has established the CALIOPE air quality system (Figure 2a) to forecast air pollution (O_3, NO_2, SO_2, PM_{10} and $PM_{2.5}$) with high spatial resolution over Europe and the Iberian Peninsula. The CALIOPE system consists in a set of models: the WRF-ARW meteorological model; the HERMES emission model (Figure2c), the BSC-DREAM8b natural dust model, and the CMAQ Chemical Transport Model (CTM). The complexity of the Iberian Peninsula forces to consider high spatial (4km x 4km) and vertical resolution (15 layers) to be able to simulate the layering of meteorology and pollutants (Pay et al., 2014; Schaap et al., 2015).



(b) PM modelling

$$PM_{CALIOPE} = PM_{CMAQ} + PM_{BSC\text{-}DREAM8b}$$

$$PM_{2.5,i,j} = [SO_4^{2-}]_{2.5,i,j} + [NO_3^-]_{2.5,i,j} + [NH_4^+]_{2.5,i,j} + [OC]_{2.5,i,j} + [EC]_{2.5,i,j} + \text{Unspeciated Mass}_{2.5,i,j}$$

$$PM_{10,i,j} = PM2.5_{i,j} + [SO_4^{2-}]_{coarse,i,j} + [NO_3^-]_{coarse,i,j} + [NH_4^+]_{coarse,i,j} + \text{Unspeciated Mass}_{coarse,i,j}$$

NOTES: HERMES-DIS indicates that HERMES model is configured with a top-down approach. HERMIS-BOUP indicates that HERMES model is run with a bottom-up approach. CMAQ-ISAM indicates the CMAQv5.0.2 includes the Integrated Source Apportionment Method. PM_{CMAQ} includes primary and secondary anthropogenic aerosol and sea salt aerosol in PM10 and PM2.5 fractions. $PM_{BSC\text{-}DREAM8b}$ includes mineral dust from deserts in PM10 and PM2.5 fractions. *i* indicates emission by tagged activity sector (diesel emission from traffic, residential combustion, shipping, etc.) and *j* indicates emission by tagged regions (urban, suburban, national, etc.). *Coarse* is the fraction of aerosol with a diameter between 10 and 2.5 µm.

(c) Emission sources accounted in CALIOPE

SNAP	Description of sectors (i)
1	Energy industry
2	Residential and commercial combustion: 2.1. Coal; 2.2. Liquid fuel; 2.3. Medium liquid fuel; 2.4. Heavy liquid fuel; 2.5. Gas; 2.6. Solid biomass.
3 and 4	Industry (combustion & processes)
5	Fugitive emissions from fuels
6	Product use including solvents
7	On-road transport: 7.1. Exhaust, gasoline; 7.2. Exhaust, diesel; 7.3. Exhaust, LPG/natural gas; 7.4. Non-exhaust, evaporation; 7.5. Non-exhaust, wear
8	Non-road transport: 8.1. shipping, diesel; 8.2 shipping, heavy fuel oil
9	Waste treatment
10	Agriculture
11	Dust, Sea Salt, Biogenic SOA

Figure 2. Modelling framework for PM source apportionment studies in the PAISA project. SNAP sector from 1 to 10 are estimated within HERMESv2 models. Dust is is accounted by the BSC-DREAM8b. Sea salt and Biogenic SOA are estimated through CMAQv5.0.2

Over the last years many efforts have been done to improve the PM representation within the CALIOPE system. At a regional scale over Europe, the introduction of desert dust aerosol from the Sahara desert on an hourly basis and inclusion of sea salt emission have been identified as key points (Pay et al., 2010). Reproducing both contributions at regional scale is essential to simulate PM at urban scales over urban/suburban location in Spain. At urban scale, the local contribution to PM has remarkably improved by means of the implementation of resuspension emissions from paved roads on an hourly basis in the HERMES model (Baldasano et al., 2011; Pay et al., 2011). This approach is accurate and effective in order to reproduce PM_{10} concentrations near road traffic. The RPR contributes to increase PM_{10} concentrations up to 7 µg m^{-3} as annual mean in or near the largest urban zones. Despite the aforementioned improvements, $PM_{2.5}$ and PM_{10} concentrations remain underestimated as in the other state-of-the-art systems. Evaluation of CALIOPE in terms of aerosol chemical composition over Spain and Europe for the year 2004 (Pay et al., 2012a,b) shows that fine carbonaceous aerosols present the highest underestimations partly due to the state-of-the-

science concerning the SOA formation pathways typically implemented in models, which do not include biogenic SOA formation from isoprene and sesquiterpenes. The predominant vegetation types in the Spanish domain favour isoprene as the main biogenic VOC. The absence of the isoprene-SOA route for SOA modelling in the domain of study may impact significantly air quality during summer, when elevated biogenic VOC emissions combine with an enhanced photochemistry. Another source of underestimation is related to uncertainties on primary carbonaceous emissions.

At urban scale, the results obtained using the CALIOPE system (Pay et al., 2014; Schaap et al., 2015) have demonstrated that high-resolution (1-4 km) and specific description of emissions are key points to simulate AQ levels over urban/suburban areas affected by traffic or industrial emissions. In this sense, the HERMES emission model developed by the group is a key and unique assess of the CALIOPE system. The High-Elective Resolution Modeling Emissions System (HERMES) model accurately characterizes the variety of emission sources, as well as uses up-to-date information and emission estimation methodologies compiling the state-of-the-art in the pollutant activities considered (Guevara et al., 2013, 2014). For Spain, the model uses a bottom-up approach for the most significant pollutant sources. Emissions from point source sectors (e.g. power plants, industries) are estimated according to a facility database (1,796 stacks included) that compiles specific information per stack including, among others, geographical location and activity/emission factors. Emissions from road transport are estimated combining the Tier 3 method described in the EMEP/EEA air pollutant emission inventory guidebook (fully incorporated in the COPERT 4 software) with a digitized traffic network (over 111,000 km) that contains specific information by road stretch for daily average traffic, mean speed circulation, temporal profiles and vehicular park profiles. For the rest of pollutant sources a combination of top-down approaches and downscaling methodologies is adopted.

Pay et al. (2014) indicated the subgrid air quality variability at 1-km resolution could not be reproduced within street canyons and/or tree canopies, because a finer spatial structure is needed. The lastest generations of mesoscale meteorological models try to incorporate urban characteristics (urban morphology, land uses, land cover, building thermal characteristics, etc.). The last example of such an urbanization process is found on the urban modules added to the mesoscale meteorological model WRF to bridge the gaps between traditional mesoscale and microscale modelling (Chen et al., 2011). For better estimating the concentration at the microscale (< 1km) 3D urban canopy models integrated in Computation Fluid Dynamics (CFD) models are required (e.g. EULAG, San José et al., 2011). Most of the studies using CFD to assess air quality are implemented over very specific spatial and temporal conditions (Lateb et al., 2016). Although future urban air quality studies will potentially improve with CFD models, at present they are not yet suited for simulating air quality integrating the contribution from different spatial scales (e.g. regional, country, long-range transport) due to the high requirements of computational resources and the spatial and temporal limitation of current CFD applications. PAISA will implement and evaluate an urban model within WRF to improve the meteorological performance over urban areas.

Currently a new version of CMAQ is being tested, namely CMAQv5.1. It includes a new aerosol module, AERO6, which contains substantial scientific improvements over the AERO4 released in version 4.5, especially devoted to improve SOA formation, aerosol dynamic (nucleation, interactions of fine and coarse aerosol), in-line calculation of photolysis rates, speciation to crustal material (Al, Ca2+, Fe, Si, and Ti) and other ions (Mg2+, K+, and Ca2+) (CMAQ, 2016). There are no studies that have evaluated the new features of CMAQv5.1 in Spain over intensive measurement campaigns for PM, their components (sulphate, nitrate, ammonia, secondary organic aerosol, black carbon) and their gas precursors (NH_3, NO_2, VOCs, SO_2). As part of PAISA, CMAQv5.1 with AERO6 will be integrated within the CALIOPE system and evaluated. Diagnostic evaluation is essential to quantify the uncertainty of the model PM prediction and define the necessities of improvement of modelling system, but also to read into the subsequence source apportionment results for PM over urban areas.

Beside the updates in the science within the modelling part, the CMAQv5.1 has been instrumented with algorithms allowing for the estimation of source contribution in just one run (CMAQ-ISAM; Kwok et al., 2013; 2015). This is an advantage, because before SA was

performed by a brute-force method zeroing out sources one by one, but this becomes computationally prohibitive if many emitters are of interest and they not able to take into account non-linarites in chemical processes. However, it requires high computational and storage resources, as well as skilled professionals to analyse the results. Others CTMs have been instrumented with SA algorithms (Wagstrom et al., 2008; Kranenburg et al., 2013) (e.g. the Particulate Source Apportionment Technology, PSAT-CAMx; and the LOTOS-EUROS). PAISA will integrate ISAM within the CALIOPE system, which includes the state-of-the-art atmospheric chemistry for gas and aerosol pollutants within CMAQv5.1.

Source apportionment modelling studies in Spain

Zero-out approaches have been traditionally used in the Earth Science Department of the BSC to perform different impact assessment for different emission sector/s or specific facilities. For instance, in traffic management to test the impact of different traffic strategies, e.g. speed reduction (Gonçalves et al., 2008) or electric vehicles replacement (Soret et al., 2014) or the impact from the energy sector (Baldasano et et al. 2014; Valverde et al., 2016a). Recently, the source apportionment algorithms implemented within the CTM have been applied for assessing the contribution of specific activity sectors on the features of secondary pollutant using the CMAQ-ISAM tool implemented in the CALIOPE system. On the one hand, CMAQ-ISAM was used to quantify the contribution of on-road traffic sector coming from Madrid and Barcelona in the O_3 concentrations over the Iberian Peninsula under representative synoptic circulation, which determined that traffic from those metropolitan areas is not the main contributor but determine the O_3 daily peaks (Valverde et al., 2016b). Following the same methodological approach, the study of the contribution of selected sources (energy, industrial and shipping) on SIA over main urban areas in Spain indicated that NH_3 emissions are controlling the formation of sulphate and nitrate in Spain, and shipping and industrial sectors are major contributor to SIA over urban areas located downwind (Pay et al., 2016). The application of CMAQ-ISAM within CALIOPE system has shown promising results, but the reliability in the technique has to be explored in detail. To meet the identified research opportunities, PAISA will explore the use of CMAQ-ISAM within CALIOPE system to obtain a precise contribution of sources to main Spanish urban PM. Figure 3 shows the urban areas with more than 500,000 inhabitants that account for 20-30% of the Spanish population, according to Tele Atlas Multinet (2011).

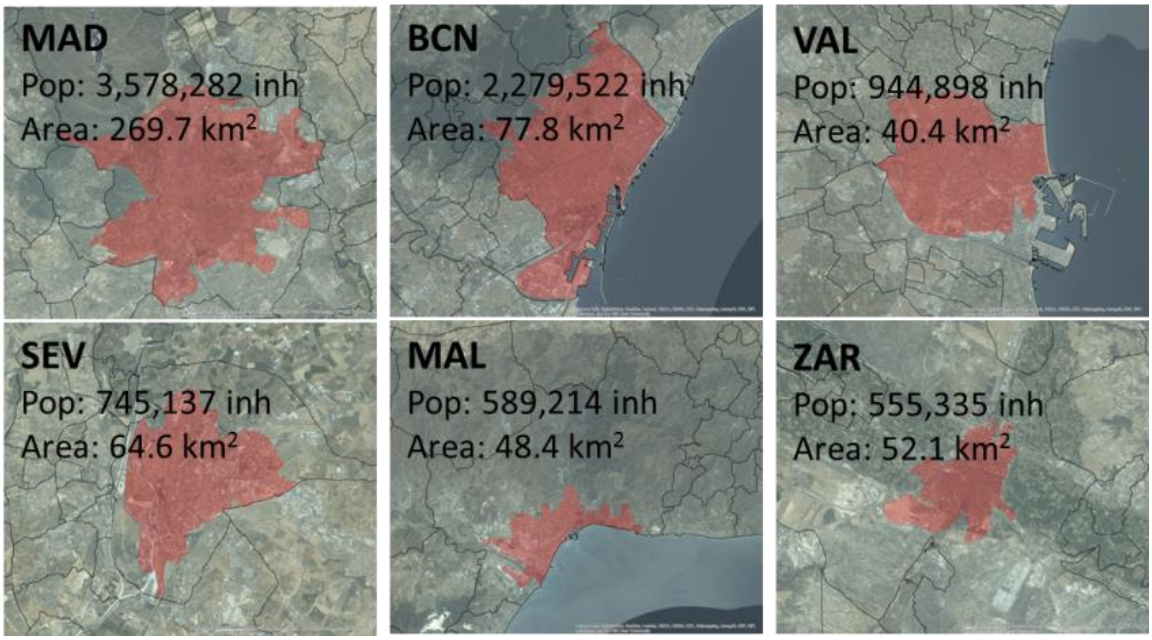


Figure 3. Top-five urban areas in Spain. Madrid (MAD), Barcelona (BCN), Valencia (VAL), Sevilla (SEV), Málaga (MAL), Zaragoza (ZAR). Red areas correspond with built-up areas as defined by Tele Atlas Multinet (2011). Pop indicate population in inhabitants.

2. Objectives

The overal scientific objective of PAISA is to quantify by photochemical modelling the contribution of emission sources (Figure 2c) and source regions (urban, suburban, national and continental) to high PM concentrations over main Spanish urban areas (Figure 3).

This goal will be achieved through three synergic objectives, which define the project's methodological approach:

1. To quantify the degree of uncertainty of the updated photochemical model to reproduce PM concentrations, both total mass (PM_{10} and $PM_{2.5}$) and PM chemical components.

2. To improve the photochemical modelling of PM concentrations in selected episodes based on detected necessities of improvement (meteorology, emissions and chemistry)

3. To quantify the contribution of the large variety of natural and anthropogenic emission sources and source regions to the PM concentrations.

The completion of PAISA's scientific objectives are expected to make a leap forward in our understanding of the origin of high PM concentrations over the main urban areas in Spain (Figure 1). The developments within PAISA are expected to be key in the design of *ad hoc* additional local actions complementing national and EU-wide strategies designed to accomplish the air quality thresholds that protect human health and ecosystems.

3. Background of the research team and other groups working in the topic

Experience of the PI: during her PhD at the UPC, **Maria Teresa Pay** developed a profound understanding of the air pollution problem at regional and urban scale over Europe and Spain using air quality models. Her work contributed to implement and improve an air quality modelling forecast system at high spatial and temporal resolution over Europe and Spain, the CALIOPE system, recently awarded with the prize of innovative applications for environment (MYGEOSS). She completed a thesis where a variety of aspects on air quality modelling: development, improvement and forecasting. She performed a deep evaluation of the CMAQ CTM. These works have allowed her to be involved in the evaluation of the CALIOPE system in different intercomparison at European scale (e.g. EURODELTA and the Task Force for Measurement and Modelling under the UNECE on trends analysis). After her PhD, the fellow moved her scientific training on air quality models from the development into an assessment approach. During her first two years as post-doctoral research at the *Laboratoire of Météorologie Dynamique (Ecole Polytechnque)*, she acquired an in-depth knowledge of the relationship between air quality and synoptic circulation patterns to explain in what extend air pollution dynamic can be explained by meteorological situations. During her last years as post-doctoral researcher, she focused on determining the role of source classes in air pollution episodes, so she studied the potential of the SA algorithms implemented in CTM, and she moved to the US Environmental Protection Agency (US EPA) to learn how to run and interpreted them under the supervision of Dr. Napelenok, developer of the new ISAM tool in CMAQ; now, the applicant is used to handle them in different configurations. This experience has allowed her to be involved as a scientific expert in the FAIRMODE WG3 on Source Apportionment to harmonize the use of SA techniques in EU. The applicant has worked in 6 leading research institutes for extended periods, published 17 scientific paper (15 publications within the Q1, an 8 h-index and 190 citations, according to SCOPUS, 5 publication as first author) with long lists of co-authors, and participated in 9 national and 6 (3 no funding) international projects. Her CV and the publication and conference participation listed therein show how those interactions have been extremely fruitful and have always resulted in publications in major journals. These experiences have permitted the applicant to create and maintain a rich network of international collaborations and led the co-direction of 1 PhD thesis on air quality.

Experience of the PhD in the Research Group: 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 is currently coordinating the development and implementation of an air quality forecast system for the Mexico DF Environment Secretary. 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 9 papers in international scientific journals and 8 communications to International conferences. He has acted as a reviewer of several International journals.

The PI and Dr. Guevara set a complementary team between the atmospheric chemistry modelling and the emission modelling, toghether with the background on meteology of the Earth Science Department. New SA techniques implemented in CTM togheter with high flexible emission models, will allow to better understand the origin of PM under pollution episodes in urban areas in Spain.

At national level, several research groups work on the use of photochemical models for source apportionment studies in Spain, but using a zero-out approach for either specific sources or regions, among them:

- Roberto San José, Grupo de Modelos y Software para el Medio Ambiente, Universidad Politécnica de Madrid. Mesoscale modeling based on CMAQv4.7.
- Rafael Borge. Tecnologías Ambientales y Recursos Industriales, Universidad Politécnica de Madrid. Mesoscale modeling based on CMAQv4.7.
- Maria Rosa Soler. Mesoscale and microscale atmospheric modelling and research group, Universidad de Barcelona. Mesoscale modeling based on CMAQv4.7
- Jose Antonio Souto González, Universidad de Santiago de Compostela. Mesoscale modeling based on CHIMERE.
- Fernando Martin, CIEMAT. Grupo de Modelización de la Contaminación Atmosférica (GMCA), CIEMAT. Mesoscale modeling based on CHIMERE.

At international level, many different research centres and universities departments works on the topic. Listed below are the most relevant ones for the project:

- The air quality group, Norwegian Institute for Air Research (NILU).
- Atmospheric Modelling and Environmental Mapping Unit, INERIS. They develop the CHIMERE model.
- Environment and sustainability department, TNO. They develop the LOTOS-EUROS model.
- Atmospheric Modeling and Analysis Division, US EPA. They develop the CMAQ model.
- System for Integrated modeLling of Atmospheric composition, FMI. They develop the SILAM model.

The Working Group includes four PhD researcher from international groups. Dr. **Sergey Napelenok** is scientific researcher at the United States Environmenta Protection Agency, in the Atmospheric Modeling and Analysis Division. His expertise includes (1) development, evaluation, and application of the CMAQ model, (2) development of formal mathematical sensitivity methods within CMAQ and their application to sensitivity analysis, and (3) implementation of state of the science PM formation and transport algorithms including secondary organic aerosols, and aqueous chemistry. Sergey Napelenok is the developer of the CMAQ-ISAM. **Dr. Claudio Belis** is a senior scientist at the Air and Climate Unit of the Joint Research Center, and he is the leader of the Working Group on Source Apportionment under FAIRMODE. **Dr. Leonor Tarrasón** is the head of the Urban Environmental and Industry Department at the Norwegian Institute for Air Research. She is responsibility for the development, application and validation of chemical air transport models for PM and photo-oxidant pollution to support the development of air emission control policies in Europe, and she is co-chairing activities of the Urban Emission Working Group under FAIRMODE. **Dr. Marisol Monterrubio** is a CONACY post-doc researcher currently working in at BSC-ES on the improvement of the HERMES emission model.

4. Societal challenges

Exposure to air pollutants is largely beyond the control of individuals and requires actions by public authorities (regional, national, and international levels) and economic sectors. In the last decades air quality has improved, but exceedances of PM concentrations are still registered in Spain. In this sense, PAISA addresses the research problem of determining the origin of PM pollution over highly populated areas in Spain and this is a twofold challenge. First, it is a scientific challenge because it requires the development/improvements of reliable, advanced and updated tools to quantify the contributions to atmospheric pollutants from a variety of sources that interact by multiple path-ways and at different spatio-temporal scales. Second, it is a societal challenge because it requires the involvement and the awareness of socio-economic sectors, governments and the society.

Only with a good understanding of air pollution causes (emission sources, transport at different scales, chemical and physical transformations), effective actions to reduce the impacts can be designed. In this sense, PAISA can provide an integrated framework to diagnose the origin of PM in urban areas in Spain because it compiles (1) the contribution from emission sectors and source areas at different scales, (2) the spatial and temporal emission variability of activity sectors (e.g. bottom-up emission from on-road traffic), (3) meteorological interactions and synoptic and mesoscales, as well as (4) the non-linear interactions of the aerosol and their precursors in the atmosphere, all together integrated in a the CALIOPE system, which runs at high spatial and temporal resolution in the MareNostum supercomputer.

The multidisciplinary character of the actors involved in PM pollution in Spain (multi-pollutant, multi-source, multi-scale, multi-effect) requires comprehensive solutions that include technological development, structural changes (e.g. optimisation of infrastructures and urban planning) and behavioural changes. PAISA can provide this multidisciplinary framework to discuss about air quality over Spanish urban areas because (1) it will quantify for every single urban area in Spain (> 500,000 inhabitants) the contribution of local activities as well as regional, national, and international contributions to the PM concentrations, and (2) it will invite local governments and companies involved to define efficient emission abatement scenarios to improve PM concentrations.

All in all, PAISA's results are expected to provide better scientific understanding of the origin of PM pollution over urban areas in Spain, whereby matching the premises of one challenge in the ***"Plan Estatal de Investigación Científica, Técnica y de Innovación 2013-2016"***: '*6.4.5. Reto en acción sobre el cambio climático y eficiencia en la utilización de recursos y materias primas*', in particular with the topic "*II. Eficiencia en la utilización de recursos y material primas"* by means the following sub-items:

(ii) "establecimiento y la operatividad de Sistemas Globales de Observación de la Tierra (GEOS)". PAISA will contribute to enhance the CALIOPE system, which is a MyGEOSS innovative application for environment, through the improvement of the simulation of PM and the implementation of a source apportionment tool.

(ix) "desarrollo y validación de modelos cuantitativos sobre el estado de la calidad del aire la influencia de variables climatológicas y geográficas". PAISA will develop and validate the CALIOPE system to improve the simulation of PM under representative episodes over most populated areas in Spain using measurements from routinely monitoring network and experimental campaigns (provided by IDAEA-CSIC) that contribute to improve the scientific confidence on the modelled PM.

(xii) "obtencion de medidas y parámetros representativos de la calidad del aire y de apoyo a la identificación de fuentes de contaminantes y procesos de formación y transformación de contaminantes atmosféricos". PAISA will augment the CALIOPE system with a source apportionment algorithm (i.e. CMAQ-ISAM) allowing the quantification of the contributions from socio-economic activities and sources at multiple scales to PM high concentrations taking into account the secondary formation of the aerosols.

PAISA will quantify the contribution of different activity sectors to the PM pollution, and specifically taking into account the fuel type in the combustion process. This outcome could

facilitate strategic choices in the energy sector, addressing the challenge *"6.4.3. Reto en energía segura, eficiente y limpia"*, and in the on-road transport sector, through the challenge *"6.4.4 Reto en transporte sostenible, inteligente e integrado".*

PAISA's outcomes are in agreement with the objectives in the current ***"Plan Nacional de Calidad del Aire y Protección de la Atmósfera 2013-2016: Plan aire"*** which identifies PM as a critical pollutants to monitor and modeling, and the emission reduction of PM precursors as one of the target. The *Plan* identifies air quality modeling as a key topic where the Spanish research community has to further increase its expertise. The *Plan* evidences the need of advanced modelling tools that allow increasing the knowledge on air pollution. These priority areas are in agreement with PAISA's main objective and tools. PAISA will improve the scientific knowledge on PM modeling within the CALIOPE system to better reproduce PM concentration and also will augment the system with a source apportionment technique to quantify the origin of high PM concentration in urban areas. The outcomes of PAISA will provide robust evidences on source contributions to develop efficient air quality management that ensure that the legal limit are not exceeded and the consequences of poor air quality are avoided.

PAISA framework 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 BSC staff, the collaboration with national and international research institutions, and the developments of cutting-edge technologies.

Likewise, PAISA's expected outcomes tightly follow the H2020 societal challenge "**Climate action, environment, resource efficiency and raw material**", via its specific objective '*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*'.

5. Methodology

To achieve the objectives mentioned above, the following tasks have been foreseen:

Task 1.1. Compilation and treatment of available PM measurements and related precursors in Spain

Maria Teresa Pay, PhD (25%)
Marc Guevara, PhD (00%)
Carles Tena (00%)
Post-doc (00%)

This task will exploit and compile historical meteorological and air quality registers in the Iberian Peninsula to be used in the selection of the episode and for the evaluation of modelled air quality concentrations. The sources of information that will be used are:

- Experimental campaigns that provides a unique dataset to develop and evaluate new modelling frameworks. E.g., DAURE ("Determination of the sources of atmospheric Aerosols in Urban and Rural Environments in the western Mediterranean") in winter and summer 2009 (http://cires.colorado.edu/jimenez-group/wiki/index.php/DAURE).
- EBAS database (http://ebas.nilu.no) which compiles observation data of atmospheric chemical composition and physical properties. This database includes European Monitoring and Evaluation Programme (EMEP) measurements.
- Airbase (http://www.eea.europa.eu/data-and-maps/data/aqereporting) the air quality monitoring data for main regulatory pollutants submitted by Member States and managed by the European Environmental Agency.
- METAR database which provides meteorological measurements at airports.
- IDAEA-CSIC (that acts as *Ente Promotor Observador, EPO*, see ANNEX) will provide air quality data related to PM and its chemical components as well as photochemical gas precursors from campaigns (see letter of support).

The main outcome of this task will be a database on air quality measurements from regular monitoring networks and campaign together with meteorological data.

Task 1.2. Characterization of selected PM episodes by using observations

Maria Teresa Pay, PhD (25%)
Marc Guevara, PhD (00%)
Carles Tena (00%)
Post-doc (00%)

From the data compiled and analysed in task 1.1, we will select PM episodes based on two criteria: (1) high PM values where observed, and (2) available experimental campaigns with detailed measurements (PM components and precursors). The selection of the PM episodes will be done through guidance of the IDAEA-CSIC with experience in PM registers in Spain. The selection of episodes will be complemented with a description of the meteorological patterns (synoptic and mesoscale) from maps using the WRF model in CALIOPE system and measurements from METAR. The outcome of this task will be a catalogue of PM episodes characterized in terms of meteorological patterns and PM levels at specific measurement points.

Task 2.1. Evaluation of the PM prediction skill during the selected episodes

Maria Teresa Pay, PhD (10%)
Marc Guevara, PhD (30%)
Carles Tena (00%)
Post-doc (20%)
Claudio Belis, PhD
Leonor Tarrasón, PhD
Segey Napelenok, PhD
Marisol Monterrubio, PhD

This task will develop an evaluation protocol based on the expertise and validation tools of the Research Group. The evaluation protocol will include statistics, both discrete (bias, root mean square error, etc.) and categorical (skill scores, probability of detection, critical success index, etc.) for the comparison of simulation data with measurements at stations. The development of a protocol for the data format will allow the automatization of the evaluation and validation process with the available data. The protocol will include the DELTA tool (http://aqm.jrc.ec.europa.eu/index.aspx), which is a software developed by FAIRMODE to evaluate air quality models in the framework of the air quality directive.

The evaluation task will cover the analysis of the model performance to simulate PM concentrations, their components and precursors. The evaluation over intensive campaign periods will help identifying necessary improvements in the PM modelling. The evaluation task will be an iterative during the implementation of an improvement/change/update in the modelling system.

The evaluation task will provide an assessment of the model uncertainty that is required to analyse and interpret the source apportionment results.

Task 2.2. Improvement of performance of the air quality system for modelling PM in source apportionment studies

Maria Teresa Pay, PhD (10%)
Marc Guevara, PhD (60%)
Carles Tena (80%)
Post-doc (30%)
Leonor Tarrasón, PhD
Segey Napelenok, PhD
Marisol Monterrubio, PhD

To improve the performance of the CALIOPE system to simulate PM over Spain (4 km x 4 km horizontal resolution), several scientific and technical improvements will be implemented in the framework of the PAISA project. Improvements on three modules of the CALIOPE system (Figure 3) are foreseen:

1. WRF meteorological model:

- Process high-resolution data of land-use (use of the CORINE database with a resolution of 100 m), topographic data (e.g., the USGS global topography data, with a resolution of 1 km), sea temperature, initial moisture and temperature of soil.
- Implement the integrated WRF/urban modelling system within WRF to targeting Spanish urban areas.

2. HERMES emission model:

- Enhance the HERMES emission database to be used for multiyear activity which facilitates the integration of any activity data from national, regional and local sources whenever it is available. This helps to perform any simulation over any selected PM episodes.
- Expansion of HERMES model with higher flexibility to output emissions by SNAP categories (Table 2). The latter will be fundamental to perform source apportionment studies on different categories (e.g. fuel type) and processes (exhaust and non-exhaust traffic emission). This is possible thanks to the HERMES modularity and its bottom-up approach in the emission estimation.
- Enhance the PM speciation database used in HERMES based on SPECIEUROPE to account for the AERO6 species.

3. CMAQ chemical transport model:

- Implementation of the CMAQ-ISAM (v5.1) that will allow the source apportionment studies for aerosol, ozone and gas precursors.
- Configuration of the system (pre- and post-processing) to work with AERO6 aerosol module.

Despite these suggested improvements, other ones can arise during the diagnostic evaluation process (task 2.1). The main outcomes of this task will be an improved and flexible version of CALIOPE system for source apportionment studies based on a robust evaluation process through comparison with measurements.

Task 3.1. Source apportionment modelling during selected PM episodes

Maria Teresa Pay, PhD (10%)
Marc Guevara, PhD (00%)
Carles Tena (20%)
Post-doc (25%)
Segey Napelenok, PhD

This task will configure and run the source apportionment tool CMAQ-ISAM within CALIOPE to track the emission sources (following Table 2) and at different source regions. Source regions will be defined according to the following categories: (1) urban (Figure 2); (2) regional (administrative *Comunidades Autonomas*); (3) national (Spain); and (4) international (contribution coming towards the domain of simulation (Iberian Peninsula). After the configuration of the source apportionment system, we will run the model for the selected episodes. The outcome of this task will be a database on PM for the whole Spain as a function of the contribution of emission sectors (Table 2) and source regions (urban, regional, national, and international) under the selected PM episodes.

Task 3.2. Quantify the contribution of source classes to PM over main urban areas in Spain

Maria Teresa Pay, PhD (20%)
Marc Guevara, PhD (10%)
Carles Tena (00%)
Post-doc (25%)
Claudio Belis, PhD
Leonor Tarrasón, PhD
Segey Napelenok, PhD
Marisol Monterrubio, PhD

The contribution of emission sources and source region will be carried out over main Spanish urban areas as defined in Figure 2 using the database obtained in task 3.1. We will define two types of indexes: (1) to determine the dominant socio-economic sector and (2) to determine the dominant region (local, regional, national, and international) on the PM concentration. This task will provide a diagnostic of the origin of PM concentrations at individual selected urban areas determining to what extend PM concentration are controlled by specific anthropogenic sources and/or regional, national or international contributions.

6. Implementation

As envisaged from its conception, PAISA has been designed with the aim of tailoring the Research Group's background, the Working Group's expertise and the facilities of the host institution, in order to ensure its successful completion. The work plan reflects this idea, where the scientific program can be implemented from head-to-tail and in autonomy. The project is divided in four work packages (WP): three for research (WPs1-3) and one for management and dissemination (WP4). Further details are provided bellow, including milestones (Ms) and deliverables (Ds). Note that the expected date is indicated in terms of the corresponding month, thereafter *pm*. The schedule of the tasks described above is presented in the following chronogram.

Project month (PM)		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
WP1	T1.1																		
	T1.2																		
WP2	T2.1																		
	T2.2																		
WP3	T3.1																		
	T3.2																		
WP4	Comm		C1																
	Dissem						Dis1						Dis2						Dis3
	Explot													E1					
Milestones				M1			M2					M3	M4						
Deliverable							D1						D2						
Meeting													Me1						
Visit													V1			V2			

Project month (PM)		19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
WP1	T1.1																		
	T1.2																		
WP2	T2.1																		
	T2.2																		
WP3	T3.1																		
	T3.2																		
WP4	Comm					C2													C3
	Dissem						Dis4						Dis5					Dis6	
	Explot								E2										E3
Milestones						M5	M6	M7									M8		
Deliverable						D3											D4	D5	
Meeting								Me2									Me3		
Visit								V3			V4					V5	V6		V7

List of work packages (description)

WP1. Selection of PM episodes. This WP will select and characterize relevant PM episodes with available measurements that cover the typical PM pollutions patterns in the Iberian Peninsula. It comprises tasks 1.1-1.2 and will be monitored by M1, M2 and D1.

WP2. Model evaluation and improvements. The objective of this WP is twofold. The first is to determine the degree of uncertainty of the air quality simulation results through modelling techniques under selected PM episodes. The second is to improve the numerical results of the CALIOPE air quality system with the aim of obtaining a better description of the PM dynamic and consequently of the source apportionment modelling. It comprises tasks 2.1-2.2 and will be monitored by M3-M6 and D2-D3.

WP3. Modelling source apportionment. This WP will determine the origin of pollution by PM using the CALIOPE system, which includes de CMAQ-ISAM model for source apportionment studies. The source apportion modelling will discriminate between (1) anthropogenic and natural contribution, (2) source areas, and (3) activity sectors. It comprises tasks 3.1-3.2 and will be monitored by M7-M8 and D4-D5.

WP4. Project management and dissemination of results. This work-package will ensure the appropriate management of the project and broadly disseminate the outputs throughout its duration. It will be feasible thanks to the Project Management Department at the host institution (BSC) and the strong group of "Earth System Services" established at the department level (BSC-ES). WP4 will monitor the progress of the project, ensure timely preparation of scientific reports (milestones and deliverables) and outreach activities (see Section C.2), facilitate communication among the Research, Working Group members' institutions and EPO (BSC, NILU, JRC, USEPA, IDAEA-CSIC, MAGRAMA) and organize the project meetings. There will be three annual meetings organized by BSC within the PAISA project to ensure that action items are under way [Me1, pm12; Me2, pm 24; and Me3, pm34]. These project meetings are not intended to be internal symposiums but open conferences, in which researchers not directly involved in PAISA, e.g. from other scientific groups in Spain (e.g. UPM, IDAEA-CSIC) will be invited. Coincidental with the project meetings, two-days visits of the Working Group members to BSC are scheduled to discuss the results, plan additional analysis and prepare the meetings [V1, pm12; V3, pm25 and V6, pm34]. Under WP4, the project will also undertake a final report that, in addition to summarizing the scientific achievements, will identify priority research lines to enhance air quality models to model PM concentration in Spain and to increase the knowledge and the confidence on the PM source apportionment studies based on those photochemical models (D5, pm35).

List of milestones (tracking progress)

- M1- Database of compiled meteorological and air quality measurements
- M2- List of selected PM episodes
- M3- Report with the necessities of improvement detected in the CALIOPE system
- M4- First project meeting
- M5- Report on achievements in the improvements of the CALIOPE air quality systems
- M6- List of emission sources and source region to perform the SA study
- M7- Second project meeting
- M8- Third project meeting

List of deliverables (tracking achievements)

- D1- Assessment of the relevant PM episodes in Spain from observation
- D2- Assessment of the CALIOPE system model uncertainty in selected PM episodes
- D3- Assessment of PM concentrations under selected episodes using improved modelling and measurements
- D4- Assessment of the origin of PM concentration under selected episodes in main urban areas in Spain
- D5- Final scientific report and recommendations

7. Technical resources

[See requested budget for details]

PAISA will have access to the BSC high performance computing facilities to run the experiments in WP2 (model improvements) and WP3 (source apportionment). The simulation of 24 hours with the CALIOPE system at 4 km over Spain requires 512 CPU hours (including emission, meteorology and chemistry). The experiments are more demanding when running the source apportionment tool. For instance, tagging 4 sources for only SIA requires 8 times a normal simulation (4096 CPU hours). This number is expected to increase with the number of activity sources and the number to regions to track and the number of episodes (5-10 days/episode). Thanks the computational resources of BSC, with the MareNostrum III (48,896 cores, 1017 TFlops) the simulation over selected episodes will be feasible in a less than 6 months.

However, additional infrastructure is needed for a successful implementation of PAISA. Due to the unusually large number of tagged species, emission sources and emission areas, is expected that a file with 24 hour presents a size of 30 Gb (> 100 variables), PAISA would need an additional infrastructure for the accomplishment of all post-processing; a fat node is the most suitable tool for handling this output, which involve two extra dimensions: ensemble-member and lead-time. On top of this, to allocate the modelled PM over selected

episodes (task 2.2), the source apportionment information (task 3.1) and the observational datasets (task 1.1), the outputs, and all post-processed variables (task 3.2), the project would also require local storage; a suite of five disks of 4 TB HDD each has been requested. Likewise, PAISA considers hiring a post-doc (see below) to complementarily deal with WP2 (task 2.1.-2.2) and WP3 (task 3.1-3.2); hence, the project would additionally need a workstation (PC) for the post-doc to work in autonomy. Finally, and in order to facilitate an efficient execution/development of the activities in missions outside the host institution, e.g. attendance to meetings, PAISA would require a laptop with an UNIX-based OS.

Software tools are already present in the BSC if required, however most are expected to be free and open-source or already exist as in-house codes such as HERMES. BSC has a well-furnished library and subscription to on-line journals.

8. Human resources

The need for a post-doc for the optimal achievement of the tasks in WP2 (task 2.1.-2.2) and WP3 (task 3.1-3.2) is justified by ambitious evaluation of the model performance and the implementation of methods (in emission, meteorology and chemistry) that contribute to the improvement of the PM model performance. On the other hand, the high number of sources (economic sectors and regions) and species to analyze require trained human resources to post-process and analyze the PM results. This diagnostic evaluation goes beyond the routinely evaluation of an air quality model. The post-doc will help the scientists of the Research and Working Group towards a better completion of these objectives. At the same time, he/she will benefit from the support of a dedicated Computer Engineer (**Carles Tena**) at BSC in charge of task 2.2 and task 3.1, an Emission Modeller (**Marc Guevara**, PhD) performing tasks 2.1 and 2.2 and an Air Quality Modeller (**Maria Teresa Pay**, PhD) coordinating tasks 2.1, 2.1, 3.1 and 3.2 and supervising the whole project. The candidate should be a recent PhD graduate in atmospheric chemistry, preferably with a robust background in air quality modelling evaluation and developments.

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C.2. IMPACTO ESPERADO DE LOS RESULTADOS

National and international impacts: scientific, social, and economic.

[See attached letters of support/interest]

Air pollution is the environmental factors with the greatest impact on health in Europe and is responsible for the largest burden of environment-related disease. PAISA will develop, implement and evaluate an extended version of the CALIOPE air quality forecast system that will allow the identification of socio-economic activities (transport, residential, commercial, energy, agriculture, etc.) and geographical areas contributing to air pollution in Spanish urban areas. CALIOPE is a robust and well-settled system that accounts with > 10,000 users in its website since 2014. It is expected that the updated version with source apportionment will increase our knowledge of PM origin in Spanish urban areas taking into account the processes that contribute to the generation of secondary pollutants and the influence of climatic and geographical variables.

In this sense, PAISA will help to a better design national/regional air quality plans to meet the Air Quality Directive in Spain, promoting the synergies between different scientific groups (experimentalist and modellers), companies and governments. With this framework, PAISA agrees with the European Air Quality Directive that highlights the necessity of having modelling tools which provide an estimation of the geographical scope of episodes and establish restrictive measurements based on source apportionment studies.

The main impacts derived from PAISA, which meets the priorities of the *"Plan Estatal de Investigación Científica, Técnica y de Innovación 2013-2016"* are:

1. Increase in the knowledge of relevant physical and chemical processes for aerosols (primary and secondary) under the influence of climatic and geographical variables, through the use of modelling and measurements during specific experimental campaigns.
2. Implementation of an advanced tool for an efficient air quality management in Spain. This will be possible thanks to the supercomputing power of MareNostrum, unique in Europe and Spain, and to the parallelized environment provided by that supercomputer.
3. Optimization in the design of national and regional air quality plans in Spain (long-term action plan). This will be based in a solid knowledge of the origin of PM sources from PAISA.
4. Contribution in the development of short-term action plans when the thresholds set by legislation are exceeded.
5. Establishment of complementary information which is needed for the assessment of atmospheric pollution (gaseous and particulate matter) related to damage to human health, vegetation and ecosystems.
6. Capacity building of national/regional authorities to develop air quality plan based on source apportionment techniques.
7. Population awareness on air pollution by providing evidences on the origin of PM pollution in cities.
8. Promotion the synergies between different scientific groups, companies, governments and citizen, identified as main actors in the PM problem.

Summarizing, PAISA 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. PAISA will cause a step forward in the development of

technology and its application, transferring knowledge on a short, medium and long-term to scientific community and environmental administrations. PAISA will provide a high-resolution tool for the management of environmental problems derived from atmospheric pollution.

Communication, dissemination and exploitation

PAISA is committed to(1) share with the scientific community the methods and novelties implemented in the project; (2) promote best practices, knowledge and technology transfer in source apportionment to private and governmental stakeholders (3) communicate the topic to society targeting broader non-specialised audiences.

Communication. As recently pointed out by the European Environmental Agency, air quality pollution messages are currently not communicated to the society in an effective and engaging way. In this sense, outreach activities are crucial to increase public awareness and understanding of science and, at the same time, to show the payback of national investment in I+D+i. PAISA activities will be communicated using a language that can be understood by non-specialists using appealing communication formats such as leaflets, explaining the scientific evidences of the origin and responsible actors from the PM problems that occur in the main Spanish urban areas [C1-C3].

Dissemination. The results will be presented in top renowned international scientific conferences and meetings [Dis1-Dis6] with the idea of engaging the target scientific community and getting new ideas and feedback. Planned European and international conferences and meetings to attend are: the FAIRMODE technical meetings (one a year), the International Technical Meeting on Air Pollution and its Application (ITM) supported by NATO, the Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (HARMO), and the Model and Analysis System (CMAS). Furthermore, it is foreseen to publish three articles in relevant peer-reviewed scientific journals following the European Commission's policy on open-access for research articles. Regarding dissemination to target stakeholders (private and governmental), The description of the project and main outcomes will be disseminated through the website of the Earth System Services. This group inside the BSC-ES is devoted to knowledge and technology transfer in air quality issues and will ensure project visibility in fora of relevance for air quality stakeholders. Finally, three open-project meetings organized by the BSC are planned with the aim to present the state and progress of the project to the local scientific staff, BSC collaborators, national and regional governments and stakeholders. The continuous presence and coordinating role of the Working Group members and the BSC-ES scientists in different international initiatives, projects and scientific activities will ensure the dissemination of the PAISA's outcomes.

Exploitation. A database for the main Spanish urban areas, indicating the source apportionment by different activity sectors as well as the contribution from surrounding regions will be generated as one of the outcomes of the PAISA project. These results can be exploited in different ways by national and regional governments. For example, this information can be translated into actionable air quality policies at the national and regional scale. In this sense, adapted talks directed to national/regional/local governments are foreseen. PAISA also plans to send annual newsletters [E1, E2] to stakeholders and the target audience (enterprises from the economic sectors included in the study), as well as a technical report [E3] that ensures a detailed communication and understanding of the project results.

Besides the reported PAISA's communication and dissemination plan, the project will take advantage from the BSC's dissemination infrastructure (i.e., Media communication manager, communication team, in-house designer, BSC website, BSC social media accounts with >2,500 followers, MareNostrum open day events with >5,000 visitors per years, etc.) to enhance the spread of the results derived from research activities among the general public, companies (e.g. automotive or gas companies) and the international scientific community.

C.3. CAPACIDAD FORMATIVA DEL EQUIPO SOLICITANTE

For the covered research problem and the structure, PAISA offers a unique opportunity to strengthen and widen the competences of the PI (Maria Teresa Pay, PhD), whereby she will have to deep her background on atmospheric aerosol modelling and establish a link to the

source apportionment studies to increase the knowledge of the origin of PM using photochemical models. Particularly effective in this regard will be the clear bottom-up nature of PAISA (from measurements, through improving the modelling, to modelling source apportionment) and the high research level of the Research and Working Groups. PAISA represents a great opportunity for the PI to develop project management skills needed to become an accomplished and multidisciplinary researcher. By doing so, and by managing a scientific problem from end to end, she will create a stream of responsibilities associated with the outcomes of the project, an important part of the training of an independent research. Thus, PAISA will provide her with the final expertise needed to lead a research group as a junior scientist.

Since its goals are clearly stated, the methodology is precise and the technical support to undertake the research is considerable (see Research Group), PAISA is very adequate for the formation of young researchers. The complex origin of PM has been cover with experts from measurement and modelling fields. Both communities agree on the missing processes that take place in the aerosol chemistry and physics (e.g. SOA and SIA) and the role of gas precursors (e.g. NH3 emissions). Source apportionment are powerful tool to get insight on the origin of PM pollution, but the PM modelling have to update the recent scientific advances in their mechanism. Training young expert on this research are will reinforce the Spanish position in the global framework. The novel approach of exploring the PM modelling performance in relevant experimental campaigns is a unique opportunity to develop and evaluate modelling framework as CALIOPE that will help to improve the simulation of formation and evolution of PM components and their precursors. This will definitely increase the capability of the Spanish scientific community, and particularly the host institution (BSC) and other experimental group like IDAEA-CSIC (see Section C.2.). The background of the PI (one directed PhD thesis) and the experience of other PhD in the Research Group provides a great opportunity for training new experts. The PhD student will also benefit from interacting with the Working Group as well as with the large amount of scientist visiting BSC-ES. Hence, PAISA provides a highly stimulating scenario for carrying a PhD thesis. Its work plan would be similar to the one in PAISA but applied to ozone, which is consider a hazard pollutant in Spain, and share the same gas precursors with PM. It could be the continuation of the work of the PhD students in the group directed by the PI (Valverde et al., 2016b).

PAISA will be developed within the BSC-ES Department which has a long record of supervising PhD theses in the doctoral programme Environmental Engineering (UPC) with MEC Excellence Mention from 2011 (MEE2011-0335), with 21 dissertations completed during the last 10 years and available in the following link: http://www.bsc.es/earth-sciences/phd-thesis). Dr. Pay has supervised 1 PhD theses: Victor Valverde (2016, UPC) – "Characterization of atmospheric pollution dynamics in Spain by means of air quality modelling", Excellent Cum Laude. BSC-ES has also experience in organizing/hosting conferences and workshops. Additionally, BSC has a specialized Education and Training Team, dedicated to establish a curricula based on cutting-edge scientific research on software tools for HPC and application areas targeting research communities and industry with HPC needs. E.g., BSC-ES offers the course "Earth Sciences Simulation Environments at BSC" every year funded by PRACE ("Partnership for Advance Computing in Europe").

BSC provides professional development plan for each member according to their profile and objectives. In this sense, BSC has been awarded with the Human Resources Excellence in Research due to its progress in aligning their human resources policies with the principles set out in the EU Charter and Code for Research.

C.4. IMPLICACIONES ÉTICAS Y/O DE BIOSEGURIDAD

Not applicable

ANNEX: Letters of support by EPO (Ente Promotor Observador)

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

CONSEJO SUPERIOR
DE INVESTIGACIONES
CIENTÍFICAS

Instituto de Diagnóstico Ambiental y Estudios del Agua (IDAEA-CSIC)

A quien pueda interesar:

Dentro de la convocatoria de Retos Investigación: Proyectos I+D+i para el año 2016 correspondientes al Program Estatal de I+D+i Orientada a los Retos de la Sociedad, en el marco del Plan Estatal de Investigación Científica y Técnica y de Innovación 2013-2016 , el Departamento de Ciencias de la Tierra del Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS) ha preparado una propuesta de proyecto titulado *"Photochemical modelling to attribute emission sources and source regions to high particulate matter concentration in urban areas in Spain (PAISA)"*

Tras la lectura de esta propuesta, el Instituto de Diagnóstico Ambiental y Estudios del Agua – Centro Superior de Investigaciones Científicas (IDAEA-CSIC) declara estar interesado en participar en este proyecto como ente promotor observador (EPO) y por ello ofrece su colaboración y apoyo en el suministro de datos experimentales de composición química de aerosoles y gases fotoquímicos para la evaluación del modelo fotoquímico incluido dentro del sistema CALIOPE (www.bsc.es/caliope). Por ello reiteramos nuestro interés en la utilización de los resultados del proyecto y nos comprometemos a hacer disponibles los resultados de nuestros experimentos al Departamento de ciencas de la Tierra del BSC.

Atentamente,

Barcelona, 13 de abril de 2016

Prof. Xavier Querol

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MINISTERIO
DE AGRICULTURA, ALIMENTACIÓN
Y MEDIO AMBIENTE

SECRETARÍA DE ESTADO DE MEDIO AMBIENTE

DIRECCION GENERAL DE
CALIDAD Y EVALUACION
AMBIENTAL Y MEDIO NATURAL

A quien pueda interesar:

Dentro de la convocatoria de Retos Investigación: Proyectos I+D+i para el año 2016 correspondientes al Programa Estatal de I+D+i Orientada a los Retos de la Sociedad, en el marco del Plan Estatal de Investigación Científica y Técnica y de Innovación 2013-2016 , el Departamento de Ciencias de la Tierra del Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS) ha preparado una propuesta de proyecto titulado *"Photochemical modelling to attribute emission sources and source regions to high particulate matter concentration in urban areas in Spain (PAISA)"*.

Tras la lectura de esta propuesta, el Área de Calidad del Aire de la Dirección General de Calidad y Evaluación Ambiental y Medio Natural expresa su interés, como potencial usuario de los resultados obtenidos, en el desarrollo del proyecto. El proyecto propuesto y los resultados derivados del mismo son esenciales para las entidades responsables de la gestión de la calidad de aire, ya que les permite tener una mejor comprensión sobre la contribución de las distintas fuentes de emisión (por región y actividad) a la contaminación atmosférica por material particulado en zonas urbanas de España que permitirán establecer planes de reducción de emisiones más eficientes.

Además, el proyecto pretende establecer de una herramienta de análisis de contribución de fuentes específica para España, que permitirá realizar el diagnóstico del origen de la contaminación durante episodios de superación de excedencias de los límites que marca la legislación, tal y como requiere la directiva de calidad del aire 2008/50/CE.

En Madrid, 13 de abril de 2016

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