AGENCIA ESTATAL DE INVESTIGACIÓN - Convocatorias 2018
Proyectos de I+D de GENERACIÓN DE CONOCIMIENTO y Proyectos de I+D+i RETOS INVESTIGACIÓN

AVISO IMPORTANTE - La memoria no podrá exceder de 20 páginas. Para rellenar correctamente esta memoria, lea detenidamente las instrucciones disponibles en la web de la convocatoria. Es obligatorio rellenarla en inglés si se solicita más de 100.000,00 €.

IMPORTANT – The research proposal cannot exceed 20 pages. Instructions to fill this document are available in the website. If the project cost exceeds 100.000,00 €, this document must be filled in English.

IP 1 (Nombre y apeliidos): Oriol Jorba Casellas

IP 2 (Nombre y apellidos):

TÍTULO DEL PROYECTO (ACRÓNIMO): Química del carbón marrón: modelización de la absorción reactiva de amoníaco en los aerosoles orgánicos secundarios y su efecto en el forzamiento radiativo (BROWNING)

TITLE OF THE PROJECT (ACRONYM): Brown carbon chemistry: Modeling the reactive uptake of ammonia on secondary organic aerosols and its effect on radiative forcing (BROWNING)

1. PROPUESTA CIENTÍFICA - *SCIENTIFIC PROPOSAL*

1.1. Antecedentes y estado actual

Brown carbon as an important absorbing aerosol

Atmospheric aerosols have a significant influence on the climate system. On average, aerosols cool the atmosphere directly by scattering solar radiation and indirectly through aerosol–cloud interactions (Myhre et al., 2013). However, some aerosol components are capable of absorbing visible solar radiation and warming the lower atmosphere. The most prevalent types of absorbing aerosols are black carbon (BC; Haywood and Boucher, 2000) and mineral dust (Usher et al., 2003). Most organic aerosols (OA) can be characterized as "white" because they efficiently scatter visible radiation. Recently, optical and thermal analyses (e.g., Kirchstetter et al., 2004) and electron microscopy (e.g., Alexander et al., 2008) from laboratory and field experiments have provided strong evidence for the existence of some OA with light absorbing properties. In recent scientific literature, the term "brown carbon" (BrC) has emerged to describe this type of OA, characterized by an absorption spectrum that smoothly increases from visible to UV wavelengths (Kirchstetter et al., 2004; Laskin et al., 2015). All aerosols capable of absorbing visible radiation tend to reduce the magnitude of the cooling attributed to aerosols (Moosmüller et al., 2009). The climate response to aerosol absorption has been found to depend strongly on the altitude of the absorbing aerosols (Hodnebrog et al., 2014; Ban-Weiss et al., 2012; Koch and Del Genio, 2010). This altitude dependence leads to an enhanced role for BrC in the net climate effects of total absorbing carbonaceous aerosols (Zhang et al., 2017). Therefore, ***accurate respresentations of the spatial and vertical distributions of BrC are essential to estimating its climate effect***.

Current climate models often assume that BC and mineral dust are the only two significant types of light-absorbing aerosols on the global scale, and they treat OA as a purely scattering component that leads to climate cooling (Bond et al., 2011; Ma et al., 2012). Feng et al. (2013) estimated for the first time the enhanced absorption of solar radiation due to BrC, only considering primary sources, in a global model. Their results suggest that the inclusion of BrC absorption produces a forcing of +0.11 Wm^{-2} for strongly absorbing BrC and +0.04 Wm^{-2} for moderately absorbing BrC at the top of the atmosphere. Such findings change the global radiative forcing of organic carbonaceous aerosols from cooling ($-0.08Wm^{-2}$) to warming ($+0.025Wm^{-2}$), with much larger potential impacts on regional climates. ***Constraining the absorbing fraction of organic aerosol is necessary to reduce this uncertainty.***

Recent studies have shown that BrC is widespread in specific geographic areas and urban environments and makes a significant contribution to total aerosol absorption (Kirchstetter

and Thatcher, 2012; Ramanathan et al., 2007). Such findings highlight the need for an improved understanding of OA absorption properties, providing motivation for laboratory and field studies focused on fundamental aspects of the chemistry of BrC and its absorption properties (Laskin et al., 2015).

Secondary formation of brown carbon and aging effects of ammonia on secondary organic aerosols (SOA)

Until recently, it was believed that BrC is produced solely by primary sources, which include residential coal combustion and biomass burning (Andreae and Gelencser, 2006; Moosmüller et al., 2009). Recent studies have challenged this view and postulated the existence of various secondary sources of BrC resulting from multi-phase reactions between gas-phase, particulate and cloud micro-droplet constituents. Examples include the reactions of OH radicals with aromatic hydroxyacids and phenols in cloud water (Gelencser et al., 2003), aqueous reactions of glyoxal and methylglyoxal with ammonium sulfate (Galloway et al., 2009), gas-to-particle uptake of glyoxal by deliquesced ammonium-sulfate aerosol (Trainic et al., 2011), aqueous reactions between glyoxal and amino acids (De Haan et al., 2009), reactions of limonene SOA with ammonia (NH_3; Laskin et al., 2010) and with ammonium-sulfate (Bones et al., 2010), heterogeneous reactions of gaseous isoprene on acidic aerosol particles (Limbeck et al., 2003), and aqueous photochemistry of pyruvic acid in the presence of common atmospheric electrolytes (Rincon et al., 2009). Currently, ***the amount of additional SOA mass and the climate effects of nitrogen-containing organic compounds produced by ammonia-driven secondary sources are highly uncertain, and require urgent attention from the atmospheric research community*** (Updyke et al., 2012).

Gas-phase ammonia interactions with SOA have also recently been shown to have complex effects on physical particle properties. Recent single-particle measurements of laboratory-generated SOA from α-pinene ozonolysis exposed to gas-phase ammonia revealed that the ammonia reaction products form a semi-solid layer on the particle surface a few nanometers thick that prevents coagulation, but which remains volatile enough to evaporate upon dilution of the gas-phase ammonia (Bell et al., 2017). These physical aerosol effects have the potential to impact aerosol optical properties in two ways. First, the concentration of light-absorbing reaction products at the surface can be expected to enhance aerosol absorption compared to the case of a well-mixed aerosol. Secondly, the semi-solid layer that forms upon reaction of gas-phase ammonia with SOA surfaces has been shown to prevent further uptake of ammonia, leading to the potential availability of more gas-phase ammonia to react with uncoated SOA particles. ***An exploration of the effects of ammonia-induced changes to aerosol morphology on the formation of BrC has not yet been reported, and may have important implications for climate and air-quality modeling***.

The effects of added ammonia on the yields and important properties of SOA has only been investigated in a limited number of chamber and field experiments. Na et al. (2007) observed a significant increase in α-pinene + O_3 SOA yields in the presence of ammonia. Huang et al. (2012) also observed that ammonia significantly increases the yield of SOA from reactions between indoor ozone and VOCs emitted from cleaning products. However, the presence of ammonia has the opposite effect on reactions of the aromatic SOA-precursor styrene; the SOA yield decreases because NH_3 facilitates the decomposition of the major SOA-forming product, 3,5-diphenyl-1,2,4-trioxolane (Na et al., 2006). Lin et al. (2013) found no strong association between isoprene-derived SOA and ammonia in samples collected in the southeastern US. Updyke et al. (2012) exposed a number of different types of SOA generated from biogenic and anthropogenic precursors to ppb levels of ammonia and found that light-absorbing nitrogen-containing organic compounds are produced inside SOA material. Recently, Liu et al. (2015) reported for the first time chemical uptake coefficients for ammonia onto SOA. They determined these coefficients to be on the order of 10^{-3}–10^{-2} for fresh SOA, and to decrease significantly below 10^{-5} after six hours of reaction. ***Clearly, the effects of ammonia on SOA yields are complex and potentially dependent on the nature of the SOA precursor, justifying a more systematic study of ammonia–SOA aging chemistry***.

Some of the first modeling studies to address the role reactive NH_3 uptake by SOA plays in air quality identified a significant impact on PM2.5 and NH_3 concentrations. Horen et al. (2018) incorporated a new surface reaction of NH_3 with SOA into an air quality model using the uptake coefficients of Liu et al. (2015). Results show that the chemical uptake of NH_3 by SOA acts as a sink for NH_3, reducing the formation of ammonium nitrate and ammonium sulfate in the particle phase. Zhu et al. (2018) extended the study to the continental scale, implementing a first-order loss rate for NH_3 onto SOA over the US using the CMAQ model. ***The impact of such a reduction in ammonium sulfate and ammonium nitrate by nitrogen-containing organic compounds on the radiative forcing of particles has not yet been quantified and warrants further research***.

Ammonia emissions are expected to increase worldwide in all future global scenarios because of the intensifying agricultural use of ammonia-based fertilizers (FAO, 2011). In addition, increases in temperature of 2ºC–4ºC due to climate change could lead to overall increases of up to 10%–27% in ammonia emissions (Skjøth and Geels, 2012). At the same time, VOC emissions are expected to increase because of the rising trend in global temperatures (Constable et al., 1999). The combination of these two trends is likely to lead to significant changes in the mass-concentrations and chemical composition of SOA. ***Both experimental and modeling efforts are required to address this critical gap in our understanding of the effect of ammonia on SOA and the resulting BrC radiative forcing***.

Aim of the proposal

In this scientific context, we propose to address the following scientific questions:

1) What is the contribution of brown carbon formed in the aging of SOA by ammonia to the total radiative forcing of organic aerosols?

2) How does this secondary formation of brown carbon contribute to total aerosol mass loading and air quality?

3) What effects can the complex chemistry and physics of SOA aging by ammonia be expected to have on the ambient environment?

To address these scientific questions, a multidisciplinary approach is planned that combines expertise in aerosol modeling, laboratory experiments, field campaign retrievals, and climate assessment. The funded project will allow the research team from the Atmospheric Composition group of the Barcelona Supercomputing Center (AC-BSC), which has wide experience in air quality and aerosol modeling at local-to-global scales, to strengthen established collaborations with: 1) University of California, Irvine (UCI) research groups focused on photochemical laboratory investigations and air quality modeling, 2) the Environmental Geochemistry Atmospheric Research IDAEA-CSIC group (EGAR), which comprises experts in field measurements of aerosol composition throughout Spain and Europe, and 3) the climate research group at NASA–Goddard Institute for Space Studies (NASA–GISS). Prof. Donald Dabdub and Prof. Sergey Nizkorodov (UCI), Dr. Xavier Querol and Dr. Andrés Alastuey (EGAR), and Dr. Kostas Tsigaridis (NASA–GISS) will participate in the project as external members of the working group. Their contributions will perfectly complement the modeling expertise of AC-BSC with lab-based research on SOA (UCI), ambient field-measurement experience and analysis (EGAR), and climate assessments of atmospheric aerosols (NASA–GISS).

Background of the AC-BSC research group and existing relationships with other research groups

The AC-BSC research group has strong expertise in air quality and aerosol modeling. Several scientific publications and PhD theses have studied air quality and atmospheric composition at the Barcelona, Spain, Europe and global scales (e.g., Jorba et al., 2004; Pineda et al., 2004; Jorba et al., 2008; Jiménez-Guerrero et al., 2008; Pérez et al., 2011; Jorba et al., 2012; Spada et al., 2013; Badia and Jorba, 2015; Badia et al., 2017). The group coordinated a national initiative to develop an air-quality forecasting system for SPAIN under the umbrella of the CALIOPE project (Baldasano et al., 2008; Pay et al., 2010; Baldasano et al., 2011; Pay et al., 2012; Basart et al., 2012a). The CALIOPE system now provides air quality forecasts for Europe at 12-km resolution and for Spain at 4-km resolution. The group

has published extensive work (Pérez et al., 2006a,b; Basart et al., 2009; Haustein et al., 2009; Basart et al., 2012b) on the evaluation of mineral dust models using lidar observations, sun-photometer data and satellite imagery. Importantly, the inclusion of dust radiative effects has been demonstrated as a means to substantially improve numerical weather prediction results through feedbacks between aerosol concentrations and meteorology (Pérez et al., 2006a).

In 2008, the group began developing a new online chemical weather prediction system, the NMMB-MONARCHv1.0 model (Pérez et al., 2011; Haustein et al., 2012; Jorba et al., 2012; Spada et al., 2013; Badia et al., 2017; DiTomasso et al., 2017), previously known as NMMB/BSC-CTM and NMMB/BSC-Dust. The model is a new fully online chemical weather prediction system for meso- to global-scale applications, and will be the primary modeling framework for the proposed work. The NMMB-MONARCHv1.0 has been developed under the umbrella of several national research projects of the Ministry of Economy and Competitiveness (CGL2006-11879/CLI, CGL2008-02818/CLI, CGL2010-19652 and CGL2013-46736-R1). The principal investigator (PI) of the present proposal has acted as PI of two of these national projects. Currently, the NMMB-MONARCHv1.0 provides operational regional mineral dust forecasts to the World Meteorological Organization's (WMO) Barcelona Dust Forecast Center (BDFC) and the Sand and Dust Storm Warning Advisory and Assessment System's (SDS-WAS) Northern Africa–Middle East–Europe (NA–ME–E) Regional Center—both centers are managed by a consortium of AEMET and AC-BSC. Additionally, NMMB-MONARCHv1.0 provides global aerosol forecasts to the International Cooperative for Aerosol Prediction (ICAP) initiative (Sessions et al., 2016). Finally, the model will be the next-generation air-quality model for the CALIOPE system, replacing the current system based on the WRF-CMAQ model, and is a candidate model for the European Air Quality Ensemble System of the Copernicus Atmosphere Monitoring Service (CAMS) initiative of the European Centre for Medium-range Weather Forecasts (ECMWF).

The AC-BSC group has established several collaborations with national research teams including AEMET, CIEMAT, IDAEA-CSIC, CEAM, the Technical University of Catalonia, the University of Murcia, and the University of the Basque Country. On an international level, ongoing collaborations have been established, among others, with the National Centers for Environmental Predictions (NCEP; USA), NASA–Goddard Institute for Space Studies (NASA–GISS; USA), the University of California, Irvine (UCI; USA), and the National Observatory of Athens. It is believed that such collaborations strongly benefit the progress of the scientific projects undertaken by AC-BSC related to developments of the NMMB-MONARCHv1.0 model. Furthermore, the group coordinates the new European COST Action "International Network to Encourage the Use of Monitoring and Forecasting Dust Products" lead by Dr. Sara Basart, a member of the research team of the present proposal.

Of particular relevance is the collaboration of AC-BSC with the University of California, Irvine. Strong synergies have been created with the Computational Environmental Sciences Laboratory managed by Prof. Donald Dabdub, an expert in air quality and SOA modeling (Pay et al., 2010; Jorba et al., 2012; Gonçalves et al., 2012; Badia et al., 2017). Currently, Prof. Donald Dabdub and Prof. Sergey Nizkorodov (Department of Chemistry, UCI) are conducting laboratory and modeling experiments to characterize ammonia-related SOA chemistry and physics (i.e., Aiona et al., 2017; Montoya et al., 2017, Horen et al., 2018; Zhu et al., 2018). ***Their findings will be the basis for regional and global modeling experiments proposed here to further advance understanding of the effects of secondary BrC formation on air quality and climate***.

Furthermore, AC-BSC has a long history of collaboration with EGAR IDAEA-CSIC (Pandolfi et al., 2014; Jorba et al., 2013; Pay et al., 2012). EGAR maintains complete laboratory facilities and state-of-the-art instrumentation for the measurement and characterization of atmospheric aerosols and trace gases. The group has an extensive database of measurements of oxidants, aerosols and optical properties in Spain, and its research objectives are in close agreement with those of the present proposal. Thus, ***the EGAR group offers an ideal synergistic complement to the AC-BSC team for the analysis of field measurements and modeling results***.

Previous project

The proposed work is a natural continuation of the project CGL2013-46736-R1 led by the PI of the present proposal. In CGL2013-46736-R1, the radiative effects of aerosols were implemented in NMMB-MONARCHv1.0, the mineral dust component of the model was improved, and the aerosol–radiation impact on meteorology was studied. The knowledge acquired during that project on aerosol properties (Obiso et al., 2017; Obiso and Jorba, 2018) and radiative effects (Gkikas et al., 2018) contributed to identifying brown carbon as an important but under-explored aerosol component that should be considered in air-quality and climate models.

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1.2. Hipóstesis de partida, objetivos generales, adecuación

Initial hypothesis:

Organic aerosols (OA) affect climate forcing and human health, but large uncertainties persist in their sources and evolution. Organic aerosols make up a large fraction of total submicron particulate matter (20% to 90%). Recent studies have shown that secondary organic aerosols (SOA) account for a large fraction of the OA burden. Most OA efficiently scatter visible radiation and contribute to a cooling of the atmosphere. However, a significant fraction of OA absorbs radiation in the near-UV and visible ranges. This fraction is generally referred to as "brown carbon" (BrC), and together with black carbon (BC) and mineral dust, contributes to a warming of the atmosphere.

The initial hypotheses supporting the objectives of the project are:

1) Current climate models assume that BC and mineral dust are the only two significant types of light-absorbing aerosols on the global scale, and they treat OA as a purely scattering component leading to climate cooling. However, recent advances in the identification and characterization of BrC indicate that BrC may contribute substantially to total aerosol absorption at specific wavelengths. **We hypothesize the inclusion of BrC in models will allow constraining the size and the sign of the radiative forcing of OA.**

2) Brown carbon is directly emitted during wood and fossil fuel combustion, but can also be formed by atmospheric oxidation of gas-phase species as a secondary pollutant. Light absorption of some SOA is enhanced after aging of the original aerosol. **We hypothesize that this 'browning' of SOA is a significant contributor to the total absorption of BrC.**

3) Recent studies have demonstrated that some initially scattering SOA undergoes browning during exposure to reduced nitrogen compounds such as ammonia, ammonium from dissolved ammonium sulfate or other salts, and amino acids. The contribution of such light-absorbing OA to the total warming effect of BrC is still highly uncertain. **We hypothesize that the warming is significant in areas with high emissions of ammonia or dissolved ammonium salts.**

4) Several field campaigns have focused on the characterization of OA. The EGAR group has conducted several field campaigns to study the processes involved in the formation of pollution episodes with formation of secondary aerosols. Last July 2018, EGAR organized a comprehensive camaign measuring relevant atmospheric pollutants (e.g., O_3, NO_2, NH_3, and secondary aerosols) toghether with aerosol optical properties. Mesurements where conducted at a site with high ozone and ammonia concentrations. Results of this campaign provide an excellent framework to further investigate the role of SOA in northeast Spain, and study the role of NH_3 in the formation of some SOA. **The optical properties measued *in situ* will provide valuable information on the presence of some absorbing secondary BrC under ambient conditions.**

Main objective:

The main objective of this proposal is to explore the effect of the reactive uptake of ammonia (NH_3) by secondary organic aerosols (SOA) on the optical properties and burden of anthropogenic and biogenic SOA using both experimental and modeling approaches. We propose implementing new NH_3-SOA chemistry from UCI and PNNL laboratory experimental results in a state-of-the-art atmospheric-chemistry model to quantify the fraction of BrC of primary and secondary origin, and the contribution of this light-absorbing SOA and BrC on the total radiative forcing of OA. We also propose the analysis of specific field campaigns

conducted in northeast Spain by the EGAR group to study the relevance of this new chemistry in a region with high NH_3 and O_3 concentrations. Surface concentration measurements of NH_3, O_3 and OA were conducted together with optical property measurements (absorbing AOD, single scattering albedo, and absorbing Ångstrom exponent). The combination of modeling studies with field campaign measurements may provide unique information on the light-absorbing contribution of secondary BrC in northeast Spain.

Appropriateness to the National and European research strategy

The topic of the present proposal covers the fifth societal challenge identified by the Spanish research strategy regarding climate change. A better understanding of the role of light-absorbing organic aerosols on the radiative balance of atmospheric models will contribute to reduce uncertainties in the quantification of radiative forcing attributed to anthropogenic and natural aerosols. Such advances will contribute to the future mitigation and adaptation measures required to face challenges that Climate Change is creating. The goals defined in HORIZON 2020 related to climate change and air quality modeling are in agreement with the strategy defined by the Spanish Government. In this sense, the improvement and evaluation of air quality modeling systems and advancement in the understanding of anthropogenic forcing that is enhancing climate change are key areas of research at the European level.

Additionally, the objectives of the present proposal are in agreement with the research lines defined by the “Estrategia Española de Ciencia Tecnología e Innovación 2013–2020” of the Ministry of Science, Innovation and Universities. The Strategy identifies aerosols as one of the critical pollutants to monitor and for which further modeling activities are required. One of the targets of the Plan is the reduction of secondary-aerosol precursor emissions. Approximately 40% of PM10 comprises secondary aerosols. Modeling tools developed as part of the proposed project will provide valuable information about the chain production of secondary aerosols and will facilitate identification of strategies that may lead to their reduction in the atmosphere. Concerning actions to promote research, the Strategy identifies air quality modeling as a key topic where the Spanish research community must further increase its expertise. Models must be improved and evaluated under a variety of conditions. The present proposal has as its primary objective to further understanding of the contribution of secondary organic aerosols to total aerosol concentrations and the impact of such aerosols on radiative forcing affecting the climate.

Finally, the Horizon 2020 2016–2017 Work Programme for the "Climate action, environment, resource efficiency and raw materials" challenge describes the European air quality economic sector as “critical to moving forward the transition to a circular economy, and also an important source of growth and jobs.” Additionally, climate action is one of the primary crosscutting actions highlighted by the Horizon 2020 program, and the effect of aerosol species on Earth’s radiative balance represents the largest uncertainty in predicting the trajectory of climate change. Thus, the expected impact of this research—to improve the prediction skills of aerosol mass and optical properties, and their impact on air quality and climate in one of the premier Spanish chemical weather prediction systems, NMMB-MONARCHv1.0—falls perfectly in line with European research priorities and concurrent initiatives.

1.3. Objetivos específicos

To achieve the main objective of the project, three specific objectives are defined:

1) Design a new mechanism for the formation and evolution of secondary BrC from the reactive uptake of ammonia into SOA for chemical transport models, and a new aerosol–radiation interaction parameterization for secondary BrC aerosol.

a. Review laboratory experiments conducted by Prof. Sergey Nizkorodov (UCI) on the reactive uptake of NH_3 on SOA and its impact on the absorption properties of the resulting particles.

b. Review laboratory experiments conducted by Dr. Alla Zelenyuk-Imre (PNNL) using single-particle measurements of SOA + NH_3 aerosols to characterize several physical aerosol properties, including density and morphology.

c. Analyze results of a field campaign conducted by Dr. Xavier Querol and Dr. Andrés Alastuey (EGAR) in northeast Spain measuring ozone, ammonia, secondary aerosols and aerosol optical properties. Measurements were performed at a countryside site in the Village of Vic, a region characterized by recurrent exceedances of ozone concentrations (>200 μg m^{-3} average hourly concentrations) during summertime, and where high concentrations of ammonia have also been measured (40 μg m^{-3} daily mean concentrations).

2) Explore the roles of the reactive uptake of NH_3 on SOA formation, and of SOA aging on the total mass of BrC, OA and particulate matter by means of atmospheric-chemistry modeling experiments conducted with the NMMB-MONARCHv1.0 model.

a. Implement a new organic aerosol tracer labelled "Brown Carbon" in the atmospheric-chemistry model. Include emission, transport and deposition of the new aerosol component.

b. Include the new NH_3-related SOA formation and aging mechanism proposed in specific objective 1 in the NMMB-MONARCHv1.0 model.

c. Evaluate the new BrC mechanism using regional modeling experiments over northeast Spain at high horizontal and temporal resolution (1 km x 1 km and hourly frequency), and global modeling experiments at medium resolution (50 km x 50 km and 3 hourly frequency).

3) Quantify the contribution of BrC to overall OA radiative forcing by means of modeling experiments.

a. Implement the parameterized scheme for BrC aerosol radiative effects in the radiation module of NMMB-MONARCHv1.0 to explicitly determine the radiative forcing from secondary BrC, following the scheme developed in Specific Objective 1.

b. Characterize the optical properties of BrC (extinction efficiency, single scattering albedo and asymmetry parameter) by means of Mie or T-Matrix calculations, while considering the effects of SOA aging on BrC optical properties.

c. Perform model experiments to quantify the radiative forcing of BrC at the global and regional scales.

d. Contribute to the AEROCOM-Phase III initiative an updated global aerosol simulation that includes a comprehensive treatment of BrC and aging processes associated with the reactive uptake of NH_3 on SOA.

1.4. Metodología

The manpower envisaged for the proposed project will be provided by the research team of the proposal (three senior researchers and an experienced technician) and Dr. Matthew L. Dawson (AC-BSC; Marie Skłodowska-Curie fellowship, atmospheric chemist and modeler). External collaborators include Prof. Sergey Nizkorodov and Prof. Donald Dabdub (University of California, Irvine; UCI) as experts on laboratory measurements and modeling of the reactive uptake of NH_3 on SOA and absorption properties; Dr. Alla Zelenyuk-Imre (Pacific Northwest National Laboratory; PNNL) as an expert on lab and field measurements of single-particle aerosol properties; Dr. Xavier Querol and Dr. Andrés Alastuey (Environmental Geochemistry and Atmospheric Research group at IDAEA-CSIC; EGAR) as experts on experimental field campaigns measuring secondary aerosols and optical properties; and Dr. Kostas Tsigaridis (NASA–Goddard Institute for Space Studies; NASA–GISS) as an expert on climate modeling, aerosol forcing, and organic aerosols. Finally, one post-doctoral researcher (PD1) with experience in atmospheric chemistry and secondary aerosol modeling will be hired, and will contribute to WP2 and WP3—implementing and assessing the impact of the new secondary BrC formation and aging mechanism.

In order to achieve the proposed objectives, we define the following methodology and working plan:

Work package 1: The science basis—design of a new BrC formation mechanism and a BrC aerosol–radiation interaction parametrization

The proper treatment of BrC in chemical transport models requires a in-depth understanding of its various formation mechanisms. Conventional knowledge associates light-absorbing OA

with primary sources and light-scattering OA with secondary sources. Well-known primary BrC sources include smoldering forest fires and residential coal combustion. However, recent work has demonstrated the existence of secondary sources of BrC that involve multi-phase reactions among gas-phase, particulate-phase and cloud micro-droplet constituents. Furthermore, browning transformations have been observed in specific SOA-aging processes. The aim of WP1 is the design of a comprehensive and computationally efficient mechanism for secondary BrC formation that accounts for state-of-the-science understanding of the processes involved in the reactive uptake of NH_3 on SOA and its effects on aerosol mass loading, optical properties and physical characteristics. Laboratory results from Prof. Sergey Nizkorodov (UCI) and Dr. Alla Zelenyuk-Imre (PNNL), and a preliminary chemical mechanism proposed by Prof. Donald Dabdub (UCI) will be the starting point of the design of the new secondary BrC mechanism. Furthermore, we propose to analyze field measurements of SOA and aerosol optical properties conducted by Dr. Xavier Querol and Dr. Andrés Alastuey (EGAR) to search for evidence of the role of NH_3 in the formation of secondary BrC. The overall outcome of WP1 will be the science details of a new secondary BrC formation mechanism and BrC aerosol–radiation interaction parameterization to be implemented in NMMB-MONARCHv1.0 model in WP2 and WP3.

Task 1.1 Review of laboratory experiments of the reactive uptake of NH_3 on SOA conducted at UCI

Prof. Sergey Nizkorodov and Prof. Donald Dabdub are currently performing chamber experiments designed to expand on their work to quantify the impact of NH_3 on SOA aging using a variety of biogenic and anthropogenic SOA precursors under various atmospherically relevant temperature and relative humidity conditions. The work proposed in this task will collaboratively parameterize their published and on-going work on the formation of light-absorbing SOA from NH_3 processing for inclusion in the NMMB-MONARCHv1.0 model. The new chemistry will expand the current implementation with a state-of-the-art secondary BrC formation and aging mechanism to quantify the effects of the new NH_3–SOA chemistry on the total OA burden. Because this new chemistry represents a sink of NH_3 that was not accounted for in previous model simulations, it is expected that the burden of secondary inorganic aerosols will change (as suggested by preliminary results of Prof. Dabdub and Prof. Nizkorodov). Prof. Sergey Nizkorodov and Prof. Donald Dabdub are already publishing their work on this new chemistry. This reduces uncertainty in the feasibility of the task due to a lack of applicable results. The expertise of the AC-BSC research team on numerical modeling and the participation of Prof. Sergey Nizkorodov and Prof. Donald Dabdub makes this task completely feasible.

Task 1.2 Review of single-particle measurements of SOA exposed to NH_3 conducted at PNNL

Dr. Alla Zelenyuk-Imre and her team at PNNL are also currently working to extend their investigation of the physical and chemical changes to aerosol particles from the interaction of gas-phase NH_3 and SOA to a variety of SOA precursors and relative humidity conditions. This task will focus on collaboratively developing a scheme to account for changes to particle coagulation and further uptake caused by the uptake of gas-phase NH_3 into SOA from various precursors. A simple core-shell or 'onion' model will be investigated for its ability to capture changes in particle-phase diffusion, uptake and coagulation, and for its feasibility for inclusion in NMMB-MONARCHv1.0. Once complete, this scheme will be coupled with the chemical and optical mechanism described in Task 1.1, and evaluated for its impact of BrC formation and lifetime. Dr. Zelenyuk-Imre and her team have already published results for α-pinene SOA interactions with NH_3 under dry conditions (Bell et al., 2017). Thus, the feasibility of having results available for the development of the physical scheme is high. Development of the scheme will leverage the modeling experience and resources of both the AC-BSC team and Prof. Dabdub's research group, adding value to the proposed work.

Task 1.3 Analysis of field measurements of ammonia, SOA and aerosol optical properties conducted by EGAR

The 'browning' of some SOA (e.g., limonene/O_3 SOA) has been observed during exposure to high-concentrations of reduced nitrogen compounds (NH_3, NH_4^+, and amino acids). This

chemistry may contribute to aerosol absorption under ambient conditions when high concentrations of reduced nitrogen compounds are present, frequent changes in relative humidity occur, and/or high photochemical activity is observed. Such conditions may exist in predominantly agricultural areas and in forested areas where high oxidant concentrations (e.g., O_3 or OH), high NH_3 concentrations, and high photochemical activity are prevalent.

There is a region in northeast Spain, located in a rural area where farming and agriculture activities are dominant, that is characterized by recurrent exceedances of ozone concentrations (>200 μg m^{-3} hourly concentrations) during summer, where high ambient ammonia concentrations are common (40 μg m^{-3} daily mean concentrations). This site, the Plana de Vic, was the location of a recent field campaign conducted by EGAR in July 2018. Measurements retrieved during the campaign were: (1) hourly concentrations of NH_3, O_3, NO_2 and VOCs at surface level; (2) daily average concentrations of organic carbon, elemental carbon, sulfate, nitrate, ammonium, mineral fraction, trace elements like levoglucosan (tracer of organic mass from biomass burning), and pH; (3) loading of BC and aerosol light absorption coefficients from a Multi-Angle Absorption Photometer; (4) aerosol light absorption coefficients (σ_{ap}) at seven wavelengths from the UV to near IR measured with an aethalometer, from which absorption Ångstrom exponents can be derived; (5) aerosol light scattering (σ_{sp}) and hemispheric backscattering (σ_{bsp}) coefficients measured at three wavelengths measured with a nephelometer, from which the scattering Ångstrom exponent and single scattering albedo can be derived; (6) the vertical structure of atmospheric aerosols from a ceilometer; and (7) quantitative measurements of the non-refractory components of submicron atmospheric aerosols (sulfate, nitrate, chloride, ammonium and OA) with a time resolution of 15 min to 1 h measured with an Aerosol Chemical Speciation Monitor (ACSM). The ACSM provides organic mass spectra, which can be analyzed by multivariate mathematical techniques, such as positive matrix factorization (PMF), to identify the OA origin/type. The most common OA sources/types are: hydrocarbon-like OA (HOA), which is related to primary engine emissions; biomass burning OA (BBOA), related to primary emissions from biomass combustion; and oxygenated OA (OOA), attributed to secondary OA (SOA).

An analysis of all the measurements combined with the model results will provide valuable information on the presence of BrC and the relevance of the reactive uptake of NH_3 on SOA in the real atmosphere. Collaborations already established with the UCI, PNNL and EGAR teams assure the feasibility of this task, as their research work is currently or soon-to-be published.

Work package 2: BrC chemistry and the role of reactive uptake of NH_3 by SOA: Model development and simulations

Work package 2 will address specific objective 2. The chemical mechanism and aerosol representation proposed in WP1 will be implemented in the NMMB-MONARCHv1.0 model. Modeling experiments will then be performed to explore the dynamics of secondary BrC formation and aging and advance the scientific community's understanding of the role of BrC chemistry in air quality.

Task 2.1 Implementation of the secondary BrC aerosol component in the NMMB-MONARCHv1.0 model

The current NMMB-MONARCHv1.0 aerosol mechanism models the life cycle of aerosol components in the troposphere that are known to have important effects on air quality and climate: mineral dust, sea salt, organic aerosol, black carbon, sulfate, nitrate and ammonium. However for calculations of aerosol radiative effects, this approach groups all primary and secondary organic carbon into a single aerosol component—organic aerosol (OA)—with no distinction of their unique optical properties. Aerosol models are constrained by optical measurements, mainly aerosol optical depth (AOD) and absorbing AOD. To calculate the total AOD from the mass concentrations solved by NMMB-MONARCHv1.0, we assume some optical properties derived from the Optical Properties of Aerosols and Clouds (OPAC) dataset. The OPAC dataset provides an OA refractive index that assumes OA is purely scattering. As discussed in Section 1, a significant fraction of OA absorbs in the UV–vis range, and this has a strong impact on the radiative forcing of OA. The inclusion of absorbing

OA will greatly improve the modeled effects of OA in the atmosphere, as it will allow a consideration of both its scattering and absorbing properties. To accomplish this, task 2.1 will add a new aerosol tracer in NMMB-MONACHv1.0— brown carbon (BrC)—for use in aerosol radiative calculations. In this work package, the refractive index for BrC will differ than that for OA, to account for the absorbing properties of BrC. Changes in the microphysical characteristics will be addressed in task 2.3. All transport, sedimentation, and dry and wet deposition processes will be the same for both organic components.

The inclusion of an explicit BrC component requires a new treatment of OA emissions and chemistry. In the new scheme, emissions of primary OA (POA) will be split in OA (purely scattering) and BrC (scattering and absorbing) components. Primary emissions of BrC are mostly from fossil fuel combustion and biomass burning Currently, particulate matter from such emissions are split into the BC and OA aerosol categories. In the new scheme, the OA fraction will be further split into 60%–70% OA and 30%–40% BrC, after selecting a value based on a review of the relevant literature. Finally, secondary formation of OA (SOA) will also be split into OA and BrC components, as there are well known reactions that form purely scattering SOA, and others that form BrC-SOA. The most relevant formation pathways in the troposphere will be implemented for both SOA and BrC-SOA. For optical calculations, OA and BrC will include both primary and secondary organic species. However, POA and SOA will be treated separately in the chemical mechanism to account for the unique chemical aging of SOA, which affects its light-absorbing properties, and will be addressed in task 2.2.

Task 2.2 Implementation of the new chemical mechanism for BrC chemistry and the reactive uptake of NH_3 on SOA in the NMMB-MONARCHv1.0 model

Following the chemistry scheme proposed in WP1, a new chemical mechanism will be implemented in NMMB-MONARCHv1.0. The new chemistry will a include chemical pathway that leads to secondary BrC formation—the reactive uptake of NH_3 on SOA. The current version of the model includes a simplified treatment of SOA with a two-product scheme that contributes to the total OA (purely scattering) mass. The new chemistry will expand the current implementation with a state-of-the-art BrC chemical mechanism to quantify the role of this new NH_3–SOA chemistry on the total OA burden. The mechanism will include an aging process for SOA that transforms pure-white organics into BrC, based on NH_3 reactive uptake. From laboratory studies it is known that the browning effect of some SOA species only lasts for a few hours, after which the aerosol recovers its purely scattering properties. This process will also be explicitly implemented in the model with a decay time of several hours (recent literature suggests a decay time of ~6 hours) from newly formed secondary BrC to purely scattering SOA.

Task 2.3 Aerosol microphysical treatment for BrC

To account for observed changes in aerosol microphysical properties upon reactive uptake of NH_3 by SOA, a new aerosol representation will be developed as task 2.3. This representation will follow the approach of current state-of-the-science approaches to modeling non-equilibrium aerosol processes at small scales (e.g., Roldin et al., 2014; Shiraiwa et al., 2010, 2012) that employ multi-layered aerosol representations. This type of approach will facilitate modeling of the formation of a solid shell by reactive uptake of NH_3 on SOA, leading to reduced coagulation and uptake of gases, and limited particle-phase diffusion, as has been observed for α-pinene-SOA reacting with gas-phase NH_3 in laboratory studies (Bell et al., 2017). To make the treatment feasible for regional and global modeling, the number of modeled aerosol layers will be reduced to 2 or 3, and applied only to BrC-containing aerosols. Dr. Zelenyuk-Imre, one of the external collaborators of this proposal, performed the laboratory studies that will be used to parameterize the new aerosol representation (Bell et al., 2017), was involved in the development of a similar model for the non-equilibrium treatments of aerosol processes at smaller scale (Rodin et al., 2014), and will be of invaluable help in the execution of task 2.3.

Task 2.4 Modeling experiments

Several numerical simulations with the new aerosol scheme implemented in NMMB-MONARCHv1.0 are planned. Two domains of study and periods of analysis are proposed:

a) Regional scale: High-resolution simulations will be conducted to explore the role of BrC chemistry in northeastern Spain at a resolution of 1 km x 1 km. Anthropogenic emissions will be provided by the HERMESv3 emission inventory developed at AC-BSC at hourly temporal resolution. Biomass burning emissions will be obtained from the CAMS Global Fire Assimilation System GFASv1.2. Biogenic emissions will be calculated online within NMMB-MONARCHv1.0 using the MEGANv2.04 model. Ground-based observations gathered as part of WP2 will be used to evaluate model performance in terms of surface concentrations of organic aerosols and to constrain the total AOD and the absorbing AOD. Retrievals of single scattering albedo and absorbing Ångstrom exponent will be used to identify periods of time when BrC is present. The period of study will be July 2018, covering the measurement period of the summer campaign in Vic conducted by EGAR.

b) Global scale: The updated model will be configured for an evaluation of the impact of NH_3 on SOA globally, at a resolution of 0.7º x 0.5º. Model input conditions, including gas and aerosol species emissions will be compiled from existing inventories: HTAPv2 for anthropogenic emissions, GFASv1.2 for biomass burning emissions, and MEGANv2.04 for biogenic emissions. Ground-based and satellite observations of key species and bulk aerosol optical properties will be used to evaluate model performance. Model results will be used to assess the impact of the newly incorporated chemistry on air quality hot spots and on the global distribution of absorbing AOD.

Results of both experiments will be discussed with UCI, PNNL and EGAR collaborators. The expertise of the AC-BSC research team on numerical modeling and the use of supercomputer resources makes this work package feasible.

Work package 3: Radiative forcing of organic aerosols
Work package 3 will cover specific objective 3. This work package is focused on quantifying the contribution of BrC and secondary BrC to the radiative forcing of organic aerosols globally. Thus, the optical properties of OA and BrC will be revised and updated, and the effect of BrC will be included in the radiative parameterizations of NMMB-MONARCHv1.0. Dr. Kostas Tsigaridis from NASA–GISS will be deeply involved in this work package: in the determination of the optical properties of BrC, the set-up of the model experiments, and the assessment of the radiative forcing of both OA and BrC. He is an expert in aerosol modeling and radiative forcing of organic aerosols.

Task 3.1 Review of aerosol optical properties: fresh, aged, coatings and water uptake
Currently, the NMMB-MONARCHv1.0 model uses the OPAC database to quantify the optical properties of each aerosol component. This information is then used to compute the aerosol optical depth and the radiative forcing of aerosols. The refractive indices from OPAC are outdated for some aerosol types (e.g., for mineral dust and organic aerosols), and water uptake is underestimated (e.g., for sulfate aerosols). In this task, we will review the optical properties for carbonaceous aerosols according to their physico-chemical state (freshly emitted, aged, with coatings of other species, such as sulfate, dry or with condensed water, etc.).

Several recent works have quantified the refractive index of organic aerosols. For reference, the OA refractive index currently used in NMMB-MONARCHv1.0 is 1.53 + 0.008i at 300 nm and 1.53 + 0.006i at 550 nm. Such values are typical of primarily scattering organic aerosols with some slight absorption. Recent work quantified the imaginary part of the refractive index for BrC as ranging from <0.0001 to 0.2 at 550 nm. This large variability indicates that BrC in regions not dominated by BC may be a significant contributor to total absorption. The choice of treatment for BrC in models, if one exists at all, may significantly affect the radiative forcing of OA.

A review of recent work quantifying the optical properties of aerosols will be conducted and a specific parameterization of optical properties will be determined for implementation in NMMB-MONARCHv1.0 as task 3.2.

Task 3.2 Implementation of BrC treatment in the radiative parameterizations of NMMB-MONARCHv1.0 and an update of aerosol optical properties

Aerosol–radiation interaction processes were implemented in NMMB-MONARCHv1.0 (previously known as NMMB/BSC-CTM) in projects CGL2006-11879 (for dust) and CGL2013-46736 (for other globally relevant aerosols: sea-salt, black carbon, organic carbon and sulfate). Following the same approach used in these projects, a treatment for BrC will be implemented as part of this project. Additionally, the contribution of SOA to the total radiative direct effect will be implemented for non-absorbing and absorbing species. The NMMB-MONARCHv1.0 atmospheric driver uses the RRTMG radiative transfer model, which permits the inclusion of aerosol effects in the radiative budget computation. In this task, we will calculate the extinction efficiency, single-scattering albedo and asymmetry factor for each aerosol size bin and wavelength with a Mie or T-matrix calculation. Complex refractive indices for aerosol components will be updated following the results of task 3.1. A weighted integration across the spectral bandwidth will then be performed using the extraterrestrial solar irradiance spectrum for the solar wavelengths and the Planck function for longer wavelengths. Mean values of optical thickness, single-scattering albedo, and asymmetry factor will then be in-turn derived for each spectral band and atmospheric layer to account for the direct radiative effect in the parameterization.

The expertise of the AC-BSC research team in numerical modeling and previous experience in similar parameterizations make this task completely feasible.

Task 3.3 Assessment of the radiative forcing of the OA and BrC components of organic aerosol

Aerosol radiative forcing is estimated as the difference in calculated radiative fluxes with all aerosols and with all aerosols except the aerosol type of interest (e.g., OA or BrC). A proper calculation of the radiative forcing of aerosols in models is done by calling the radiation scheme twice during a specific time step of the model. The first call is done considering the effect of all aerosols in the radiative balance, and the second call is done without the aerosol type of interest, or excluding all aerosols if the total effect is desired. Then, the difference in radiative fluxes provides the radiative forcing of only the aerosol type of interest. This approach is used in climate models to avoid considering secondary forcings due to changes in cloud formation attributed to numerical perturbations of aerosols far away from their area of influence. This methodology will be implemented in NMMB-MONARCHv1.0 as task 3.3. This will allow the model to calculate the instantaneous radiative forcing at specific time steps or average values over a specific time period (e.g., annual or monthly).

With this detailed methodology implemented, the radiative forcing of all organic aerosols, both OA and BrC, and their contribution to total aerosol forcing will be quantified using NMMB-MONARCHv1.0. To accomplish this, a global experiment will be prepared based on the configuration defined in task 2.3b. A 10-year run will be conducted under present-time conditions. Globally and regionally averaged values of forcing will be quantified, together with various temporal averagings. The internal variability of the forcing will be quantified and compared with current estimates of climate models. Results of this experiment will contribute to the AEROCOM-Phase III global aerosol model intercomparison initiative.

The expertise of the AC-BSC research team in using supercomputer resources assures the success of the numerical experiments planned for this task.

Work package 4: Project management and dissemination of results

Work package 4 is devoted to management, monitoring and dissemination activities.

Task 4.1 Project management

Management of the project will primarily involve communicating with and reporting to the Ministry. Reports will be provided annually. Monitoring of the project will assure its successful development. Corrective actions will be applied, if required, to reduce deviations from the original plan. Achievement of milestones will provide a means to quantify the proper development of the project.

Task 4.2 Dissemination of project results

The dissemination of results will be accomplished through: 1) participation in international conferences, symposia, and other scientifically related activities to present the on-going work of the project and discuss with the scientific community its impact, 2) publication in peer-reviewed journals of high-impact, and 3) presentation on the Barcelona Supercomputing Center (BSC) and Earth Sciences Department websites. Model developments will be reported on the model webpage. Public access to the model code will be provided at the end of the project.

1.5. Descripción medios materiales, infraestructuras y equipamientos

BSC will provide access to all key research facilities, infrastructure and equipment required to carry out the planned research. BSC hosts MareNostrum 4 (Spain's largest supercomputer and one of the six Tier-0 nodes of PRACE) and other HPC specialized machines and research prototypes. MareNostrum 4 has a performance capacity of 13.7 Petaflop/s. This new machine has two distinct parts. The general-purpose element, provided by Lenovo, has 48 racks with more than 3,400 nodes with next generation Intel Xeon processors and central memory of 390 Terabytes. Its peak power is over 11 Petaflop/s, ten times more than MareNostrum 3. Despite this increase in capacity, it consumes only 30% more power, reaching only 1.3 MW/year. The second element of MareNostrum 4 will comprise clusters of three different technologies that will be added and updated as they become available. These are technologies currently being developed in the US and Japan to accelerate the arrival of next-generation pre-exascale supercomputers. Like its predecessors, MareNostrum 4 will also be connected to the network of European research centers and universities through the RedIris and Geant networks. In addition, one or two proposals will be submitted to the Red Española de Supercomputacion to have complementary access to supercomputing resources.

1.6. Cronograma

The figure below shows a chronogram of the project along its 36 months of duration. Deliverables (D) and milestones (M) are indicated, and the contributions of each member of the group and external collaborators are detailed for the various tasks.

Objectives		1st year												2nd year												3rd year											
	HHRR	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
WP1																																					
T1.1	PI, EC1, EC2			M1.1																																	
T1.2	PI, RG1, EC6						D1.1																														
T1.3	PI, PD1, EC3, EC4																								D1.2												
WP2																																					
T2.1	RG1, RG3												M2.1																								
T2.2	PI, RG3, PD1, EC6																	M2.2																			
T2.3	RG2, EC6																			M2.3																	
T2.4	PD1, PI, RG3, EC1																													D2.1							
WP3																																					
T3.1	PD1, PI, RG1, EC5																								M3.1												
T3.2	RG2, PD1																														M3.2						
T3.3	PD1, PI, EC2, EC6																																				D3.1
WP4																																					
T4.1	PI												D4.1												D4.2												D4.3
T4.2	all												M4.1					M4.1							M4.1					M4.1							M4.1

Principal Investigator (PI): O. Jorba | Research Group: E. DiTomasso (RG1), S. Basart (RG2), F. Benincasa (RG3) | External collaborators: D. Dabdub (EC1), S. Nizkorodov (EC2), X. Querol (EC3), A. Alastuey (EC4), K. Tsigaridis (EC5), M. Dawson (EC6) | Hired Personnel: Post-Doc1 (PD1)

List of Deliverables (tracking achievements):

D1.1: Design of the secondary BrC formation mechanism: chemistry and aerosol microphysical treatment.

D1.2: Evidence of the reactive uptake of ammonia on SOA in field measurements.

D2.1: Report describing new BrC component in NMMB-MONARCHv1.0 and experimental results.

D3.1: Assessment of the radiative forcing of BrC.

D4.1: First annual report to the Ministry.
D4.2: Second annual report to the Ministry.
D4.3: Third annual report to the Ministry.

List of Milestones (tracking progress):
M1.1: Scientific review of laboratory experiments conducted at UCI on the reactive uptake of ammonia on SOA and the chemical mechanism design.
M2.1: BrC component implemented in NMMB-MONARCHv1.0.
M2.2: New NH_3–SOA chemistry implemented in NMMB-MONARCHv1.0.
M2.3: BrC microphysical treatment implemented in NMMB-MONARCHv1.0.
M3.1: Scientific review of aerosol optical properties.
M3.2: BrC direct effects implemented in the radiative scheme of NMMB-MONARCHv1.0.
M4.1: Presentation at international conferences of the ongoing results of the project.

C.1.7. Contratación de personal
A post-doctoral researcher (PD1) will be hired for two years to ensure the success of the present proposal.

PD1 will work in the design and implementation of the chemistry of secondary BrC in the NMMB-MONARCHv1.0 model. PD1 will be directly involved in:
- WP1, Task 1.3: Analysis of the EGAR field campaign of July 2018 to identify evidence of the reactive uptake of ammonia on SOA in the field. Comparison of model experiments with field campaign results.
- WP2, Task 2.2: Contribution to the implementation of the secondary BrC chemical mechanism in NMMB-MONARCHv1.0. Inclusion of chemical reactions described in WP1 Task 1.1.
- WP2, Task 2.4: PD1 will be responsible for conducting the numerical experiments to study the role of BrC chemistry in air quality. She/He will evaluate surface concentrations of organic aerosols, ammonia and ozone, and the aerosol optical depth, absorption and scattering. She/He will assemble data from various measurement networks—e.g., AERONET, satellite data, and campaign data.
- WP3, Task 3.1: PD1 will conduct a review of the state-of-the-art regarding optical properties of organic aerosols with an emphasis on BrC.
- WP3, Task 3.2: PD1 will contribute to the implementation of a new parameterization for BrC–radiation interactions in NMMB-MONARCHv1.0.
- WP3, Task 3.3: Analysis of the radiative forcing of secondary BrC at the global scale.
- WP4, Task 4.2: PD1 will contribute to the dissemination of results. PD1 will participate in international and national conferences and will be involved in the preparation of scientific publications.

2. IMPACTO ESPERADO DE LOS RESULTADOS - *EXPECTED RESULTS IMPACT*
2.1. Impacto científico-técnico, social y económico
Long-term societal impacts of this work will come through an improved understanding of the key precursors and reaction pathways leading to the formation of atmospheric particulate matter. These aerosol particles reduce visibility, have adverse human health effects and impact Earth's climate through their ability to scatter and absorb solar radiation. However, mechanisms by which aerosol particles form and age are complex and still relatively poorly understood. In fact, the effect of aerosols remains the largest uncertainty in predicting climate change. SOA accounts for an important but not well quantified fraction of total atmospheric aerosol mass. This work will represent an important step forward in developing next generation atmospheric chemistry models that provide accurate weather and air quality predictions, and allow the key precursors and chemical pathways leading to SOA formation to be identified. This is an essential part of developing effective emissions reduction strategies to mitigate the deleterious effect of aerosol particles on human health and Earth's climate.

The proposed work will result in an updated NMMB-MONARCHv1.0 model that will be immediately available for weather and air quality predictions, as well as for aerosol predictions as part of the International Cooperative for Aerosol Prediction Multi-Model

Ensemble (http://icap.atmos.und.edu/) and the CALIOPE Air Quality forecast system for Spain (http://www.bsc.es/caliope/es). These projects directly inform European and international legislators' work to develop air quality policy and regulations. The expected impact of this research—to improve the quality of predictions of aerosol mass and optical properties, and their impact on air quality and climate in one of the premier Spanish chemical weather prediction systems, NMMB-MONARCHv1.0—falls perfectly in line with European research priorities and concurrent initiatives.

2.2. Plan de difusión e internacionalización

Dissemination. Results from the proposed work will be disseminated through several channels. First, results will be prepared as a series of scientific articles submitted for publication in GMD, ACP, JGR and/or PNAS. The research group has a history of publishing in these and other high-impact journals; the Earth Sciences Department of BSC has produced more than 100 scientific publications in the last three years. Additionally, a project web portal will be developed for communication of project information, progress and results to researchers and the general public. The NMMB-MONARCHv1.0 model will be disseminated to the community via the web portal through a versioning control system under development at BSC. Results from the proposed work will be presented at EGU, AGU and other appropriate international conferences. Presentation of the research conducted in the project will be included in the annual BSC Doctoral Symposium, for the PhD-students and post-doctoral researchers involved in the project.

Exploitation. The results from the proposed work will be immediately and straightforwardly exploited for the benefit of European citizens and air-quality and climate researchers globally. First, the updated NMMB-MONARCHv1.0 model will be immediately available for weather and air quality predictions, as well as for aerosol predictions as part of the ICAP-MME and CALIOPE projects. Finally, the results of this work will be made immediately available for exploitation by air quality and climate researchers in several ways:

- The assessment of the potential impact of NH_3 on aerosol mass and optical properties on the global scale will inform funding agencies and laboratory and field researchers as they allocate resources and propose future research into the complex processes at work in the interactions of NH_3 with gas- and particle-phase species.
- The updated chemistry module, made publicly available on the web portal, will facilitate the straightforward exploitation of this detailed SOA treatment by researchers in the field as they work to improve SOA predictions in other regional- and global-scale models.
- The NMMB-MONARCHv1.0 chemical weather prediction model will be exploited as the base model for future enhancements, including developing aqueous-phase aerosol and cloud chemistry treatments, for which an accurate, detailed organic and inorganic aerosol module is needed.

Communication of research results and public engagement will be a key focus of the proposed work, and is included in WP4. The research group has a strong history in the presentation of research results at scientific conferences, and engagement with the public through publications to the media via the BSC Communication department. Indeed, BSC has dedicated staff and several operational programs in place to communicate activities to other researchers, students, and the general public that will be exploited by the research group as part of WP4. First, important results and milestones will be published in the BSC newsletter for communication to the general public. Existing routes of communication at BSC (website, brochures, presentations, etc.) will also be employed to communicate project information, progress and results. Specific details of the communication through these channels will be developed in conjunction with BSC staff as part of WP4. Members of the research group will further participate in MareNostrum open days, for students and the general public, and professional tours, which exceed 5000 per year. The BSC operates as a PRACE Advanced Training Centre with a mission to provide training and education related to the utilization of European supercomputing resources, including for environmental simulation. As part of WP4, members of the research group will participate in the PRACE training program modules related to atmospheric modelling. Finally, results will be presented approximately once a year as part of the BSC Research Seminar Lecture series.

2.3. Transferencia de resultados

Results of the project will consist of an improved atmospheric chemistry forecasting system, a better understanding of the radiative forcing of the organic aerosols, and the impact of the direct effect of organic aerosols on meteorological forecasts and climate. In this sense, the transfer of knowledge will be organized into two main plans. First, the improved NMMB-MONARCHv1.0 model will be transfered to the *CALIOPE: Air Quality Forecasting System for Spain* as the main model kernel. The new SOA mechanism and the inclusion of BrC will improve the aerosol predictions of the system. The contribution of AC-BSC to ICAP-MME global aerosol forecasts will be updated with predictions based on the new NMMB-MONARCHv1.0 model. Furthermore, the products obtained with the new aerosol mechanism will be transferred to the World Meteorological Organization's (WMO) Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS), the Northern Africa-Middle East-Europe (NA-ME-E) Regional Center and the Barcelona Dust Forecast Center. The centers will distribute internationally the improvements achieved in model forecasts. In addition, the scientific results will be disseminated through presentations at international conferences, workshops and publication in international journals. Through these dissemination efforts, contacts may be made in the scientific community to exchange experience and knowledge in related fields of study. Several institutions have expressed interest in the project results: NASA–Goddard Institute for Space Studies (NASA–GISS; USA), the University of California Irvine (UCI; USA), AEMET Izaña Atmospheric Research Center (Spain), CSIC-Institute of Environmental Assessment and Water Research (Spain), and the Barcelona Dust Forecast Center (Spain).

3. CAPACIDAD FORMATIVA - *TRAINING CAPACITY*

3.1. Programa de formación

The training plan envisaged for the pre-doctoral contract in the project context will address the acquisition of competence in atmospheric modelling, secondary organic aerosol chemistry and radiative forcing. This transition will be ensured by his/her participation in the proposed project and following a training schedule organized by the Earth Sciences Department of BSC that takes advantage of its experience in these areas. The overall objective of the training program is the transfer of knowledge from BSC to the pre-doctoral student in the field of advanced atmospheric and aerosol modelling. The acquisition of expertise in the following scientific topics has been identified as the principal training objective: 1) meteorology–air quality modelling (emission processes, transport in the atmosphere, cloud processes, and dry and wet deposition); and 2) aerosol radiative forcing (optical properties of aerosols, radiative transfer models for SW and LW, the direct effect of aerosols, and meteorological feedbacks). This training will be developed in the framework of the PhD program in the Environmental Engineering department at UPC. This doctoral program had the MEC Quality Mention until 2010 (MCD2004-00394), presently has the MEC Excellence Mention since 2011 (MEE2011-0335), and is currently registered in the VERIFICA process of the ANECA evaluation agency (RUCT: 5600080).

The BSC is dedicated to providing high-quality pre-doctoral training that draws upon its experience in developing specific technical and scientific skills, as well as the complementary skills required for efficient research execution and communication. The candidate will have the oportunity to participate in some of the courses organized by the BSC as a member of the PRACE consortium. PRACE, the Partnership for Advanced Computing in Europe, appointed BSC as one of the first PRACE Advanced Training Centres (PATC). The mission of PATC is to carry out and coordinate training and education activities that enable the European research community to utilise the computational infrastructure available through PRACE. The envisaged courses where the candidate may participate are: PRACE PATC Course Earth Sciences Simulation Environments, and PRACE PATC Course PUMPS Summer School.

The pre-doctoral candidate will conduct a short-term visit of 4 months with the research groups of Prof. Donald Dabdub from the Department of Mechanical and Aerospace Engineering at the University of California, Irvine, and of Prof. Sergey Nizkorodov from the Chemistry Department at the University of California, Irvine. During this visit, the pre-doctoral contract will gain knowledge in the chemistry formation of secondary organic aerosols and

their optical transformations in the presence of high NH_3 concentrations. Additionally, the pre-doctoral contract will contribute to the implementation of the new chemistry proposed by the groups of Prof. Sergey Nizkorodov and Prof. Donald Dabdub in the chemistry model being developed as part of the present proposal.

3.2. Relación de tesis realizadas o en curso en los últimos 10 años
PhD thesis defended in the last 10 years:

1) Vicenzo Obiso. "Assessment of Dynamic Aerosol-Radiation Interaction in Atmospheric Models". 7/3/2018. Obiso et al. (2017 JAS), Obiso and Jorba (2018 JAS).
2) Lluís Vendrell Miquel. "Modeling the dust life cycle and its associated meteorological processes from global to regional scales". 10/11/2017.
3) Michele Spada. "Development And Implementation Of A Fully Coupled Global Aerosol Model Within The Chemical Non-Hydrostatic Multiscale Model (NMMB/BSC-CHEM)". 23/11/2015. Spada et al. (2013), Spada et al. (2015).
4) Alba Badia Moragas. "Implementation And Development Of A Gas-Phase Chemical Mechanism Within The Global/Regional Atmospheric Chemical Nonhydrostatic Multiscale Model (NMMB/BSC-CHEM)". 12/12/2014. Badia and Jorba (2014 AE), Badia et al. (2017 GMD).
5) Albert Soret Miravet. "Air Quality Management: Assessing The Impacts Of On-Road Transport Strategies And Industrial Emissions In Urban Areas". 18/12/2014. Soret et al. (2011 APR), Soret et al. (2014 AE).
6) Marc Guevara Vilardell. "Desarrollo De Un Modelo Para La Estimación De Las Emisiones Atmosféricas En España Orientado A La Modelización De La Calidad Del Aire". 17/12/2014. Guevara et al. (2014 AE).
7) Ángel Rincón Rodríguez. "Sistema De Pronóstico De Radiación Solar A Corto Plazo A Partir De Un Modelo Meteorológico Y Técnicas De Post-Proceso Para España". 28/06/2013.
8) Simone Marras. "Variational Multiscale Stabilization Of Finite And Spectral Elements For Dry And Moist Atmospheric Problems". 10/12/2012. Marras et al. (2013ab JCP),
9) Karsten Haustein."Development Of An Atmospheric Modeling System For Regional And Global Mineral Dust Prediction". 31/01/2012. Haustein et al. (2012 ACP).
10) Sara Basart Alpuente."Mineral Dust Model Validation Through Ground Based And Satellite Observation In North Africa And Europe". 30/01/2012. Basart et al. (2009 ACP), Basart et al. (2012 ACP), Basart et al. (2012 Tellus).
11) María Teresa Pay Pérez. "Regional And Urban Evaluation Of An Air Quality Modelling System In The European And Spanish Domains". 22/11/2011. Pay et al. (2010ab AE), Pay et al. (2011 AE), Pay et al. (2012 AE).
12) María Gonçalves Ageitos. "Assesing Variations In Urban Air Quality When Introducing On-Road Traffic Management Strategies By Means Of High-Resolution Modelling. Application To Barcelona And Madrid Urban Areas". 09/03/2009. Gonçalves et al. (2008 AE), Gonçalves et al. (2008 STOTEN), Gonçalves et al. (2009 AE), Gonçalves et al. (2009 STOTEN).

PhD thesis under development:
1) Jaime Pérez Benavides. "Development And Evaluation Of An Air Quality Modelling System Over Barcelona: From Regional To Street Scale". Expected date: July 2019.

3.3. Desarrollo científico - profesional de los doctores egresados del equipo de investigación
N/A

3.4. Contexto científico-técnico y formativo del equipo y de la institución
The BSC is a public consortium composed of: the Spanish Ministry of Economy, Industry and Competitiveness, the Catalan government and the Universitat Politècnica de Catalunya (UPC). The mission of the BSC is to research, develop and manage information technology in order to facilitate scientific progress. The BSC is one of the first eight recipients of the Spanish “Severo Ochoa Centre of Excellence” award given by the Spanish Government, and one of the four host members of the European PRACE Research Infrastructure FP7 project.

The BSC hosts the MareNostrum 4 supercomputer, used in a Tier-0 PRACE system with 13Pflop/s capacity.

The Earth Sciences Department of BSC (ES-BSC) is focused on carrying out research in Earth system modeling. The high performance capabilities and close collaboration with the Computer Sciences department allow an increase in the spatial/temporal resolution of atmospheric modeling systems to improve our knowledge of dynamic patterns of air pollutants in complex terrains and the atmospheric interactions/feedbacks of physico-chemical processes. ES-BSC produces daily operational air quality and mineral dust forecasts for scientific purposes and to support national initiatives for air quality interventions. In addition, ES-BSC is an active air quality model developer, including emission models, aerosol models and chemistry models. Thus, ES-BSC is an appropriate place to conduct the proposed research, which falls within the ES-BSC mission scope, and ES-BSC provides the computational infrastructure required to successfully execute the proposal.

The BSC provides a 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 because of its progress in aligning their human resources policies with the principles set out in the EU Charter and Code for Research. Additionally, BSC organizes doctoral symposia to allow its PhD students to present and discuss their own research with the professors and researchers of the center.

4. IMPLICACIONES ÉTICAS Y/O DE BIOSEGURIDAD - *ETHICAL AND/OR BIOSAFETY IMPLICATIONS*

None.