Convocatoria 2019 - «Proyectos de I+D+i»

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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 €, this document must be filled in English.

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TÍTULO DEL PROYECTO (ACRÓNIMO): eValuación del ImpacTo de medidAs de mobiLIdad urbana Sobre la calidad del airE y la salud pública (VITALISE)

TITLE OF THE PROJECT (ACRONYM): *eValuating the ImpacT of urbAn mobiLIty measureS upon air quality and public hEalth (VITALISE)*

1. PROPUESTA CIENTÍFICA - *SCIENTIFIC PROPOSAL*

1.1. Antecedentes, estado actual y justificación de la propuesta

Air pollution as a key problem in urban areas

Air pollution remains as a key unresolved problem in many urban areas. In 2016, more than 70% of urban population in Europe were exposed to $PM_{2.5}$ concentrations exceeding the World Health Organization (WHO) air quality guidelines (AQGs) (10 $\mu g \cdot m^{-3}$) (EEA, 2018). At the same time, the annual limit value for nitrogen dioxide concentrations (NO_2) established in the 2008/50/EC EU Ambient Air Quality Directive (AQD) is also widely exceeded across Europe, with around 11.5% of all reporting stations recording concentrations above the threshold value (40 $\mu g \cdot m^{-3}$) in 2016. ***Approximately 88% of the exceedances of the NO_2 annual limit value were observed in traffic stations, highlighting the contribution of road transport to population exposure to ambient concentrations***.

In the city of Barcelona (Spain), chronic NO_2 and $PM_{2.5}$ exceedances are also recorded in urban traffic stations (ASPB, 2018). This is despite the downward concentration trends observed in Spain during the last decade due the implementation of major policy actions (Querol et al., 2014; Cuevas et al., 2014). The high vehicle density (5500 vehicles km^{-2}) and coastal emplacement of the city (i.e. dominance of sea breeze during the warm season, shallow boundary layer development and recirculation of air pollutants; Jorba et al. (2004)) are the main causes for the poor air quality. Studies have shown that the urban plume of Barcelona very often also causes severe ozone (O_3) episodes in the northern plains and valleys especially in the Vic Plain (Querol et al., 2016; Valverde et al., 2016). ***Clearly, the road transport emissions released in Barcelona have an impact both at urban and regional scales.***

Air pollution is also a problem in terms of health of citizens. In the recent years, multiple studies have highlighted the impacts of air pollution on public health, especially in urban areas like Barcelona. Persistent exposure to high $PM_{2.5}$ and NO_2 atmospheric concentrations can play an active role on human fertility rate (Nieuwenhuijsen et al., 2014) and cause detrimental health effects in children such as reduction in cognitive functions (Sunyer et al., 2015).

Assessing the impact of mobility plans at the local scale

Public administrations are currently testing several management strategies to reduce on–road traffic emissions. Due to the failed outcomes in reducing NO_x by the reduction of vehicle emissions (i.e. the diesel gate scandal, Jonson et al. (2017)), local authorities are focusing on mobility policies that try to reduce the number of circulating vehicles within the city. These policies include the implementation of Low Emission Zones (LEZ), congestion charges, car sharing schemes and the promotion of eco-driving (reduction of driving speed), among others (Holman et al., 2015). Following, these lines, the city of Barcelona has recently presented the new Urban Mobility Plan (UMP 2019-2024), whose guiding principle is to increase mobility on foot while reducing the use and presence of private motorized transport.

The application of numerical models in combination with monitoring data is highlighted in the AQD as a fundamental tool to better assess and manage air quality, encouraging their use in the preparation of air quality plans (Miranda et al., 2015). This fact is particularly relevant for Barcelona, where the monitoring network is not dense enough for properly characterising population exposure and therefore needs to be combined with models (Duyzer et al., 2015). ***Air quality models should be used for both assessment and planning; but to do so, the modelling chain has to be fit-for-purpose and properly checked and verified.***

Mesoscale Eulerian Chemical Transport Models (CTMs), which require as input data estimated emissions and meteorological variables, are currently the most widely used when performing the evaluation of the potential emission reductions (e.g. Pisoni et al., 2019). These air quality systems are usually combined with Traffic and travel demand models (TDM) (Barceló, 2010) to simulate the effect of restrictions on the traffic activity (e.g. traffic flow, speed) across the city (e.g. San José et al., 2018). The application of such an integrated modelling approach allows estimating the changes induced by the mobility action not only in the implementation area (e.g the LEZ) but also, more generally, in the city where it is located and surroundings. Therefore, possible rebound effects such as the increase of urban O_3 levels due to the traffic NO_x emission reductions (Saiz-Lopez et al., 2017) can be accounted for when using a CTM.

Despite a satisfactory performance of the CTMs, several studies have identified emissions as one of the main sources of uncertainty in the air quality modelling chain. In the particular case of road transport, the quality of the estimated emissions largely depends on the representativeness and accuracy of the: vehicle emission rates, vehicle activity patterns (traffic flow, speed) and vehicle fleet distribution (Smit et al., 2010). In the macroscopic approach, emissions for a specific vehicle category are obtained using average-speed (e.g. COPERT) or traffic situation (e.g HBEFA) emission factor models (e.g. Borge et al., 2012). On the other hand, in the microscopic approach emission traffic models are based on vehicle-specific instantaneous engine or state data (e.g. speed, acceleration) (e.g. PHEM, VERSIT+) (Borrego et al., 2016). Microscopic models provide emissions at higher temporal resolution compared to macroscopic models (Quaassdorff et al., 2016), yet are more data-intensive and their use is mostly limited to the analysis of very small areas (e.g. intersections). The comparisons of model-based emission factors against real-world measurements have shown significant discrepancies and the need to apply correction factors to the models (e.g. Ntziachristos et al., 2016). In terms of activity data, the use of information derived from traffic cameras (Perez et al., 2019) is also gaining more attention for the compilation of urban traffic emissions. ***Overall, the combination of state-of-the-art estimation approaches and local activity and emission measurements is key for the compilation of reliable urban traffic emissions.***

Another important limitation of CTMs is that due to limited spatial resolution the strong urban pollutant concentration gradients, usually associated to high road traffic flows, cannot be reproduced (Borge et al., 2014). ***In order to depict street level concentration gradients, local–scale tools are needed, either high–resolution flow models that consider the buildings (e.g. Computational Fluid Dynamic (CFD) models or Large Eddy Simulation (LES) models) or semi–empirical street canyon models based on Gaussian dispersion curves (e.g. ADMS-URBAN, OSPM) able to capture this local variability***. Coupling regional and urban scales by downscaling the regional CTMs using a dispersion kernel has been successfully applied in several cities during the last years (e.g. Borge et al., 2014; Jensen et al., 2017; Kim et al., 2018; Hood et al., 2018; Benavides et al., 2019). Other studies have also proved valid the use of CFD for assessing street-scale air quality levels (e.g. Santiago et al., 2017), their main limitation being that they are very computationally expensive and can only be applied to spatially and temporally restricted domains (i.e. not entire cities).

Besides improving the performance of grid-based CTMs, the application of a hybrid air quality modelling approach (i.e. the combination of mesoscale and street-scale dispersion models) can also lead to more detailed results when evaluating urban mobility plans. As reported by Borge et al. (2018), while the response of both mesoscale and microscale models to the same emission perturbation is rather consistent, the actual effect on exposure may change substantially for each specific street in the latter (e.g. larger concentration reductions in heavily trafficked streets when compared to pedestrian streets). CTMs can provide an overview of the citywide effect of a mobility action, but microscale models give details attributable to local-scale dispersion. ***Therefore, urban air quality plans should be assessed under a multi-scale modelling approach for an optimal result.***

Mesoscale CTMs have been widely used in health studies to estimate air pollutant exposures and the effect of reduction policies (e.g. Boldo et al., 2014; Anenberg et al., 2017). More recently, hybrid air quality modelling approaches have also begun to be implemented to estimate exposure to traffic-related air pollutants in urban areas (Isakov et al., 2014). Nevertheless, there has been little work done in using these hybrid modelling approaches for quantifying the impact of traffic management strategies on public health (Bigazzi and Rouleau, 2017). In the case of Barcelona, studies of health effects have typically relied on the application of land-use regression techniques (e.g. Eeftens et al., 2012) or on the use of the ADMS-Urban street canyon model (Rojas-Rueda et al., 2012). Nevertheless, when using ADMS-Urban, the model is not coupled to a mesoscale CTM, and background concentration levels are based on data from a background station located on the coast in the north of Catalonia. This fact implies that none of the Barcelona studies have considered the contributions from photochemical interactions or the dynamics of long-range (regional) transport. Therefore, when such methodologies have been applied for scenario assessment, the non-linearity of atmospheric chemistry processes have been neglected considering the impact of reducing only one pollutant (i.e., NO_2). ***A refinement in the characterization of air pollutants (composition of gas and particle phase, size distribution of particles) and their chemical evolution under different conditions may provide an added value to advance our knowledge on the health impact of mobility plans.***

Aim of the proposal

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

- To what extent can current and future local traffic management strategies improve urban and regional air quality levels (NO_2, O_3, $PM_{2.5}$)?
- How does the use of hybrid air quality models in comparison to traditional mesoscale models affect the estimation of air pollution and public health impacts when evaluating urban mobility plans?

We will address these scientific questions using the city of Barcelona as our region of study. The Atmospheric Composition group of the Barcelona Supercomputing Center (AC-BSC) has a large experience in air quality modelling studies in Barcelona (see subsection on the background of the group). For the present proposal, a multidisciplinary approach is planned that combines expertise in emission and air quality modeling, transport modeling, field measurements and health impact assessment. The funded project will allow the research team from the AC-BSC, which has wide experience in air quality and emission modeling at local-to-global scales, to strengthen established collaborations with: 1) the inLab-FIB research and innovation laboratory of the Universitat Politècnica de Catalunya (inLab FIB UPC), a research group focused on traffic and travel demand modelling, 2) the Environmental Geochemistry Atmospheric Research IDAEA-CSIC group (EGAR), which comprises experts in field measurements of air quality throughout Spain and Europe, and 3) the Barcelona Institute for Global Health (ISGlobal), which performs exposure assessment, epidemiological and health impacts studies on a range of urban-related exposures including air pollution.

Novelty of the proposal

Table 1 summarizes the most up-to-date works that have evaluated the impact of urban mobility actions in terms of air quality and/or public health in Spain (Borge et al., 2018; San José et al., 2018; Mueller et al., 2019). All three works included the use of a TDM to simulate the impacts of traffic restrictions on emissions. One of the main limitations of Borge et al. (2018) and Mueller et al. (2019) is the non-inclusion of $PM_{2.5}$ and O_3 in the impact assessment. San José et al. (2018) includes $PM_{2.5}$ but the approach is based on a mesoscale system ($1km^2$) and do not consider the street level concentration gradients. In the case of Borge et al. (2018), it uses a multi-scale modelling approach, which combines a mesoscale CTM for the entire city ($1km^2$) with a CFD. Nevertheless, the use of a CFD model limits the spatial and temporal coverage of the study (e.g. limited domain, short-term measure and limited number of scenarios). On the other hand, Mueller et al. (2019) includes the quantification of the annual preventable premature mortality related to NO_2 but relies on a rather simple modelling approach that does not consider the non-linearity of atmospheric chemistry processes.

The novelty of VITALISE relies on the following points:

- ***Combination of scenarios:*** *The project will not only perform the air quality and health impact assessment of a single traffic measure but of a combination of many (e.g. implementation of the superblock model + unification of Barcelona's tram + implementation of congestion charge + electrification of the vehicle fleet).*
- ***Multipollutant and multiscale assessment:*** *The assessed air quality impacts will not be limited to NO_2 but will also include $PM_{2.5}$ and O_3 at both urban and regional level*.
- ***Spatial and temporal coverage:*** *The microscale domain will include the whole city of Barcelona. The assessment will cover short (specific pollution episodes) and long (annual mean values) term periods.*
- ***Climate change:*** *The estimation of impacts on greenhouse gases will allow quantifying other co-benefits such as the decarbonization of the urban transport.*

Table 1 Recent works on modelling the impact of urban mobility actions in Spain

Ref. City	Assessed impacts	Modelling approach	Limitations
Borge et al. (2018) Madrid	Urban NO_2 (hourly maximum)	Mesoscale CTM for the entire city (1km) + CFD for a microscale domain in the city center. Traffic restrictions modelled with a TDM.	- No inclusion of urban $PM_{2.5}$ or regional O_3 - No inclusion of health impact assessment - Microscale domain not covering the entire city
San José et al. (2018) Madrid	- Urban NO_2 and $PM_{2.5}$ (daily average) - Daily mean change of mortality	Mesoscale CTM for the entire city (1km). Traffic restrictions modelled with a TDM. Health impacts modelled with exposure-response functions	- No inclusion of regional O_3 - No inclusion of a microscale modelling approach to consider street level concentration gradients.

Mueller et al. (2019) Madrid	- Urban NO_2 (anual mean) - Preventable premature mortality	Street scale dispersion model coupled with background observations. Traffic restrictions modelled with a TDM. Health impacts modelled with exposure-response functions	- No inclusion of urban $PM_{2.5}$ or regional O_3 - Non-consideration of the non-linearity of atmospheric chemistry processes - Modelling at the census-track level

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

The AC-BSC research group has strong expertise in emissions and air quality 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; Jiménez-Guerrero et al., 2008; Jorba et al., 2012; Spada et al., 2013). 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). The CALIOPE system operationally provides air quality forecasts for Europe at 12-km resolution and for Spain at 4-km resolution using mesoscale meteorological and chemical transport models, and has been used for air quality assessment in main urban regions (Barcelona and Madrid at 1-km resolution). 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; Badia et al., 2017), a fully online chemical weather prediction system for meso- to global-scale applications that is currently a candidate model of the Regional Production Service CAMS50 of the European Copernicus program.

The group has published extensive work on the assessment and evaluation of traffic emission abatement measures on Barcelona using the CALIOPE system. The works performed include the evaluation of the impact on emissions and air quality of: (1) the 80 km h^{-1} speed limit in the access roads of the Barcelona Metropolitan area (Gonçalves et al., 2008), (2) the introduction of natural gas vehicles (Gonçalves et al., 2009), (3) the implementation of superblocks (Soret et al., 2011) and (4) the electrification of the fleet composition (Soret et al., 2014).

During the last years, the AC-BSC research group has worked towards the improvement of the estimation of high-resolved emissions as well as the modelling of air pollution at the urban scale. Concerning the first point, the group has developed the High-Elective Resolution Modelling Emission System version 3 (HERMESv3), a stand-alone multiscale atmospheric emission modelling framework that processes and computes gaseous and aerosol emissions for use in atmospheric chemistry models (Guevara et al., 2019). In the case of road transport, HERMESv3 estimates hourly and street-level emissions for both criteria pollutants (i.e. NO_x; CO; NMVOC; SO_x; NH_3; PM10 and PM2.5) and greenhouse gases (CO_2 and CH_4) associated to cold-start, hot exhaust, wear and resuspension processes using emission factors derived from the COmputer Programme to calculate Emissions from Road Transport version 5 (COPERT 5; https://copert.emisia.com/), and Amato et al. (2012). Regarding the second point, the CALIOPE mesoscale forecasting system has successfully been coupled with the Research LINE urban dispersion model (RLINE; Snyder et al., 2013; Valencia et al., 2018). The coupled regional to street-scale modelling system, namely CALIOPE-Urbanv1.0, is capable of providing high-spatial and high-temporal-resolution (up to 10 m×10 m and hourly) NO_2 concentrations for the city of Barcelona (Benavides et al., 2019). The temporal and spatial variability of CALIOPE-Urbanv1.0 has been evaluated against measurements from traffic and background sites as well as passive dosimeters distributed across Barcelona. Additionally, the dispersion of black carbon in the city modeled by CALIOPE-Urbanv1.0 has been compared with novel measurements of horizontal and vertical profiles described in Amato et al. (2019).

The AC-BSC group has established several collaborations with national research teams including AEMET, CIEMAT, IDAEA-CSIC, inLab FIB UPC, ISGlobal, 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 European Center for Medium-Range Weather Forecasting (ECMWF; EU), The Netherlands Organisation for Applied Scientific Research (TNO), Le Centre national de la recherche scientifique (CNRS), NASA–Goddard Institute for Space Studies (NASA–GISS; USA) and the University of California, Irvine (UCI; USA). It is believed that such collaborations strongly benefit the progress of the scientific projects undertaken by AC-BSC. Furthermore, the principal investigator (PI) of the present proposal currently coordinates the work package on service evolution of the Global and Regional Emission Service CAMS81 of the Copernicus program of the European Commission. The PI also co-chairs the working group on emission inventories of the Forum for Air quality Modeling (FAIRMODE). In the recent months, the PI was invited to participate in the emissions working group of the Multi-Scale Chemistry Modeling (MUSICA) initiative, lead by the National Center for Atmospheric Research (NCAR).

More recently, the AC-BSC group started a collaboration with inLab FIB UPC with the aim of integrating the emission and transport modelling tools developed by each group. This joint effort is currently materialized through a PhD thesis that is being co-directed by the IP of this proposal and Dr. Josep Casanovas, and that has the objective of integrating the HERMESv3 emission system with the Virtual mobility lab transport model (VLM). The VML tool is a detailed multimodal transport modeling of the First Crown of the Metropolitan Area of Barcelona that integrates both the offer of all modes of public transport, as well as the road by the private vehicle and the demand for updated mobility. The VML model relies on the VISUM mesoscale traffic model (http://vision-traffic.ptvgroup.com), and is capable of supporting decision-makers in mobility policies. ***This state-of-the-art transport modelling tool developed will be key for the correct assessment and evaluation of the mobility policies.***

Furthermore, AC-BSC has a long history of collaboration with EGAR IDAEA-CSIC (Viana et al., 2005; Jorba et al., 2013; Pay et al., 2012; Obiso et al., 2017; Benavides et al., 2019). 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 gases and aerosols in Barcelona. ***Thus, the EGAR group offers an ideal synergistic complement to the AC-BSC team for the analysis of field measurements and modeling results.***

Air quality concentrations modelled with CALIOPE have been used in the past by ISGlobal for epidemiological research and health impact studies (Aguilera et al., 2013; de Keijzer et al., 2016). Currently, a collaborative study on the diesel-gate impact on air quality and health is also being conducted between AC-BSC and ISGlobal. The institution has a large experience in compiling mortality data and quantifying the associations between exposures and mortality in Barcelona, and its research objectives are in line with those of the present proposal. ***The epidemiological databases generated by ISGlobal past and ongoing studies can be exploited with the exposure metrics derived with the AC-BSC modelling tools.***

Initial hypothesis

The initial hypotheses of the project are as follows:

1) Recent field campaigns have demonstrated that traffic emission models tend to underestimate vehicle emissions. During 2017, the Barcelona city performed a remote sensing device campaign to measure thousands of vehicles and obtain real data on traffic emissions. **We hypothesize that these in-situ measurements, to which the AC-BSC has access, will dramatically correct the current underestimation in vehicle emissions.**

2) Traditional surrogates of exposure (e.g. land-use regression techniques) used in health impact studies do not capture potentially important influences on spatial variability and temporal variability of traffic-related air pollutants. **We hypothesize that the use of emission and hybrid air quality models will substantially reduce uncertainty in exposure estimates and allow more reliable health impact assessments**

3) CTMs are not able to adequately reproduce the concentration gradients that typically occur near heavily trafficked street. A hybrid approach (coupling of CTMs with a urban dispersion model) is needed to correctly simulated street-level concentrations. **We hypothesize that when evaluating the impact of a traffic management strategy, the responses obtained with a CTM and a hybrid modelling approach will change substantially.**

4) Following with the previous hypothesis, **we hypothesize that a hybrid modelling approach will estimate more detailed exposure metrics when compared to CTMs and that this will affect the results obtained in terms of health impact assessment.**

5) Current health studies mostly focus on the impact of mobility policies to individual pollutants (NO_2) and neglect potential cofounding effects on other pollutants also affected by the emission reductions (O_3). **We hypothesize that a multi-pollutant modelling approach will lead to a much very detailed quantification of the attributable preventable mortality burden.**

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1.2. Objetivos generales y específicos

Main objective

The overall scientific objective of VITALISE is to quantify the impact of Barcelona's urban mobility plans and policies upon local and regional air quality and public health. The project will use a comprehensive multi-scale modeling approach and target NO_2, $PM_{2.5}$ and O_3.

Specific objectives

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

1) Compiling mobility scenario-dependent and very high-resolution road transport emissions

Emissions are generally recognized as key inputs to air quality systems due to the large uncertainty that they introduce in the modelling chain. In the case of road transport, main uncertainties arise from: 1) the traffic activity data used as input, which is usually based on static information such as traffic counts and vehicle census information, and 2) the vehicle emission rates, which tend to underestimate real circulation driving emissions. In order to overcome these limitations, the HERMESv3 road transport emission module will be refined by using on-road emission measurements. Moreover, HERMESv3 will be coupled with the Barcelona's Virtual mobility lab transport model in order to simulate the impact of urban mobility actions on traffic dynamics and emissions. These two actions will allow improving the representativeness a reliability of the emissions considered for the assessment study.

2) Advancing the current knowledge of the characterisation of street-canyon and near-road atmospheric chemistry processes for both gas and condensed-phase pollutants

A correct modelling of street canyon principal effects on dispersion is key in order to reproduce the high pollution levels that are usually observed in these spots. The R-LINE gaussian dispersion model implemented within CALIOPE-Urbanv1.0 includes a parametrization to reproduce the channeling effect along street canyons. Nevertheless, it does not account for other street canyons effects such as pollutants trapped in recirculation regions, exchange of pollution in inter-section links or wall effects. At the same time, when assessing the impact of emission abatement measures on $PM_{2.5}$ concentrations, it is important to reproduce not only the dispersion of the total mass across the urban geometry but also the formation of secondary aerosol components. In its current version, the CALIOPE-Urbanv1.0 system uses the R-LINE Generic Reaction Set NO_x photolytic chemistry module, which accounts for fast, near-road oxidation of NO by O_3 to form NO_2. Nevertheless, for PM_{10} and $PM_{2.5}$ R-LINE only models the dispersion of primary species (e.g. black carbon) as inert tracers and do not predict the formation of secondary pollutants (e.g. secondary inorganic and organic aerosols). In order to overcome these obstacles, new parametrizations will be include in CALIOPE-Urbanv1.0 to better assess the canyon effect and to predict the formation of secondary aerosols.

3) Assessing the impact of individual and combined urban mobility policies on local and regional air quality and public health.

A multiscale and multipollutant approach is needed when assessing the impact of urban mobility policies in order to consider both the regional and urban effects as well as potential rebound effects. A set of urban mobility policies (changes of traffic volume, vehicle speeds and technologies) will be defined and then modelled combining the transport-emission coupled model and the mesoscale CALIOPE and microscale CALIOPE-Urbanv1.0 systems. For each case, expected changes in the air pollutant concentrations will be combined with exposure-response functions to quantify the impact on public health. The proposed approach will allow identifying combinations of urban mobility options that can achieve significant reductions of urban and regional air pollution and mortality in Barcelona.

The figure below shows the workflow that will be applied to fulfill the aforementioned objectives.

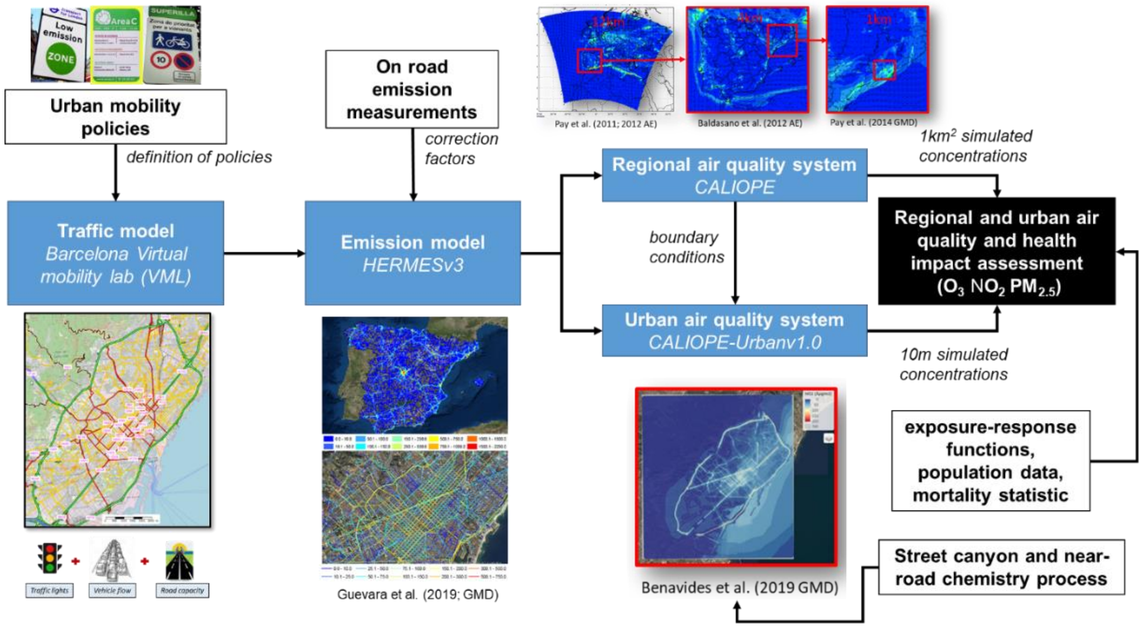

Figure 1. Workflow of VITALISE for assessing the impact of urban mobility policies.

1.3. 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 and resource efficiency and raw materials. Particularly, it addresses the thematic priority of using and improving environmental engineering tools for the monitoring, assessment and design of environmental policies. VITALISE addresses the research problem of determining the impact of local mobility plans on urban and regional air quality levels 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 impact of specific traffic management measures at a multi-scale level. 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.

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, which includes NO_x and VOC from traffic activities. Modeling tools developed as part of the proposed project will provide valuable information about how the implementation of mobility policies can impact the formation of secondary aerosols. 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. VITALISE has as its primary objective to further understanding the performance of hybrid air quality modelling tools, which combine mesoscale and microscale models, and the role of refined traffic emissions for assessing street level pollutant concentrations.

Finally, the Horizon 2020 2018–2020 Work Programme for the "Climate action, environment, resource efficiency and raw materials" challenge describes the importance of understanding, assessing and measuring the potential contribution of natural-based solutions in combating air pollution and regulating greenhouse gases in cities. VITALISE will evaluate mobility actions such as the implementation of superblocks, which have the objective of pacifying areas and generating new green spaces within the city. The modelling tools and methodologies developed will contribute to filling these knowledge and evidence gaps and, subsequently, will make a strong case for wide deployment of such solutions.

1.4. Metodología y plan de trabajo

The manpower envisaged for the proposed project will be provided by the AC-BSC research team of the proposal (three senior researchers and an experienced technician). External collaborators include Dr. Josep Casanovas and Dr. Maria de la Paz Linares (inLab FIB UPC) as expert on transport modelling; Dr. Fulvio Amato (EGAR) as expert on experimental field campaigns measuring gases and aerosols in urban areas and Dr. Mark Nieuwenhuijsen (ISGlobal), as expert on exposure assessment, epidemiological and health impacts studies. Finally, one post-doctoral researcher (PD1) with experience in urban air quality modeling will be hired, and will contribute to WP1 – Air quality evaluation of the emission-transport coupled system, WP2 – advancing the street canyon and the near-road atmospheric chemistry processes in the CALIOPE-Urbanv1.0 system and WP4 – dissemination of project results.

The methodology and working plan is defined as follows:

Work package 1: Refinement of the HERMESv3 road transport emission module and coupling with the Barcelona VML transport model

The aim of WP1 is to refine the current road transport emission module implemented in the HERMESv3 system by: 1) using up-to-date emission measurements available from local campaigns and scientific literature to refine the default emission factors used and 2) coupling the HERMESv3 system with the Barcelona virtual mobility lab (VML) transport model to have dynamical information on the traffic flow and travelling speed at the road link level. The overall outcome of WP1 will be a refined coupled transport-emission system for Barcelona to be used in the CALIOPE-Urbanv1.0 system in WP2 and WP3.

Task 1.1 Refinement of the traffic emission module in the HERMESv3 system

The work proposed in this task will include a review and collection of traffic-related observational data that will be used to refine the traffic emission module of the HERMESv3 system. This dataset will include the results of a remote sensing device campaign performed during 2017 by the Barcelona city council, which reports measured emission rates per vehicle category (NO_x, CO, PM, HC) and information on the vehicle fleet composition that circulates throughout the city. The dataset is composed by more than 90,000 individual measurements performed in 31 locations inside the city of Barcelona and its surroundings. The vehicle specific emission factors will be compared against the ones reported by COPERT 5, which is used by HERMESv3, in order to identify potential discrepancies and propose correction factors. Other measurements performed under real world driving conditions and reported by the current scientific literature will be also considered. The parametrizations and correction factors proposed by the literature will be integrated within the HERMESv3 system.

Task 1.2 Coupling between HERMESv3 and the virtual mobility lab transport model

The virtual mobility lab (VML) tool, which relies on the VISUM traffic model, includes a road network with detailed information about maximum speeds and capacities, permitted turns, etc. as well as patterns of mobility defined according to matrices of mobility derived from mobile phone Call Detail Records. Previously to the coupling with HERMESv3, a calibration process will be performed to ensure that the traffic intensity and average speed simulated are correct. For that, a base case simulation will be performed and the traffic volumes and average speeds obtained will be compared against observational data. For the traffic volumes, data from the Barcelona traffic count network (more than 150 sites) will be used, while the modelled speed will be contrasted against floating car data compiled by TomTom GPS data. Both datasets have already been acquired by AC-BSC. As a function of the discrepancies found between modelled and observed data, calibration of the VML input parameters will be performed based on the expertise of Dr. Josep Casanovas and Dr. Maria de la Paz Linares (Inlab FIB UPC). In the framework of the current PhD co-directed between the AC-BSC and Inlab FIB UPC groups, some preliminary runs of the virtual mobility lab (VML) tool have already been performed in the AC-BSC group, which guarantees its use during the development of the project. Once the calibration process is finished, the VML model will be coupled with HERMESv3. For that, a processing function to adapt the VML outputs (i.e. traffic intensity and average speed at link level with 1-h resolution) to the format required by HERMESv3 will be implemented.

Task 1.3 Inter-comparison with other existing inventories and air quality evaluation

The coupled transport-emission system will be used to run one year emission simulation over Barcelona. The obtained street-scale emissions will be compared against results simulated by the current non-refined version of HERMESv3 as well as other existing emission datasets, such as the official inventory provided by the Barcelona City. Since no emission inventory can be defined as the "true" reference, an air quality simulation will be also performed in order to see the impact of the new coupled transport-emission system on the air quality levels. The CALIOPE and CALIOPE-Urbanv1.0 modelling systems will be run over Europe (EU-12km), the Iberian Peninsula (IP-4km), the region of Catalonia (CAT-1km) and Barcelona (BCN-10m) for a period of one year. For the EU-12km domain, meteorological and chemical boundary conditions will be derived from the ECMWF and Copernicus products ERA5 and CAMS, while the CAMS-REG_AP European emission inventory will be processed (i.e. spatial remapped to the working domain, temporally disaggregated to the hourly level and speciated) using the HERMESv3 system. For the other mesoscale domains (IP-4km and CAT-1km) all the Spanish emissions will be estimated using the multiple bottom-up approaches and local activity data included in HERMESv3. Finally, for the BCN-10m domain the previously street-scale and hourly emissions already estimated will be used as input for modelling the dispersion of traffic emissions. It is important to note that in CALIOPE-Urbanv1.0 the hourly, link-specific emissions results are consistently used for both the microscale (BCN-10m) and the mesoscale modelling domains (IP-4km and CAT-1km). The air quality results simulated in the CAT-1km and BCN-10m domains will be used to evaluate the model performance in terms of surface concentrations (NO_2, $PM_{2.5}$, O_3). Ground-based concentrations will be compiled from the official observational network as well as from specific field campaigns performed by the EGAR group in Barcelona. The simulated concentrations will be used as a base case to evaluate the effect of the new parametrizations implemented with the CALIOPE-Urbanv1.0 system in WP2.

Work package 2: Advancing the street canyon and the near-road atmospheric chemistry processes within the CALIOPE-Urbanv1.0 system

Work package 2 will address specific objective 2, which includes the improvement of the street canyon effect and simulation of near-road chemistry processes within the CALIOPE-Urbanv1.0 system. Modeling experiments will then be performed to explore and evaluate the effect of the new parametrizations implemented.

Task 2.1 Modelling the street canyon effect

A parametrization to consider the street canyon effects in CALIOPE-Urbanv1.0 will be implemented during this task. For that, a review of the current methodologies used in other urban dispersion tools applied over whole city domains such as ADMS-Urban, OSPM uEMEP or SinG will be performed. Details on the dispersion calculations will be first collected and then implemented in the CALIOPE-Urban system. It is important to mention that current LES or CFD urban models use methodologies that are not feasible to apply over a large city domain for multiple scenario-runs due the extremely high computational resources needed. In this sense, although such methodologies will be revised no plans to implement them are foreseen.

Task 2.2 Modelling the near-road atmospheric chemistry processes

Chemical reactions between NO_x, VOC, SO_2 and other compounds in the air to produce particulates will be introduced in CALIOPE-Urbanv1.0. For that, the Chemistry Across Multiple Scales (CAMP; Dawson et al., 2019) chemical solver will be used. CAMP allows a flexible configuration of the chemistry in atmospheric models and it is already used in NMMB-MONARCH model by AC-BSC. CAMP will allow a simple and fast configuration of different chemical mechanisms in CALIOPE-Urbanv1.0. Considering that most state-of-the-art urban dispersion models consider simplified aerosol chemistry (i.e only sulfate chemistry in ADMS-Urban) this task will advance and propose appropriate chemical mechanisms to describe the street-level concentrations of primary and secondary gas and condensed-phased pollutants when background concentrations are mixed with freshly emitted emissions

Task 2.3 Evaluation of the new parametrizations
A set of sensitivity tests will be performed in order to quantify what is the impact of the new parametrizations developed in tasks 2.1 and 2.2 on the street-level modelled concentrations. The sensitivity runs will cover periods where specific field campaigns performed by the EGAR group were conducted in Barcelona characterizing the composition of particulate matter. The same strategy defined in Task 1.3 will be conducted with the new model. An annual simulation for the Barcelona domain (10-m) will be performed using the boundary and initial conditions of the base case simulation (CAT-1km) performed in task 1.3. A comparison between the two annual simulations and observations will allow identifying potential changes in the performance of the system. Depending on the results obtained, a posterior refinements of the parametrizations developed in tasks 2.1 and 2.2 will be done and simulations will be rerun.

Work package 3: Mobility scenarios: definition and impact assessment
The aim of WP3 is to assess the impact of specific urban mobility actions on air quality and public health considering a multiscale and multipollutant approach. Individual policies will be defined and evaluated in a single and combined way in terms of air quality and public health.

Task 3.1 Definition and modelling of the traffic management strategies
The work proposed in this task will review and define a series of urban mobility actions for its subsequent evaluation with the modeling tools developed in WP1 and WP2. The new Barcelona's Urban Mobility Plan (UMP 2019-2024) will be used as a basis for the definition of the strategies to be considered (e.g. implementation of a low emission zone and of superblocks or the unification of the Barcelona's tram). A review of other actions that are currently being implemented (or planned to be implemented) in other cities such as congestion charge or electrification of the vehicle fleet composition will be also considered. This review will be performed in close collaboration with all the external collaborators (EGAR, Inlab FIB UPC and ISGlobal), in order to consider a multidisciplinary point of view. The criteria for selecting the measures will be based on: 1) their relevance, 2) the feasibility of implementing them within the current socioeconomic context of the city and 3) the feasibility of modelling them with the available tools. Once all the traffic management strategies are selected, their impact in terms of traffic activity and emissions will be modelled. For that, the coupled transport-emission model prepared in WP1 will be used. The traffic restrictions associated to each action will be translated into specific modifications of the input datasets of the VML transport model (e.g. changes on the road network impedances, modal transport shares). This work will be performed in close collaboration with Dr. Josep Casanovas and Dr. Maria de la Paz Linares (Inlab FIB UPC) to ensure the maximum representativeness of the traffic restrictions. On the other hand, restrictions related with changes in vehicle technologies (e.g. low emission zone) will be implemented by modifying the input database of HERMESv3. The system considers more than 400 vehicle categories as a result of the combinations of vehicle type characteristics (depending on fuel, age, weight, engine size). The modelling of the selected measures will be performed individually but also in a combined way when feasible (e.g. superblocks +

interconnection of the Barcelona's tram + congestion charge). The individual and/or combination of measures that implies a larger impact in terms of traffic activity will be selected for the air quality and health impact evaluation performed in tasks 3.2 and 3.3.

Task 3.2 Assessment on emissions and air quality levels

Several scenarios will be developed to examine associations between traffic restrictions and change in urban and regional pollutant concentrations. The first scenario (i.e. base case scenario) will consider the current traffic situation (i.e. no measures applied). Following with the simulations performed in Task 1.3, the CALIOPE-Urbanv1.0 modelling system will be run over Europe (EU-12km), Iberian Peninsula (IP-4km) the region of Catalonia (CAT-1km) and Barcelona (BCN-10m) for a period of one year. For the multiple traffic restriction scenarios, the same configuration and input data will be maintained for EU-12km and IP-4km, while new traffic emissions will be estimated for CAT-1km and BCN-10m taking into account the traffic scenarios selected and modelled in the previous task (Task 3.1). Emissions for all the other anthropogenic sectors will be estimated by HERMESv3 and kept constant for all the proposed scenarios. The difference between the base case scenario and each traffic restriction scenario will give us the contribution of traffic restriction measures to reduce both emissions and concentrations of pollutants in the streets of Barcelona and the region of Catalonia. In terms of emissions, the analysis will consider both criteria pollutants (i.e. NO_x; CO; NMVOC; SO_x; NH_3; PM10 and PM2.5) and greenhouse gases (CO_2 and CH_4). The inclusion of the greenhouse gases will allow quantifying the impact of the measures on the decarbonisation of the city. Regarding air quality concentrations, the analysis will focus on NO_2, O_3 and $PM_{2.5}$ (total mass) annual mean values as well as hourly maximum values occurred during specific air pollution episodes. An assessment of individual $PM_{2.5}$ components such as organic carbon (OC) will be performed based on the success of the chemical implementations performed in Task 2.2. Reductions in air pollutant levels between scenarios will be quantified both at the mesoscale (outputs of CAT-1km) and microscale (outputs of BCN-10m) level with the aim of quantifying the consistency in the response of both modelling approaches. The results of this task will allow quantifying the impacts of the traffic measures both at the local and regional scale as well as for the short (specific episodes) and long (annual mean values) term period.

Task 3.3 Assessment on health impacts

The modelled concentrations corresponding to the base case and all the different mobility scenarios will be processed for the performance of a health impact assessment. Model-based exposure metrics for NO_2, O_3, $PM_{2.5}$ will be calculated from the hourly predictions simulated by the CALIOPE-Urbanv1.0 system and will be temporally and spatially averaged according to the requirements established by Dr. Mark Nieuwenhuijsen (ISGlobal). This will include, for instance, the estimation of annual average concentrations for $PM_{2.5}$ and of daily maximum eight-hour mean values for O_3, following the methodology recommended for European health impact assessments by the Health risks of air pollution in Europe (HRAPIE) project of the WHO. Similarly, the simulated concentrations in the BCN-10m domain will be spatially averaged to the same track census areas for which ISGlobal has information on population data and mortality statistics. Once the original outputs have been processed, expected changes in the air pollutant concentrations between scenarios will be estimated and the results will be delivered to ISGlobal for the quantification of the health impact assessment. The relationship between exposure variables and their effects on health will be modelled by ISGlobal using specific exposure-response functions (ERFs). The combination of exposure data with the ERFs, population data and mortality statistic will allow calculating the population attributable fractions and therefore quantify the attributable preventable mortality burden for each one of the simulated scenarios. Concentrations from both the mesoscalte (CAT-1km) and microscale (BCN-10m) simulations will be considered with the aim of quantifying the effect of the different scales on the health impact results. Similar to the previous tasks, the health impact assessment of specific $PM_{2.5}$ components (e.g. OC) will be performed based on the success of the implementations performed in Task 2.2.

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 following the Ministry requirements (mid-term and final report). Monitoring of the project will assure its successful development. Corrective actions will be applied, if required, to reduce deviations from the original plan. Regular meetings will be organized with the external collaborators of the project to promote a smooth and fruitful exchange of results and scientific discussions. Achievement of milestones detailed in Section 1.6 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 data produced will be provided at the end of the project. Currently the Earth Sciences Department of the BSC is deploying a THREADS system to disseminate model results to the scientific community and uses a Gitlab repository system to distribute in-house software like HERMESv3.

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 currently 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. Recently, the European Commission (EC) has announced that EuroHPC has selected BSC as one of the institutions that will host a pre-exascale supercomputer in the high-capacity supercomputer network promoted by EC. MareNostrum 5, the future BSC's supercomputer, is one of the pre-exascale machines. It will have a peak performance of 200 petaflops (200 x 1015 floating-point operations per second) and will come into operation on 31 December 2020. In addition, one proposal will be submitted to the Red Española de Supercomputación to have complementary access to supercomputing resources. Apart from the supercomputing resources, the Earth Sciences Department hosts a data storage system of 3.6 PBytes where all the data produced during the project will be stored.

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, EC1, EC2, RG3								M1.2																												
T1.3	PI, EC1, EC2, EC3, RG1, PD1												D1.1																								
WP2																																					
T2.1	PD1, RG3														M2.1																						
T2.2	PD1, RG2, RG3																								M2.2												
T2.3	PD1, PI, RG2, EC3																											D2.1									
WP3																																					
T3.1	RG1, RG2, EC1, EC2, EC3, EC4																		M3.1																		
T3.2	RG1, PI																														M3.2						
T3.3	PI, EC4, RG1, RG2																																			M3.3	D3.1 D3.2
WP4																																					
T4.1	PI																		D4.1																		D4.2
T4.2	all												M4.1												M4.2												M4.3

Principal Investigator (PI): M Guevara | Research group: A. Soret (RG1), M.T. Pay (RG2), C. Tena (RG3) | External collaborators: J.M. Casanovas (EC1), M.P. Linares (EC2), F. Amato (EC3), M. Nieuwenhuijsen (EC4) | Hired personnel: Post-Doc1 (PD1)

<u>List of Deliverables (tracking achievements):</u>

- D1.1: Evaluation of the coupled transport-emission system
- D2.1: Description of the new street canyon and near-road atmospheric chemistry in CALIOPE-Urbanv1.0 and evaluation results.
- D3.1: Assessment of air quality and health impacts derived from the mobility actions.
- D3.2: Best practices document for the evaluation of urban mobility policies.
- D4.1: Mid-term annual report to the Ministry.
- D4.2: Final annual report to the Ministry.

<u>List of Milestones (tracking progress):</u>

- M1.1: Refinement of the HERMESv3 traffic emission component
- M1.2: Coupling between HERMESv3 and VML finished.
- M2.1: New street canyon refinements implemented in CALIOPE-Urbanv1.0.
- M2.2: Near-road atmospheric chemistry implemented in CALIOPE-Urbanv1.0.
- M3.1: Definition of the urban mobility policies to be evaluated.
- M3.2: Assessment of the air quality impacts finished.
- M3.3: Assessment of the public health impacts finished.
- M4.1/4.2/4.3: Presentations at international conferences of the ongoing results.

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 street canyon effect and the near-road atmospheric chemistry processes in the CALIOPE-Urbanv1.0 system. PD1 will be directly involved in:

- WP1, Task 1.3: PD1 will contribute to the evaluation of the road transport emissions derived from the coupled transport-emission system (HERMESv3 and VLM) using CALIOPE-Urbanv1.0. This task will allow PD1 to get familiarized with the AC-BSC modelling tools and to better assess the current limitations of CALIOPE-Urbanv1.0.
- WP2, Task 2.1: PD1 will be responsible for the implementation of a new parameterization for street canyon effect in CALIOPE-Urbanv1.0.
- WP2, Task 2.2: PD1 will be responsible for the implementation of a simplified near-road atmospheric chemistry in CALIOPE-Urbanv1.0.

- WP2, Task 2.3: PD1 will contribute to the evaluation of the new parametrizations implemented in CALIOPE-Urbanv1.0. Comparison of model experiments with observational data will be performed.
- WP4, Task 4.2: PD1 will contribute to the dissemination of results. PD1 will participate in 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

During the last years, several works have studied the impact of urban mobility actions in terms of air quality and/or public health in Spain. Nevertheless, all the studies performed so far include limitations either in terms of modelling scales and/or pollutants covered. From the air quality modelling perspective, most studies have limited their application to a mesoscale approach, which do not allow depicting street level concentration gradients. More recently, new efforts were performed to investigate the effect of measures at street level in microscale domains, but they have been limited to city centre areas and did not include the health aspect. On the other hand, and from the epidemiological point of view, recent health impact assessment studies have mainly focussed on quantifying the number of preventable deaths attributed to reductions in NO_2, ignoring potential confounding effects by co-pollutants such as PM2.5 or O_3. The consideration of these co-pollutants is key considering the rebound effects that the reduction of NO_x traffic emissions may have on other secondary pollutants (O_3).

VITALISE proposes for the first time assessing the air quality and health impacts of urban mobility actions under a multi-scale modelling approach and a multi-pollutant focus (NO_2, O_3 and total PM2.5 and components). In this sense, the present proposal will contribute to advance the scientific community's understanding on how does the use of hybrid air quality models in comparison to traditional mesoscale models affect the estimation of air pollution and public health impacts when evaluating urban mobility plans. At the same time, the outputs obtained with this approach will be of high value for the epidemiological community, which typically uses surrogates of exposure (e.g. traffic volumes on nearby roadways) and land-use regression techniques to estimate exposure and health impacts. Therefore, long-term societal impacts of this work will come through an improved understanding of the air quality and public health impact that traffic measurement restrictions have.

The developments within VITALISE, which will serve to identify urban mobility options that can achieve significant reductions of air pollution and mortality in Barcelona, are also 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. Moreover, and with the aim of extrapolating all the knowledge and experience acquired to other urban areas, the methodology developed within the project will be used to elaborate an integrated guidance document on the best practices for the evaluation of urban mobility actions. Finally, the proposed work will result in an updated HERMESv3 and CALIOPE-Urbanv1.0 system that will be immediately available for emission and air quality modelling as part of the Air Quality forecast system for Spain (http://www.bsc.es/caliope/es). This project 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 urban scale emissions and air quality concentrations —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 and/or AE. 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. Results from the proposed work will be presented at EGU and other appropriate international conferences. The guidance document on the best practices for the evaluation of urban mobility actions will be shared within FAIRMODE. 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 researchers. First, the updated CALIOPE-Urbanv1.0 and HERMESv3 systems will be immediately available for emission modelling and air quality predictions as part of the CALIOPE project. Second, the results of this work will be made immediately available for exploitation by epidemiological researchers.

Communication of research results and public engagement will be a key focus of the proposed work. 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. 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) will also be employed to communicate project information, progress and results. 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 emission and air quality 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 multiscale air quality modelling system and a better understanding of the impacts of traffic restriction measures on urban and regional air quality and public health. In this sense, the transfer of knowledge will be organized into two main plans. First, the improved CALIOPE-Urbanv1.0 and HERMESv3 systems will be transferred to the CALIOPE Air Quality Forecasting System as the main model kernel. The refinement of the traffic emission module in HERMESv3 and of the street canyon parametrization and near-road atmospheric chemistry implemented in CALIOPE-Urbanv1.0 will improve the air quality predictions of the system. Second, the results obtained from the simulation of mobility scenarios will be transferred to the epidemiological community so that they can be exploited in future works related to health impacts. In addition, the scientific results will be disseminated through presentations at 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.

3. CAPACIDAD FORMATIVA - *TRAINING CAPACITY*

3.1. Programa de formación

The training plan envisaged for the pre-doctoral contract will address the acquisition of competence in atmospheric modelling, secondary organic aerosol chemistry and urban scale dispersion. 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 air quality modelling. The acquisition of expertise in the following scientific topics has been identified as the principal training objective: 1) emission modeling (emission inventories, methodologies to estimate traffic emissions); 2) air quality modeling (mesoscale photochemistry, urban scale dispersion); and 3) health impacts (air pollution information used in health impact assessments). 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 it holds de ANECA certification (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 opportunity 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 utilize 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.

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". 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. " Development of a high- resolution emission model for air quality modelling in Spain". 17/12/2014. Guevara et al. (2013 AE), Guevara et al. (2014ab 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: February 2020.
2) Daniel Rodríguez Rey. “Evaluation of mobility policies impact on air quality through the development of an integrated air quality modeling system”. Expected date: April 2021.

3) Vanessa Nogueira Dos Santos "An integrated modelling assessment of PM2.5 for the European agriculture sector." Expected date: June 2022.

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

Dr. Albert Soret is currently the group leader of the Earth System Services of the BSC, while Dr. Maria Teresa Pay is a postdoctoral researcher leading the research line on source apportionment. More details on their trajectories is described in their CVs.

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 currently hosts the MareNostrum 4 supercomputer, used in a Tier-0 PRACE system with 13Pflop/s capacity. Recently, the EC has announced that EuroHPC has selected BSC as one of the institutions that will host a pre-exascale supercomputer in the high-capacity supercomputer network promoted by EC. MareNostrum 5, the future BSC's supercomputer, is one of the pre-exascale machines. It will have a peak performance of 200 petaflops (200 x 1015 floating-point operations per second) and will come into operation on 31 December 2020.

The Earth Sciences Department of BSC (ES-BSC) is focused on carrying out research in Earth system modeling. The high performance capabilities 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 physicochemical 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. CONDICIONES ESPECÍFICAS PARA LA EJECUCIÓN DE DETERMINADOS PROYECTOS - *SPECIFIC CONDITIONS FOR THE EXECUTION OF CERTAIN PROJECTS*

None