# Horizon 2020

# Call: H2020-MSCA-IF-2016

(Marie Skłodowska-Curie Individual Fellowships)

# Topic: MSCA-IF-2016

# Type of action: MSCA-IF-EF-ST

(Standard EF)

# Proposal number: 747048

# Proposal acronym: ACRoNNIM

Deadline Id: H2020-MSCA-IF-2016

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*How to fill in the forms?*

The administrative forms must be filled in for each proposal using the templates available in the submission system. Some data fields in the administrative forms are pre-filled based on the previous steps in the submission wizard.

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

# 1 - General information

| | |
|---|---|
| Topic | MSCA-IF-2016 |
| Call Identifier | H2020-MSCA-IF-2016 |
| Type of Action | MSCA-IF-EF-ST |
| Deadline Id | H2020-MSCA-IF-2016 |

| | |
|---|---|
| Acronym | ACRoNNIM |
| Proposal title | Aerosol and Climate Response to NH3 in the NMMB/BSC Inter-Scale Model |

*Note that for technical reasons, the following characters are not accepted in the Proposal Title and will be removed: < > " &*

| | |
|---|---|
| Duration in months | 24 |
| Scientific Area | ENV |

*Please select up to 5 descriptors (and at least 3) that best characterise the subject of your proposal, in descending order of relevance.*

| | | |
|---|---|---|
| Descriptor 1 | *Atmospheric chemistry, atmospheric composition, air pollution* | |
| Descriptor 2 | *Climatology and climate change* | |
| Descriptor 3 | *Environment chemistry* | Remove |
| Descriptor 4 | *Meteorology, atmospheric physics and dynamics* | Remove |
| | | Add |

| | |
|---|---|
| Free keywords | *secondary organic aerosol, ammonia, atmosphere, global model, NMMB/BSC, CACM, MPMPO* |

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

## *Abstract*

*Atmospheric particulate matter reduces visibility, adversely affects human health and impacts Earth's climate. Recent laboratory research has identified NH3 as a potentially important reactive species in the formation and aging of SOA, a significant but not-well-quantified class of aerosol particles. The goal of this proposal is to answer the questions: How does NH3 affect aerosol mass loadings and optical properties on a global scale? And, what impact do these effects have on air quality and climate? This will be accomplished by incorporating NH3-related SOA chemistry, currently being investigated by collaborators at the University of California, Irvine (UCI) into the state-of-the-art CACM/MPMPO SOA module. The updated module will be deployed in the NMMB/BSC global chemical weather model, maintained at the Barcelona Supercomputing Center (BSC). Model predictions will be validated by field measurements collected during an IDAEA-CSIC campaign that the experienced researcher (ER) will participate in, as part of this proposal. This will result in one of the most advanced SOA treatments available in global models, and allow an investigation of the impact of NH3 on global SOA, air quality and climate, thus directly impacting a crosscutting issue of the Horizon 2020 Program, climate action. The ER has experience using laboratory results to develop mechanisms for aerosol processes, and in the development of CACM/MPMPO as a graduate and postdoctoral researcher at UCI. This experience, coupled with training in global model development at BSC, will provide ideal conditions to successfully execute this proposal, and strengthen the collaboration between the European BSC and IDAEA-CSIC, and US-based UCI teams. By the end of the Fellowship, the ER will have hands-on experience in field, laboratory and computational aerosol research, uniquely positioning him to develop and carry out comprehensive, collaborative research initiatives and opening up improved career opportunities.*

Remaining characters 4

Has this proposal (or a very similar one) been submitted to a Horizon 2020 Marie Skłodowska-Curie Individual Fellowship call? ○ Yes ◉ No

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

## Declarations

| | |
|---|---|
| 1) The applicant (future beneficiary) declares to have the explicit consent of all partner organisations (if applicable) on their participation and on the content of this proposal. | ☒ |
| 2) The information contained in this proposal is correct and complete. | ☒ |
| 3) This proposal complies with ethical principles (including the highest standards of research integrity — as set out, for instance, in the European Code of Conduct for Research Integrity — and including, in particular, avoiding fabrication, falsification, plagiarism or other research misconduct). | ☒ |

4) The applicant (future beneficiary) confirms:

| | |
|---|---|
| - to have carried out the self-check of the financial capacity of the organisation on https://ec.europa.eu/research/participants/portal/desktop/en/organisations/lfv.html or to be covered by a financial viability check in an EU project for the last closed financial year. Where the result was "weak" or "insufficient", the applicant (future beneficiary) confirms being aware of the measures that may be imposed in accordance with the H2020 Grants Manual (Chapter on Financial capacity check); or | ○ |
| - is exempt from the financial capacity check being a public body including international organisations, higher or secondary education establishment or a legal entity, whose viability is guaranteed by a Member State or associated country, as defined in the H2020 Grants Manual (Chapter on Financial capacity check); or | ◉ |
| - as sole participant in the proposal is exempt from the financial capacity check. | ○ |

5) The applicant (future beneficiary) hereby declares:

| | |
|---|---|
| - it is fully eligible in accordance with the criteria set out in the specific call for proposals; and | ☒ |
| - it has the financial and operational capacity to carry out the proposed action. | ☒ |

The applicant (future beneficiary) is only responsible for the correctness of the information relating to his/her own organisation. Where the proposal to be retained for EU funding, the applicant (future beneficiary) will be required to present a formal declaration in this respect.

According to Article 131 of the Financial Regulation of 25 October 2012 on the financial rules applicable to the general budget of the Union (Official Journal L 298 of 26.10.2012, p. 1) and Article 145 of its Rules of Application (Official Journal L 362, 31.12.2012, p.1) applicants found guilty of misrepresentation may be subject to administrative and financial penalties under certain conditions.

**Personal data protection**

Your reply to the grant application will involve the recording and processing of personal data (such as your name, address and CV), which will be processed pursuant to Regulation (EC) No 45/2001 on the protection of individuals with regard to the processing of personal data by the Community institutions and bodies and on the free movement of such data. Unless indicated otherwise, your replies to the questions in this form and any personal data requested are required to assess your grant application in accordance with the specifications of the call for proposals and will be processed solely for that purpose. Details concerning the processing of your personal data are available on the privacy statement. Applicants may lodge a complaint about the processing of their personal data with the European Data Protection Supervisor at any time.

Your personal data may be registered in the Early Warning System (EWS) only or both in the EWS and Central Exclusion Database (CED) by the Accounting Officer of the Commission, should you be in one of the situations mentioned in:
-the Commission Decision 2008/969 of 16.12.2008 on the Early Warning System (for more information see the Privacy Statement), or
-the Commission Regulation 2008/1302 of 17.12.2008 on the Central Exclusion Database
(for more information see the Privacy Statement) .

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

# List of participants

| # | Participant Legal Name | Country |
|---|---|---|
| 1 | BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION | Spain |

*Proposal ID* **747048** *Acronym* **ACRoNNIM** *Short name* **BSC**

# 2 - Administrative data of participating organisations

## Future Host Institution

| ***PIC*** | ***Legal name*** |
|---|---|
| *999655520* | *BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION* |

*Short name: BSC*

*Address of the organisation*

Street Calle Jordi Girona 31

Town BARCELONA

Postcode 08034

Country Spain

Webpage www.bsc.es

*Legal Status of your organisation*

Research and Innovation legal statuses

Public body ..... yes
Non-profit ..... yes
International organisation ..... no
International organisation of European interest ..... no
Secondary or Higher education establishment ..... no
Research organisation ..... yes
Small and Medium-sized Enterprises (SMEs) ..... no
Academic Sector ..... yes

Legal person ..... yes

NACE Code: 72 - Scientific research and development

Does this participant deliver doctoral degrees that are recognised as such by the relevant national authorities? ○ Yes ◉ No

*Proposal ID* **747048** *Acronym* **ACRoNNIM** *Short name* **BSC**

## *Department(s) carrying out the proposed work*

**Department 1**

Department name: Earth Sciences ☐ not applicable

☐ Same as organisation address

Street: Jordi Girona, 29

Town: Barcelona

Postcode: 08034

Country: Spain

If the location of the Department carrying out the proposed work is not the same as the location of the Host Institute, please note that although the proposal submission system calculates the budget of the project based on the location of the Host Institute, the budget of the project for the grant agreement will be calculated by using the country coefficient of the location of the Department carrying out the proposed work.

*Proposal ID* **747048** *Acronym* **ACRoNNIM** *Short name* **BSC**

## *Researcher*

The name and e-mail of the Researcher and Supervisor are read-only in the administrative form, only additional details can be edited here. To give access rights and contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

| | | | |
|---|---|---|---|
| Researcher ID | *If you have a researcher identifier number (e.g. ResearcherID, ORCID) please enter it here.* | | |
| Last Name* | DAWSON | Last Name at Birth | Dawson |
| First Name(s)* | Matthew | Gender* | (•) Male ( ) Female |
| Title | Dr. | Country of residence* | United States |
| Nationality* | United States | Nationality 2 | |
| Date of Birth (DD/MM/YYYY) | 14/03/1978 | Country of Birth* | United States |
| | | Place of Birth | Pittsburgh, PA |

## *Contact address*

| | | | |
|---|---|---|---|
| Current organisation name | | | |
| Current Department/Faculty/Institute/ Laboratory name | | | |
| | ☐ Same as organisation address | | |
| Street | 7084 Friars Road Apt 431 | | |
| Postcode/Cedex | 92108 | Town | San Diego, CA |
| Phone | +1-412-352-2732 | Country | United States |
| Phone2 / Mobile | *+xxx xxxxxxxxx* | | |
| E-Mail* | mattldawson@gmail.com | | |

*Proposal ID* **747048** *Acronym* **ACRoNNIM** *Short name* **BSC**

## *Qualifications*

| | | |
|---|---|---|
| University Degree | Date of award (DD/MM/YYYY) | 25/04/2009 |
| Doctorate (in progress) | Date of award (DD/MM/YYYY) | |
| Doctorate | Date of award (DD/MM/YYYY) | 20/09/2014 |
| Full time postgraduate research experience | Number of months | 20 |
| Other Academic qualifications | Date of award (DD/MM/YYYY) | |

## *Place of activity/place of residence (previous 5 years - most recent one first)*

Indicate the period(s) and the country/countries in which you have legally resided and/or had your main activity (work, studies, etc) during the last 5 years up until the deadline for the submission of the proposal. Please fill in this section without gaps, until the call deadline (14/09/2016).

| Period from | Period to | Duration (days) | Country |
|---|---|---|---|
| 14/03/1978 | 14/09/2016 | 14065 | United States |
| | Total | 14065 | |

*Proposal ID* **747048** *Acronym* **ACRoNNIM** *Short name* **BSC**

## *Supervisor*

The name and e-mail of the Researcher and Supervisor are read-only in the administrative form, only additional details can be edited here. To give access rights and contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name*: **Oriol** Last name*: **Jorba**

E-Mail*: **oriol.jorba@bsc.es**

Position in org.: Atmospheric Composition Group Manager

Department: Earth Sciences

[ ] Same as organisation address

Street: Jordi Girona, 29

Town: Barcelona Post code: 08034

Country: Spain

Website:

Phone: +34 93 413 4050 Phone 2: *+xxx xxxxxxxxx* Fax: +34 93 413 7721

## *Other contact persons*

| ***First Name*** | ***Last Name*** | ***E-mail*** | ***Phone*** |
|---|---|---|---|
| Dorota | Chmielewska | dorota.chmielewska@bsc.es | +34 93 413 40 82 |

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

# 3 - Budget

Is the Researcher eligible for family allowance? (•) Yes ( ) No

| Participant Number | Organisation Short Name | Country | Country Coefficient | Number of Months | Researcher Unit Cost | | | Institutional Unit Cost | | Total |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Living Allowance | Mobility Allowance | Family Allowance | Research, training and networking costs | Management and Overheads | |
| 1 | BSC | ES | 0,976 | 24 | 108921,60 | 14400,00 | 12000,00 | 19200,00 | 15600,00 | 170121,60 |
| Total | | | | 24 | 108921,60 | 14400,00 | 12000,00 | 19200,00 | 15600,00 | 170121,60 |

Partner Organisation from Third Country does not sign the Grant Agreement, does not recruit the researcher and does not directly claim costs from the action. The entire EC contribution is transmitted to the Host organisation located in Members States or Associated Countries.

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

# 4 - Ethics issues table

| 1. HUMAN EMBRYOS/FOETUSES | | Page |
|---|---|---|
| Does your research involve Human Embryonic Stem Cells (hESCs)? | ○ Yes ◉ No | |
| Does your research involve the use of human embryos? | ○ Yes ◉ No | |
| Does your research involve the use of human foetal tissues / cells? | ○ Yes ◉ No | |
| **2. HUMANS** | | **Page** |
| Does your research involve human participants? | ○ Yes ◉ No | |
| Does your research involve physical interventions on the study participants? | ○ Yes ◉ No | |
| **3. HUMAN CELLS / TISSUES** | | **Page** |
| Does your research involve human cells or tissues (other than from Human Embryos/ Foetuses, i.e. section 1)? | ○ Yes ◉ No | |
| **4. PERSONAL DATA** | | **Page** |
| Does your research involve personal data collection and/or processing? | ○ Yes ◉ No | |
| Does your research involve further processing of previously collected personal data (secondary use)? | ○ Yes ◉ No | |
| **5. ANIMALS** | | **Page** |
| Does your research involve animals? | ○ Yes ◉ No | |
| **6. THIRD COUNTRIES** | | **Page** |
| In case non-EU countries are involved, do the research related activities undertaken in these countries raise potential ethics issues? | ○ Yes ◉ No | |
| Do you plan to use local resources (e.g. animal and/or human tissue samples, genetic material, live animals, human remains, materials of historical value, endangered fauna or flora samples, etc.)? | ○ Yes ◉ No | |
| Do you plan to import any material - including personal data - from non-EU countries into the EU? | ○ Yes ◉ No | |
| Do you plan to export any material - including personal data - from the EU to non-EU countries? | ○ Yes ◉ No | |
| In case your research involves low and/or lower middle income countries, are any benefits-sharing actions planned? | ○ Yes ◉ No | |
| Could the situation in the country put the individuals taking part in the research at risk? | ○ Yes ◉ No | |

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

| 7. ENVIRONMENT & HEALTH and SAFETY | | Page |
|---|---|---|
| Does your research involve the use of elements that may cause harm to the environment, to animals or plants? | ○ Yes ◉ No | |
| Does your research deal with endangered fauna and/or flora and/or protected areas? | ○ Yes ◉ No | |
| Does your research involve the use of elements that may cause harm to humans, including research staff? | ○ Yes ◉ No | |
| **8. DUAL USE** | | **Page** |
| Does your research involve dual-use items in the sense of Regulation 428/2009, or other items for which an authorisation is required? | ○ Yes ◉ No | |
| **9. EXCLUSIVE FOCUS ON CIVIL APPLICATIONS** | | **Page** |
| Could your research raise concerns regarding the exclusive focus on civil applications? | ○ Yes ◉ No | |
| **10. MISUSE** | | **Page** |
| Does your research have the potential for misuse of research results? | ○ Yes ◉ No | |
| **11. OTHER ETHICS ISSUES** | | **Page** |
| Are there any other ethics issues that should be taken into consideration? Please specify | ○ Yes ◉ No | |

I confirm that I have taken into account all ethics issues described above and that, if any ethics issues apply, I will complete the ethics self-assessment and attach the required documents. ☒

How to Complete your Ethics Self-Assessment

*Proposal ID* **747048** *Acronym* **ACRoNNIM**

# 5 - Call specific questions

## *Eligibility Researcher (future fellow)*

1. Were you in the last 5 years in military service? ○ Yes ◉ No

## *Other Questions*

For communication purposes only, the REA asks for permission to publish the name of the researcher (future fellow) should the proposal be retained for funding.

1. Does the researcher (future fellow) give this permission? ◉ Yes ○ No

2. Is there a secondment in Member States or Associated Countries envisaged in Part B of this proposal? ◉ Yes ○ No

In which sector is the secondment in Member States / Associated Countries foreseen?

☐ Academic ☒ Non Academic

Do you already know the organisation to which this secondment will be? ◉ Yes ○ No

Name: Spanish Council for Scientific Research

Country: Spain

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## *Data management activities*

A new focus within Horizon 2020 is data management, for example through the use of Data Management Plan (DMP).

DMPs detail what data the project will generate, whether and how it will be exploited or made accessible for verification and re-use, and how it will be curated and preserved.

The use of a DMP is required for projects participating in the Open Research Data Pilot in the form of a deliverable in the first 6 months of the project (possible updates during the project).

Other projects are invited to submit a DMP if relevant for their planned research.

| Are data management activities relevant for your proposed project? | ○ Yes | ◉ No |
|---|---|---|

## *Open Research Data Pilot in Horizon 2020*

All applicants can participate in the Pilot on Open Research Data in Horizon 2020[1] on a voluntary basis. This Pilot aims to improve and maximise access to and re-use of research data generated by actions.

Participants in the Pilot will be invited to formulate a Data Management Plan (DMP). DMPs detail what data the project will generate, whether and how it will be exploited or made accessible for verification and re-use, and how it will be curated and preserved.
Participating in the Pilot is flexible in the sense that it does not mean that all research data needs to be open. Rather, projects can define certain datasets to remain closed via a Data Management Plan (DMP).

Please note that participation in this Pilot does not constitute part of the evaluation process. Proposals will not be evaluated favourably because they participate in the Pilot on a voluntary basis.

| We wish to participate in the Pilot on Open Research Data in Horizon 2020 on a voluntary basis | ○ Yes | ◉ No |
|---|---|---|

[1] *According to article 43.2 of Regulation (EU) No 1290/2013 of the European Parliament and of the Council, of 11 December 2013, laying down the rules for participation and dissemination in "Horizon 2020 - the Framework Programme for Research and Innovation (2014-2020)" and repealing Regulation (EC) No 1906/2006.*

**DOCUMENT 1**

# START PAGE

MARIE SKŁODOWSKA-CURIE ACTIONS

## Individual Fellowships (IF)
## Call: H2020-MSCA-IF-2016

PART B

"ACRoNNIM"

"**A**erosol and **C**limate **R**esponse t**o** **N**$H_3$ in the **N**MMB/BSC **I**nter-Scale **M**odel"

**This proposal is to be evaluated as:**

**Standard EF**

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## List of Participating Organisations

| Participating organisations | Legal Entity Short Name | Academic (tick) | Non-academic (tick) | Country | Dept./ Division / Laboratory | Supervisor | Role of Partner Organisation |
|---|---|---|---|---|---|---|---|
| Barcelona Supercomputing Center | BSC | X | | Spain | Department of Earth Sciences | Dr. Oriol Jorba | Host organization |
| Spanish Council for Scientific Research | IDAEA-CISC | X | | Spain | Institute of Environmental Assessment and Water Research | X. Querol, | Partner Organization |

# 1. Excellence

## 1.1 Quality and credibility of the research/innovation action (level of novelty, appropriate consideration of inter/multidisciplinary and gender aspects)

- Introduction, state-of-the-art, objectives and overview of the action

The oxidation of volatile organic species to form low-volatility products is an important source of aerosol mass in the global atmosphere. Due to the climate, health and visibility effects of particulate matter, inclusion of this so-called secondary organic aerosol (SOA) into regional and global weather and climate models is the focus of on-going research. Complicating these efforts are the large number of species and oxidation pathways involved, their seasonally, spatially, and diurnally varying importance, and the complex physical processes controlling their phase partitioning. Regional and global chemical transport models (CTMs) generally under-predict SOA mass in the atmosphere compared to field measurements, suggesting the presence of as-yet unidentified sources or unaccounted-for physical processes.[1]

As computational ability has improved, global CTMs have begun incorporating more complex treatments of SOA that until recently had only been accessible to smaller-scale models. These include, *e.g.*, the re-evaporation of semi-volatile species (equilibrium partitioning), aqueous-phase SOA production, and variations of the Volatility Basis Set (VBS) model to account for SOA aging.[2] The Caltech Atmospheric Chemistry Mechanism (CACM) coupled with the Model to Predict the Multiphase Partitioning of Organics (MPMPO) is one of the most advanced treatments of SOA available for box and regional-scale modelling.[3] It has been developed over the last 15 years to accurately predict SOA formation over a wide range of conditions, both urban[4] and remote.[5] CACM/MPMPO is a lumped model that uses the Equilibrium Partitioning scheme of Pankow and co-workers, and utilizes a fully coupled mixed-phase aqueous/organic aerosol scheme. However, its complexity has precluded its inclusion in global models to date.

As modellers work to incorporate existing treatments of SOA into global CTMs, laboratory and field research continues to identify new precursors and routes to SOA formation. Recently, ammonia has been identified as a potentially important species in the formation and aging of SOA. However, the reactions of ammonia with gas- and aerosol-phase organic species are complex, affecting both SOA yields[6] and aerosol optical properties,[7] with implications for air quality and climate. Collaborators at the University of California, Irvine (UCI) are currently investigating the role of $NH_3$ in SOA aging using aerosol chamber experiments and advanced instrumentation for measurement of gas-phase species, and aerosol composition and optical properties, towards the goal of developing an updated aerosol chemistry and physics model that accounts for the role of $NH_3$ in SOA processes. They have considerable experience employing these techniques to investigate SOA chemistry and physics, including identifying the reactions of $NH_3$ with biogenic-derived SOA to form highly conjugated light-absorbing N-containing species.[8] Indeed, the way $NH_3$ affects the optical properties of aging SOA is one of the most intriguing aspects of recent findings, as it would introduce a secondary source of brown carbon, which has been shown to have important effects on the global climate.[9]

The goal of this proposal is to answer the questions: **How does $NH_3$ affect aerosol mass loadings and optical properties on a global scale? And, what impact do these effects have on air quality and climate?** This will be accomplished by working remotely with collaborators at UCI to incorporate their current and on-going observations of ammonia-related SOA chemistry and physics into CACM/MPMPO and then to implement the updated SOA module into the online multi-scale NMMB/BSC CTM. The NMMB/BSC CTM is a chemical weather prediction system maintained by the Barcelona Supercomputing Center (BSC) and includes modules for dust, sea

[1] Volkamer et al., *Geophys. Res. Lett.*, vol. 33, 2006. doi: 10.1029/2006GL026899.
[2] Tsigaridis et al., *Atmos. Chem. Phys.*, vol. 14, 10845–95, 2014.
[3] Griffin, Dabdub and Seinfeld, *J. Geophys. Res: Atmospheres*, vol. 107, 2002, doi: 10.1029/2001JD000541; Pun et al., *J. Geophys. Res.: Atmospheres*, vol. 107, 2002, doi: 10.1029/2001JD000542; Griffin et al., *J. Geophys. Res: Atmospheres*, vol. 107, 2002, doi: 10.1029/2001JD000544; Griffin, Dabdub and Seinfeld, *J. Geophys. Res.: Atmospheres*, vol. 110, 2005, doi: 10.1029/2004JD005219.
[4] Carreras-Sospedra, Griffin and Dabdub, *Environ. Sci. Technol.*, vol. 39, 1724-1730, 2005; Cohan et al., *Int. J. Environ. Poll.*, vol. 52, 206-224, 2013; Vutukuru and Dabdub, *Atmos. Environ.*, vol. 42, 375-364, 2008; Dawson et al., *Geosci. Model Dev.*, vol. 9, 2143-2151, 2016.
[5] Ashworth et al., *Geosci. Model Dev.*, vol. 8, 3765-3784, 2015.
[6] Na, Song and Cocker, *Atmos. Environ.*, vol. 40, 1889–1900, 2006,.; Na et al., *Environ. Sci. Technol.*, vol. 41, 6096–6102, 2007.
[7] Bones et al., *J. Geophys. Res.*, vol. 115, 2010, doi: 10.1029/2009JD012864.
[8] Bones et al., *J. Geophys. Res.*, vol. 115, 2010, doi: 10.1029/2009JD012864.
[9] Feng et al., *Atmos. Chem. Phys.*, vol. 13, 8607-8621, 2013.

salt, sulphate, and primary organic aerosol, along with a 2-product SOA module.[10] NMMB/BSC is a fully coupled, online chemical/meteorological model that is replacing the CALIOPE modelling system as the primary weather and air quality model at BSC, and operates as part of the International Cooperative for Aerosol Prediction Multi-Model Ensemble (ICAP-MME).[11] As part of a planned upgrade in 2017, the MareNostrum supercomputer at BSC will undergo hardware improvements increasing peak performance by a factor of 10. These improvements will facilitate the incorporation of the detailed CACM/MPMPO chemistry and physics. The updated model including $NH_3$ chemistry and physics is hereafter referred to as NMMB/BSC-CACM/MPMPO-$NH_3$. A multi-scaled approach will be employed in which NMMB/BSC-CACM/MPMPO will be deployed with local (Spain), and global model domains to evaluate the role of $NH_3$ in SOA formation and aging, and its effects on air quality and climate.

The experienced researcher (ER) has several years of experience incorporating new chemistry into the CACM/MPMPO module, and collaborating with its primary developer, Prof. R. Griffin (Rice University, Houston, USA), who has provided a letter of support for this proposal (Section 7). Additionally, the ER has a history of collaboration with the team at UCI, which when coupled with the computational nature of the proposal, will allow a close, but remote, collaboration that will not include travel to UCI, and will incur no separate cost as part of this proposal. Prof. D. Dabdub (UCI), a co-PI on the team investigating new $NH_3$-related SOA chemistry has served as a post-doctoral mentor to the ER, and has also provided a letter of support for this proposal (Section 7).

Collaborators at IDAEA-CISC will conduct a field measurement campaign beginning July 2017 in the region surrounding Barcelona, Spain to investigate the spatial variability in ozone, ultrafine particle and secondary aerosol generation. Importantly for this proposal, their campaign will include gas-phase measurements of key oxidants and volatile organic SOA precursors along with gas-phase ammonia, and a variety of aerosol techniques, including TAG-AMS[12] organic aerosol measurements. The campaign domain includes the Osona region in Spain (NE of Barcelona), which is an ammonia hot spot due to intensive farming activity. Thus, the campaign results will provide an ideal means to evaluate the ability of NMMB/BSC-CACM/MPMPO-$NH_3$ to predict SOA concentrations and aerosol optical properties in areas with high ammonia concentrations. A secondment to IDAEA-CISC is included as part of this proposal that will allow the ER to participate in this campaign, gaining experience with the measurement techniques used and with the compilation of field measurement data for model evaluation. Prof. X. Querol (IDAEA-CSIC, Spain), PI of the field measurement campaign, will serve as supervisor during the secondment and has provided a letter of support (Section 7).

The Fellowship will open several future opportunities for the career of the ER. First, experience with the development and implementation of aerosol modules into a global chemical weather prediction model will perfectly complement the ER's previous work with smaller-scale regional and plume models. Second, participation in the Osona region field campaign will provide the ER first-hand experience with state-of-the-art field measurement techniques. This experience, coupled with the continued collaboration with computational modellers and laboratory-based researchers at UCI will lead to stronger, more comprehensive future research collaborations that integrate laboratory, field, and modelling efforts. Finally, the Fellowship will expand the professional network of the ER, opening up the possibility of future collaborations with BSC and IDAEA-CSIC as well as European-based researchers met as part of the dissemination of the results of this work at European scientific conferences. The proposed work would also strengthen the current collaboration between the UCI and BSC teams, leading to expanded future collaborative opportunities.

Research methodology and approach: The project will be carried out as follows:

1. Compile **observational data** for model evaluation. A combination of ground and satellite data will be compiled and used to evaluate the updated NMMB/BSC model. This work will be carried out at IDAEA-CSIC.
    a. Compile data from the DUARE campaign[13] for evaluation of local (Spain) simulations. Measurements using a variety of techniques for inorganic and organic aerosol, and VOCs were taken at an urban/coastal site and a remote site, and thus can be used to evaluate model performance over a range of $NO_X$ conditions.
    b. Supplement the DUARE data with data from the IDAEA-CSIC campaign planned for the Osona region of NE Spain described in the introduction, as they become available (see letter of support in Section 7).

[10] Spada et al, Geophys. *Model. Dev.*, submitted.
[11] Sessions et al., *Atmos. Chem. Phys.*, vol. 15, 335-362, 2015.
[12] Williams et al., *Aerosol Sci. Technol.*, vol. 48, 358-370, 2014.
[13] Pandolfi et al., *J. Geophys. Res.*, vol. 119, 4978-5010, 2014.

c. Datasets from the European Environment Agency's EMEP network will be assembled for comparison with global simulation results over Europe, following the methodology employed by the BSC team previously.[14]

d. EMEP data will be combined with a suite of datasets including those from the IMPROVE, EANET, and AERONET ground-based networks, and the MODIS and MISR satellite networks, following the methodology employed by the BSC team previously, for comparison with global simulations.[15]

2. **Implement CACM/MPMPO into NMMB/BSC**. The base SOA module used for this work will be aroCACM/MPMPO 1.0,[16] which includes an updated treatment of aromatic-derived SOA, an important SOA precursor in urban areas. The following will be accomplished in this phase:

   a. Reconfigure the gas-phase CACM to make use of the Kinetic Pre-Processor (KPP) package used in NMMB/BSC for gas-phase mechanisms.

   b. Incorporate the revised gas-phase chemistry described by Ashworth et al.[17] related to peroxy-radical chemistry and isoprene-derived organic nitrate formation, which are important in remote environments with low levels of oxides of nitrogen ($NO_X$), and in areas with large biogenic emissions that are influenced by high-$NO_X$ plumes, respectively.

   c. Adapt emissions schemes currently in use in the NMMB/BSC model with the CB-05 gas-phase mechanism for use with CACM gas-phase species.

   d. Configure NMMB/BSC-CACM/MPMPO for a run covering Spain at a resolution of 4 km x 4 km using emissions calculated using the HERMES[18] model, and following the general procedure used by the BSC team for regional (Spain) simulations using the CALIOPE model.[19] Results will be compared to observational data compiled as described in Part 1.

3. Incorporate new **$NH_3$-related SOA formation and aging.** Collaborators at UCI 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 here will collaboratively parameterize their published and on-going work on the formation of light-absorbing SOA from $NH_3$ processing for **inclusion into CACM/MPMPO**. The updated module will then be incorporated into the NMMB/BSC CTM to evaluate the impact of $NH_3$ chemistry first on a local (Spain) scale, then on a global scale.

   a. Updates to the CACM/MPMPO module will be incorporated into the NMMB/BSC CTM.

   b. Updated emissions for any new gas-phase species will be assembled as described in Part 2.

   c. NMMB/BSC-CACM/MPMPO-$NH_3$ will be configured for a run covering Spain as described in Part 2. Results will be evaluated using data collected as part of the IDAEA-CSIC field campaign described above.

4. Evaluate NMMB/BSC-CACM/MPMPO-$NH_3$ results at the **global scale**. The updated model will be configured for an evaluation of the impact of $NH_3$ on SOA globally, at a resolution of 50 km x 50 km. Model input conditions, including gas and aerosol species emissions will be compiled from existing inventories and models, following procedures used previously for NMMB/BSC.[20] 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 global climate, through a parameterization of $NH_3$ optical effects on aerosol properties based on results from the UCI team. Model results will be analysed to answer the key research questions, related to the importance of $NH_3$ on SOA formation and optical properties, and how these impact air quality and climate.

Originality and innovative aspects of the research programme: The proposed work will result in the inclusion of a **state-of-the-science SOA module into the multi-scale NMMB/BSC chemical/meteorological model**. This

[14] Pay et al., *Atmos. Environ.*, vol. 44, 3322-3342, 2010.
[15] Spada et al, Geophys. *Model. Dev.*, in preparation.
[16] Dawson et al., *Geophys. Model Dev.*, vol. 9, 2143-2151, 2016.
[17] Ashworth et al., *Geophys. Model Dev.*, vol. 8, 3765-3784, 2015.
[18] Guevara et al, *Atmos. Environ.*, vol. 81, 209-221, 2013.
[19] Pay et al., *Atmos. Environ.*, vol 46, 376-396, 2012.
[20] Badia et al., *Geophys. Model Dev.*, doi:10.5194/gmd-2016-141, in review; Spada et al., *Geophys. Model Dev.*, in preparation.

innovation will permit a detailed assessment of key precursors and chemical pathways involved in SOA formation and aging on a local (Spain) to global scale using the latest understanding of the chemistry and physics of SOA.

Using the new capabilities of NMMB/BSC-CACM/MPMPO, the role of $NH_3$ on global aerosol mass loading and optical properties will be evaluated. Collaborators at UCI are currently investigating SOA aging by $NH_3$ in a 5 $m^3$ Teflon smog chamber using advanced analytical instrumentation, including PTR-MS[21] for gas-phase measurements, ToF-AMS[22] for single-particle composition measurements, and nanoDESI/HR-MS[23] for high resolution bulk aerosol composition. The multidisciplinary approach proposed here combines this cutting-edge laboratory-based research (see letter of support in Section 7) with the advanced modelling techniques employed by the Earth Sciences BSC (ES-BSC) team, and the work of the ER on the continuing development of the CACM/MPMPO SOA model, and the field measurement data and expertise of the IDAEA-CSIC team.

This work will foster **continuing collaboration** between ES-BSC, IDAEA-CSIC, the UCI team, and the ER. ES-BSC and UCI have established a long-term scientific collaboration with more than 10 years of academic collaboration and several joint publications.[24] The successful deployment of CACM/MPMPO into the global NMMB/BSC model will also permit future collaboration between ES-BSC and the developers of CACM/MPMPO.

### 1.2 Quality and appropriateness of the training and of the two way transfer of knowledge between the researcher and the host

As part of a post-doctoral appointment, the ER has gained knowledge in the development of SOA modules for regional-scale and plume models. This work has included the implementation of new aromatic-derived SOA chemistry into the version of CACM/MPMPO used in the UCI-CIT regional air quality model, as well as incorporating the CAPRAM model for aqueous SOA formation into the particle-resolved aerosol model Part-MC to evaluate the impact of aerosol mixing state on cloud formation and processing of SOA.[25] The work proposed here will bring the knowledge gained by the ER related to the development of SOA models to the ES-BSC team as they work to incorporate detailed SOA chemistry and physics into the NMMB/BSC model. The incorporation of a detailed SOA module into the NMMB/BSC model is an enhancement that directly contributes to the NMMB/BSC's role in the ICAP aerosol-forecasting ensemble.[26]

Conversely, the training on the Marenostrum supercomputer and the NMMB/BSC CTM critical to this proposal will provide the ER with a solid background in global chemical/meteorological modelling that will complement his experience in laboratory-based experimentation, and further his training in computational atmospheric modelling that began during his post-doctoral career. Additionally, the secondment at IDAEA-CSIC will give the ER first-hand experience with field measurement techniques, and data collection and processing. **This training will result in a closely coupled set of transferrable skills that will directly impact the ability of the ER to develop and participate in comprehensive, multi-discipline research projects related to atmospheric aerosol science.** Specific short and long term objectives of the training will be discussed with the research supervisor prior to the fellowship and described in the Career Development Plan, to be developed as part of Work Package (WP) 1.

### 1.3 Quality of the supervision and of the integration in the team/institution

Qualifications and experience of the supervisor(s). *Dr. Oriol Jorba*, leader of the BSC-ES Atmospheric Composition group since 2008. He has participated in projects funded by the European Commission on air quality, specifically in aerosols, (APPRAISAL, EARLINET, FIELD-AC, ACTRIS1, ACTRIS2) and in the application of atmospheric modeling in HPC (IS-ENES, IS-ENES2, RETHINK big). He has lead the research project on the development of the multiscale chemical weather forecasting system NMMB/BSC-CTM (CGL2008-02818, CGL2013-46736) which is the official model used by the Barcelona Dust Forecast Center (BDFC), the World Meteorological Organization (WMO) Regional Meteorological Center specializing in Atmospheric Sand and Dust. He has performed air quality impact assessment projects for companies (PRySMA Calidad y Medioambiente, S.A., IBERDROLA, Gas Natural, PB Powers, SGS TECNOR, S.A., INYPSA Informes y proyectos, S.A.). He has been a Spanish representative member of the management committee of COST Actions ES1002 and ES1004, and is part

[21] Jordan et al., *Int. J. Mass Spectrom.*, vol. 286, 32-38, 2009.
[22] DeCarlo et al., *Analyt. Chem.*, vol. 78, 8281-8289, 2006.
[23] Laskin et al., *Analyt. Chem.*, vol. 84, 7179-7187, 2012.
[24] Jimenez et al., *Atmos. Environ.*, vol. 37, 4179-4194; Pey et al., *Atmos. Environ.*, vol. 44, 3322-3342, 2010; Jorba et al., *J. Geophys. Res.*, vol. 117, D13301, doi:10.1029/2012JD017730, 2012; Badia et al., *Geophys. Model Dev. Discuss.*, doi:10.5194/gmd-2016-141, in review
[25] Dawson et al., *Geophys. Model Dev.*, vol. 9, 2143-2151, 2016; Dawson et al., in preparation.
[26] Sessions et al., *Atmos. Chem. Phys.*, vol. 15, 335-362, 2015.

of the International Technical Meeting on Air Pollution Modelling and its Application (ITM) scientific committee since 2012. He is an active member of the International Cooperative for Aerosol Prediction (ICAP) and the Air Quality Modelling Evaluation International Initiative (AQMEII). Additionally, he maintains regular collaborations on aerosol modelling with the NASA Goddard Institute for Space Studies, National Center for Environmental Prediction, University of California Irvine, Finish Meteorological Institute, among others. A scientific reviewer of the Scientific Commission of the Spanish National Research Program, his research expertise includes high resolution mesoscale meteorology and air quality, development of online meteorology-chemistry models, boundary layer, atmospheric chemistry studies and environmental impact assessment. He has co-authored more than 50 papers in international scientific journals, over 100 communications in international conferences and directed 6 PhD theses. Additionally, he has been the mentor of two national FPI PhD fellowships, has been part of the research group in charge of one Marie Curie Intra-European Fellowship in the call FP7-PEOPLE-2013-IEF, and acts as supervisor for one Marie Skłodowska-Curie Individual Fellowship in the call H2020-MSCA-IF-2015.

Hosting arrangements. During the fellowship, the ER will work as part of the ES-BSC team, co-led by Dr. Jorba. State-of-the-art supercomputing facilities along with the benefits of working in a large multi-disciplinary institution make BSC an ideal environment for this type of research. BSC will provide the ER with all appropriate accommodations for the proposed work, including office and storage space, and a laptop computer. BSC also has a complete scientific library, including subscriptions to all relevant journals in the field. Additionally, Dr. Jorba and the team of researchers at ES-BSC maintain a large professional network of collaborators and colleagues that will be of direct benefit as the ER continues to develop his professional network of contacts. And, BSC itself offers a diverse research environment with many opportunities to interact with researchers in a variety of fields.

The standard fellowship agreement based on Horizon 2020 contractual rules and the Spanish fiscal and social security laws will be prepared by the BSC support services, and the financial issues related to the fellowship will be handled by the financial services; both groups have substantial experience in this regard, based on a large number of previous EU contracts. The set of measures aiming to foster research careers and strengthen internal training are based on the principles of the European Charter for Researchers and on the Code of Conduct for Recruitment and have been awarded the badge of Human Resources Excellence in Research (HRS4R) by the European Commission.

### 1.4 Capacity of the researcher to reach or re-enforce a position of professional maturity/independence

The graduate work of the ER involved using experimental laboratory techniques to characterize and quantify new pathways to aerosol formation in the atmosphere, specifically those related to the reactions of methanesulfonic acid, amines and water.[27] As a post-doctoral researcher, he was introduced to atmospheric modelling techniques and has been part of several successful collaborations focused on the development of advanced models for the treatment of SOA. These include contributions to the on-going development of CACM/MPMPO, along with its evaluation within the UCI-CIT regional air quality model.[28] Additionally, he has implemented the CAPRAM aqueous chemistry model in the stochastic particle-resolved aerosol/cloud plume model Part-MC.[29] He has presented the results of these projects at numerous scientific conferences, and is author or co-author on nine peer reviewed journal articles, all of which deal with aerosol science. This background, especially his experience with CACM/MPMPO, makes the ER a prime candidate to carry out the proposed work.

The opportunity to carry out this Fellowship at BSC, by providing an expanded network of potential collaborators and an improved research tool-kit, will greatly improve the capacity of the ER to contribute to the development and execution of cutting-edge, collaborative research proposals that integrate laboratory, field and modelling work. Specifically, the training provided at BSC will increase the experience of the ER in SOA module development to include deployment in global models, thus improving his ability to take on atmospheric modelling projects at any scale. The secondment at IDAEA-CSIC will allow the ER to gain first-hand knowledge in the collection and processing of field measurement data for regional and global model evaluation. Additionally, the Fellowship will improve the project development and management skills of the ER, towards the goal of becoming a successful researcher in the fields of atmospheric modelling and aerosol science. Finally, through collaborations at BSC and IDAEA-CSIC, along with networking opportunities involved in the presentation of research results at European scientific conferences, including EGU, the professional network of the ER will be expanded, thus opening

[27] Dawson et al., *PNAS*, vol. 109, 18719-18724, 2012.
[28] Dawson et al., *Geophys. Model Dev.*, vol. 9, 2143-2151, 2016
[29] Dawson et al., in preparation.

opportunities for future collaboration, and improved career prospects. To ensure the career prospects of the ER benefit from the Fellowship to the fullest extent possible, a **customized Career Development Plan (CDP)** will be formulated for the ER at the beginning of the Fellowship, as part of WP1.

# 2. Impact

## 2.1 *Enhancing the potential and future career prospects of the researcher*

**Comprehensive research experience**. Combining laboratory-based experimentation with computational modelling and field measurement campaign data makes for competitive, comprehensive research proposals. The Fellowship will provide a means for the ER to complement his experience with laboratory-based experimentation on aerosol process acquired during graduate school and his post-doctoral experience in computation modelling, by adding two new skills that will be readily transferable to future projects focused on atmospheric aerosol science.

- **Global modelling**. The proposed research will provide training in global modelling techniques that will extend the ER's knowledge of regional-scale and plume models. Competence in simulating atmospheric processes at every scale will allow the ER to develop comprehensive, competitive and productive research projects.
- **Field campaign data**. Through the secondment at IDAEA-CSIC, the ER will gain experience in the compilation and processing of field measurement data for evaluation of predictive models. An understanding of the technological capabilities and limitations related to field measurement techniques will be acquired, and the use of field measurement data to gain insight into the processes at work in aerosol formation, growth and aging will be experienced first-hand.

The net effect of the research-related experience gained through the Fellowship will be to enhance the potential of ER to develop and execute comprehensive, collaborative research proposals on atmospheric aerosol science. By the end of the Fellowship, the ER will have first-hand experience in laboratory, field, and computational modelling research along with a unique perspective of the potential synergies and challenges in combining the three approaches into focused, unified scientific investigations. This ability will make the ER unique in the field, and open up the possibility of a productive future career.

**Expanded professional network and new cultural experience.** The ER performed his graduate work in the Department of Chemistry and his post-doctoral research in the Department of Mechanical and Aerospace Engineering, both at the University of California, Irvine. He has also participated in collaborative projects with researchers at Pacific Northwest National Lab, Rice University and the University of Illinois at Urbana-Champaign. The Fellowship will expose the ER to the new interactions and approach to research that come from working at a different primary institution. It will also expand the professional network of the ER to include both the BSC and IDAEA-CSIC teams, and bring him into closer proximity to European research teams in the field whose research the ER is well acquainted with, but with whom he has not had the opportunity to interact with in person. This will be accomplished through the travel-related funding provided by the Fellowship that will primarily be used to attend and present research results at various European scientific conferences, including the European Geophysical Union (EGU) annual meetings. This is aided by the close proximity of the BSC and IDAEA-CSIC facilities, which will result in minor travel expenses being associated with the secondment. Finally, the opportunity to live in Spain and be exposed to a new culture will greatly expand the international experience of the ER, whose history of travel outside of the United States only includes Canada.

## 2.2 *Quality of the proposed measures to exploit and disseminate the action results*

**Dissemination.** Results from the proposed work will be disseminated through several channels. First, results will be prepared as two-to-three articles covering WP 2-5 and submitted for publication in GMD, ACP and/or PNAS. The ER and the BSC and IDAEA-CSIC teams have a history of publishing in these and other high impact journals; two IDAEA-CSIC team members are included in the 2014 and 2015 list of the 1% most cited authors in Geosciences according to Thompson Reuters. Additionally, a project web portal will be developed for communication of project information, progress and results to researchers and the general public. The updated CACM/MPMPO-$NH_3$ module for KPP will be disseminated to the community via the web portal. Results from the proposed work will be presented at EGU and other appropriate European conferences. Presentation of the NMMB/BSC-CACM/MPMPO-$NH_3$ development process and results will be included in the annual BSC Doctoral Symposium, for early PhD and post-doctoral students.

**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/BSC-

CACM/MPMPO-$NH_3$ CTM 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. These projects directly inform European and international legislators' work to develop air quality policy and regulations. 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 quality of predictions of aerosol mass and optical properties, and their impact on air quality and climate in one of the premier European chemical weather prediction systems, NMMB/BSC, falls perfectly in line with European research priorities and concurrent initiatives. 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 CACM/MPMPO-$NH_3$ module redesigned for use with the KPP and 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/BSC-CACM/MPMPO-$NH_3$ global 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.

### *2.3. Quality of the proposed measures to communicate the action activities to different target audiences*

Communication of research results and public engagement will be a key focus of the proposed work, and is included in WP1. The ER has a strong history in presentation of research results at scientific conferences, and engagement with the public through, *e.g.,* participation in local middle school science fairs and giving the keynote address at the annual awards dinner for the local high school American Chemical Society (ACS) chapter. Additionally, 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 ER as part of WP1. 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 WP1. The ER 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 utilization of European supercomputing resources, including for environmental simulation. As part of WP1, the ER 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.

## 3. Quality and Efficiency of the Implementation

### *3.1 Coherence and effectiveness of the work plan*

| **WP1: Management and dissemination** | **Deliverables** | **Date** |
|---|---|---|
| **Aim**: overall management, dissemination and outreach activities.<br>**Tasks:**<br>**T1.1** General management<br>**T1.2** Career development plan<br>**T1.3** Progress monitoring<br>**T1.4** Dissemination and public engagement<br>**T1.5** Participation in PRACE training | **D1.1** Management plan | M1, 5,13, 20 |
| | **D1.2** Career Development Plan | M2 |
| | **D1.3** Progress monitoring reports | 3-monthly |
| | **D1.4** Final report | M24 |
| | **D1.5** Publication on WP2-3 | M11 |
| | **D1.6** Publication on WP4 | M18 |
| | **D1.7** Publication on WP5 | M24 |
| **WP2: CACM/MPMPO deployment** | **Deliverables** | **Date** |
| **Aim**: Compile observational data at IDAEA-CSIC | **D2.1** Local (Spain) | M23 |

| | | |
|---|---|---|
| **Tasks:**<br>**T2.1** Assemble DUARE campaign data for Spain<br>**T2.2** Participate in CSIC campaign in Osona region of NE Spain<br>**T2.3** Participate in second phase of Osona regional field campaign | observational dataset from DUARE campaign | |
| | **D2.2** Local (Spain) observational dataset from Osona region campaign (July, 2016 and 2017) | M16 |
| **WP3: CACM/MPMPO deployment** | **Deliverables** | **Date** |
| **Aim**: Implement CACM/MPMPO into NMMB/BSC<br>**Tasks:**<br>**T3.1** Modify CACM/MPMPO for KPP<br>**T3.2** Incorporate CACM/MPMPO module into NMMB/BSC CTM<br>**T3.3** Update emission schemes for CACM species<br>**T3.4** Configure NMMB/BSC-CACM/MPMO for regional (Spain) run at 4 km x 4 km resolution<br>**T3.5** Compile model input conditions for comparison with DUARE campaign<br>**T3.6** Model run and evaluation | **D3.1** NMMB/BSC-CACM/MPMPO configuration for regional (Spain) run | M9 |
| | **D3.2** Evaluation of NMMB/BSC-CACM/MPMPO results with DAURE campaign measurements | M11 |
| **WP4: $NH_3$ chemistry incorporation** | **Deliverables** | **Date** |
| **Aim**: Implement new $NH_3$-related SOA chemistry/physics into NMMB/BSC-CACM/MPMPO<br>**Tasks:**<br>**T4.1** Work with UCI collaborators to develop module for $NH_3$-related SOA formation and aging<br>**T4.2** Incorporate $NH_3$-SOA module into NMMB/BSC-CACM/MPMPO<br>**T4.3** Compile model input conditions for comparison with NE Spain campaign field measurements<br>**T4.4** Model run and evaluation | **D4.1** Evaluation of updated CACM/MPMPO-$NH_3$ module based on chamber experiment results | M14 |
| | **D4.2** Deployment of CACM/MPMPO-$NH_3$ into NMMB/BSC | M15 |
| | **D4.3** Evaluation of NMMB/BSC-CACM/MPMPO-$NH_3$ results with NE Spain field campaign | M18 |
| **WP5: Impact of $NH_3$-related SOA chemistry on the global scale** | **Deliverables** | **Date** |
| **Aim:** Evaluate the impact of $NH_3$ on aerosol mass loadings and optical properties globally<br>**Tasks:**<br>**T5.1** Configure NMMB/BSC-CACM/MPMPO-$NH_3$ for global run at 50 km x 50 km resolution<br>**T5.2** Compile model input conditions including global emissions scenarios<br>**T5.3** Evaluate model output using available ground-based and satellite measurements<br>**T5.4** Evaluate the impact of $NH_3$ on climate, through a parameterization of $NH_3$-related aerosol optical effects. | **D5.1** Evaluation of $NH_3$ on SOA globally | M24 |

- List of major milestones

| | |
|---|---|
| **MILESTONE (m1)**: Career Development Plan | **Date:** M2 |
| **MILESTONE (m2):** Deployment and evaluation of CACM/MPMPO in NMMB/BSC | **Date**: M11 |
| **MILESTONE (m3):** Incorporation of $NH_3$-related SOA chemistry into NMMB/BSC-CACM/MPMPO and evaluation based on field measurements | **Date:** M18 |
| **MILESTONE (m4):** Evaluation of the impact of $NH_3$-related SOA chemistry on global aerosol mass loadings and climate | **Date:** M24 |

### *3.2. Appropriateness of the allocation of tasks and resources*

WP1 covers the **project management and dissemination** of results and includes preparation of manuscripts and presentations. These tasks will be carried out over the course of the project and will correspond to approximately

1.5 person months. The bulk of this time will be spent in communication and dissemination activities and preparing manuscripts, and is appropriate based on previous experience.

WP2 covers the **compilation of observational datasets for model evaluation**, and participation in the Osona region campaign described in the introduction. This work project will be carried out as a secondment at IDAEA-CSIC, which is appropriate as the DUARE and future field campaign described in the introduction are IDAEA-CSIC projects, and the work progress will benefit from easy access to researchers familiar with the campaigns. Additionally, participation in the Osona region campaign will afford the ER with first-hand experience in the measurement techniques used to collect the data that will be used to evaluate the model simulations. This work project will take 4 person months, which is appropriate based on the experience of the BSC team compiling similar sets of observational data for model evaluation.

WP3 and the remaining work projects will be carried out at BSC, where the BSC-ES Atmospheric Composition team will provide necessary training and support. WP3 covers the **implementation of CACM/MPMPO into the NMMB/BSC CTM**. This work project will result in the availability of the fully evaluated NMMB/BSC-CACM/MPMPO CTM, corresponding to milestone M1. This work project will take 6.5 person months, which is ambitious but realistic considering the ER's knowledge of CACM/MPMPO and the availability of tools for fast analysis/manipulation of the model code.

WP4 covers updating CACM/MPMPO to include relevant **$NH_3$-related SOA chemistry**, and deployment into NMMB/BSC-CACM/MPMPO. This work project will result in the availability of the fully evaluated NMMB/BSC-CACM/MPMPO-$NH_3$ CTM, corresponding to milestone M2. This work project will take 6.5 person months, which is appropriate based on previous experience implementing new chemistry into the CACM/MPMPO module.

WP5 covers the evaluation of NMMB/BSC-CACM/MPMPO-$NH_3$ on the **global scale**. This work project will result in both the evaluation of the model, and an assessment of the role of $NH_3$ on SOA formation and aging in the global atmosphere. The completion of this work project corresponds to milestone M3 and the conclusion of the project. This work project will take 5.5 person months, which is appropriate based on the experience of the BSC team with the configuration of NMMB/BSC and the CALIOPE CTM for similar model domains and conditions.

### *3.3 Appropriateness of the management structure and procedures,* including risk management

Organisation and management structure. Within BSC, a qualified project manager will support the researcher in all the legal, financial and administrative arrangements needed and work in close contact with Education, Human Resources and Communications departments for all training arrangements and dissemination and outreach activities. Finances of the project will be managed according to MSC funding rules signed at the grant agreement and will follow the established processes at the host organization, which has considerable experience in managing such projects. The ER will work in close contact with the supervisor and the staff, who will review the progress of the work through progress reports compiled every three months as part of WP1. This will allow the evaluation of the progress against the work plan, and increase assistance in a timely manner if the necessity arises. Management planning is scheduled as part of WP1 to occur one month in to WPs 3, 4, and 5. Thus, preliminary experience in each new WP, along with attendant obstacles and newly identified risks, can be evaluated and the project management plan can be adjusted as needed.

Research and/or administrative risks that might endanger reaching the action objectives. ES-BSC provides an ideal infrastructure to carry out the proposed research in a manner that maximizes the potential for success, and minimizes administrative and research risks. It provides state-of-the-art high-performance computing infrastructure and personnel, computational and multidisciplinary science knowledge resources, a large, well respected international scientific network, and experience in the administration of European Union projects. More specifically, three areas of potential research-related risk have been identified: 1.) Technical difficulties in the implementation of CACM/MPMPO into the NMMB/BSC model, 2.) Delays in the availability of field data from the Osona campaign, and 3.) Delays in the availability of laboratory data from the UCI team on $NH_3$-related SOA chemistry. The first risk is mitigated by the experience of the ER with the development of CACM/MPMPO, the pledged support of the BSC team related to NMMB/BSC development, and the history of collaboration with Prof. Griffin (Rice Univ.), the primary developer of CACM/MPMPO (see letter of support in section 7). The second risk is mitigated by the availability of existing field data, including that from the DUARE campaign, which could be used in the event of a delay in the Osona campaign. The third risk is mitigated by the availability of some published laboratory research on $NH_3$-related SOA chemistry by the UCI team that could be used as a basis for the

NMMB/BSC-CACM/MPMPO-$NH_3$ model until new data become available. Further contingency planning will be carried out as part of WP1.

### *3.4 Appropriateness of the institutional environment (infrastructure)*

The BSC is a public consortium composed of: the Spanish Ministry of Economy and Competitiveness, the Catalan government and 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-CNS 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 III supercomputer, used in a Tier-0 PRACE system with 1Pflop/s capacity.

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

IDAEA-CSIC is beginning a 3-year campaign to investigate and characterize atmospheric aerosol and trace gas species in the emission plume exiting the Barcelona region and extending to rural environments. Included in the emission plume and sampling region is the Osona region of NE Spain, an area with high $NH_3$ emissions due to concentrated farming activities. The results of this campaign will provide an ideal means to evaluate the $NH_3$-related SOA chemistry that will be incorporated into the NMMB/BSC model as part of this proposal. IDAEA-CSIC features complete laboratory facilities and state-of-the-art instrumentation for the measurement and characterization of atmospheric aerosols and trace gases. Additionally, they have many years of experience performing field measurements related to aerosol and trace gas species in urban and rural environments; include some of the top-cited researchers in the field; and, have a history of collaboration with the computational modelling team at ES-BSC. Thus, IDAEA-CSIC offers the ideal synergistic complement to the ES-BSC host organization.

IDAEA-CSIC have committed to provide the ER with the training and supervision, along with the requisite office space and computer hardware, necessary to participate in the Osona campaign and compile field measurement data from the DUARE and Osona campaigns for evaluate of the NMMB/BSC-CACM/MPMPO-$NH_3$ model (see letter of support in section 7). This secondment will provide the ER with first-hand experience in the accumulation and processing of field measurement data, which will be of significant and immediate benefit to the execution of the proposed research, as it relates to evaluation of the updated NMMB/BSC-CACM/MPMPO-$NH_3$ model. Additionally, it will complement the laboratory and modelling experience of the ER, and result in long-term benefits to his ability to participate in the development and execution of comprehensive, collaborative research projects that integrate laboratory, field, and modelling work.

## Project Gantt Chart

| Month | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **WP1 – Project Management** | D1.1 Mgmt Plan | D1.2 Career Dev. Plan | D1.3 Prog Rpt | | D1.1 Mgmt Plan | D1.3 Prog Rpt | | | D1.3 Prog Rpt | | | D1.3 Prog Rpt | D1.1 Mgmt Plan | | D1.3 Prog Rpt | | | D1.3 Prog Rpt | | D1.1 Mgmt Plan | D1.3 Prog Rpt | | | D1.4 Final Rpt |
| **WP1 - Dissemination** | | | | | | | | | | | D1.5 Paper | | EGU Conf. | | | | | D1.6 Paper | | | | | | D1.7 Paper |
| **WP2 – Data Compilation** | | | D2.1 DUARE data | Osona Phase 1 | | | | | | | | | | | | D2.2 Osona Phase 2 | | | | | | | | |
| **WP3 – CACM/ MPMPO** | | | | | | | | | D3.1 Up-date | | D3.2 Eval | | | | | | | | | | | | | |
| **WP4 – $NH_3$ Chemistry** | | | | | | | | | | | | | | D4.1 Dev | D4.2 Up-date | | | D4.3 Eval | | | | | | |
| **WP5 – Global Simulation** | | | | | | | | | | | | | | | | | | | | | | | | D5.1 Global Sim |
| **Milestones** | | M1 | | | | | | | | | M2 | | | | | | | M3 | | | | | | M4 |
| **Secondment IDAEA-CSIC** | | | | | | | | | | | | | | | | | | | | | | | | |

**DOCUMENT 2**

# 4. CV of the Experienced Researcher

**CURRICULUM VITAE**
Matthew L. Dawson

**EDUCATION**

**University of California, Irvine** *Irvine, CA*
Postdoctoral Research in Mechanical and Aerospace Engineering **2014-2016**
Advisor: Prof. Donald Dabdub

**University of California, Irvine** *Irvine, CA*
Ph.D. in Chemistry **2009-2014**
GPA: 3.997
Advisor: Prof. Barbara J. Finlayson-Pitts

**University of Pittsburgh** *Pittsburgh, PA*
B.S. in Chemistry, summa cum laude **2007-2009**
GPA: 3.976
Advisor: Prof. Sunil Saxena

**Community College of Allegheny County** *Pittsburgh, PA*
GPA: 4.000 **2005-2006**

**RESEARCH EXPERIENCE**

**Postdoctoral Researcher** **2014-2016**
University of California, Irvine *Irvine, CA*

- Incorporated recently identified chemical processes related to the oxidation of aromatic species into the UCI-CIT regional air quality model.
- Developed an aqueous-phase cloud chemistry module for the stochastic model of aerosol and cloud formation in emission plumes, Part-MC.
- Evaluated and improved predictions of aerosol mass in the UCI-CIT regional air quality model using advanced models for estimating thermodynamic parameters of chemical species.
- Developed software tools for the efficient processing of large sets of emissions data.
- Routinely worked with scientific models written primarily in FORTRAN and C, and designed for High Performance Computing using openMPI. Some experience with Java, C++, VB, mySQL, NetCDF and Python.

**Graduate Research Assistant** **2009-2014**
University of California, Irvine *Irvine, CA*

- Developed a new method for measuring gas-phase ammonia and amines at the part- per-trillion level in air that includes a novel extraction/analysis technique using ion chromatography.
- Identified and characterized a new source of aerosol particles in the atmosphere through laboratory flow-reactor experiments.
- Tested a new kinetics mechanism for aerosol formation in a comprehensive aerosol chemistry and physics model.

**Undergraduate Research Assistant** **2008-2009**
University of Pittsburgh *Pittsburgh, PA*

- Modeled conformational isomers of the spin-labeled EcoRI protein by molecular dynamic simulations to aid in the interpretation of experimental electron spin resonance (ESR) data.

**AWARDS**

*Metrohm Young Chemist Award* **October 2012**

An award for novel research or an innovative approach to the applications of titration, ion chromatography and/or electrochemistry

*ARCS Scholar* **September 2012**

ARCS Foundation advances science and technology in the United States by providing financial awards to academically outstanding U.S. citizens studying to complete degrees in science, engineering and medical research.

*Gebel Award, UC Irvine* **May 2011**

An award recognizing excellence in graduate environmental chemistry research and service to the community

*Contributions to Education by a Chemistry Department TA, UC Irvine* **May 2011**

*Phillips Medal, University of Pittsburgh* **May 2009**

An award presented to the senior chemistry major with the most outstanding academic record

**TEACHING EXPERIENCE**

**Teaching Assistant** **Summer 2011, 2012, 2013** *Irvine, CA*
AirUCI Summer Teacher Workshop

**Laboratory Assistant** **Fall 2009**
University of California, Irvine **Winter–Spring, 2010**
General, Advanced Analytical, and Quantitative Analytical **Winter 2011**
Undergraduate Chemistry Labs *Irvine, CA*

**Tutor** **Fall–Winter 2006**
Community College of Allegheny County *Pittsburgh, PA*
Introductory Computer Courses and Java Programming

**ORGANIZATIONS**

American Association for Aerosol Research **2011–Present**

**REFEREED JOURNAL PUBLICATIONS**

Dawson, M.L., Xu, J., Griffin, R.J., Dabdub, D., Development of aroCACM/MPMPO 1.0: A Model to Simulate Secondary Organic Aerosol from Aromatic Precursors in Regional Models, *Geosci. Model Dev*. **9**, 2143–2151 (2016).

Perraud V., Horne, J.R., Martinez, A.S., Kalinowskic, J., Meinardi, S., Dawson, M.L., Wingen, L.M., Dabdub, D., Blake, D.R., Gerber, R.B., Finlayson-Pitts, B.J., The Future of Airborne Sulfur-Containing Particles in the Absence of Fossil Fuel Sulfur Dioxide Emissions, *PNAS* **112**, 13514–13519 (2015).

Chen, H., Ezell, M.J., Arquero, K.D., Varner, M.E., Dawson, M.L., Gerber, R.B., Finlayson-Pitts, B.J. New Particle Formation and Growth from Methanesulfonic Acid, Trimethylamine and Water, *Phys. Chem. Chem. Phys*. **17**, 13699–13709 (2015).

Dawson, M.L., Varner, M.E., Perraud, V., Ezell, M.J., Wilson, J., Zelenyuk, A., Gerber, R.B., Finlayson-Pitts, B.J. Amine-Amine Exchange in Aminium-Methanesulfonate Aerosols, *J. Phys. Chem. C* **118**, 29431–29440 (2014).

Dawson, M.L., Perraud, V., Gomez A., Arquero, K.D., Ezell, M.J., and Finlayson-Pitts, B.J. Measurement of Gas-Phase Ammonia and Amines in Air by Collection onto an Ion Exchange Resin and Analysis by Ion Chromatography, *Atmos. Meas. Tech.* **7**, 2733–2744 (2014).

Nishino, N., Arquero, K.D., Dawson, M.L., Finlayson-Pitts, B.J. Infrared Studies of the Reaction of Methanesulfonic Acid with Trimethylamine on Surfaces, *Environ. Sci. Technol*. **48**, 323–330 (2013).

Dawson, M.L., Varner, M.E., Perraud, V., Ezell, M.J., Gerber, R.B., Finlayson-Pitts, B.J. New Particle Formation from Methanesulfonic Acid, Amines and Water: Experiment, *ab initio* Calculations and a Simplified Mechanism. *PNAS* **109**, 18719–18724 (2012).

Doezema, L.A., Longin, T., Cody, W., Perraud, V., Dawson, M.L., Ezell, M.J., Greaves, J., Johnson, K.R., Finlayson-Pitts, B.J. Analysis of Secondary Organic Aerosols in Air using Extractive Electrospray Ionization Mass Spectrometry (EESI-MS). *RSC Advances* **2**, 2930– 2938 (2012).

Gratien, A, Johnson, S.N., Ezell, M.E., Dawson, M.L., Bennett, R, Finlayson-Pitts, B.J. Surprising Formation of *p*-Cymene in the Oxidation of *α*-Pinene in Air by the Atmospheric Oxidants OH, $O_3$, and $NO_3$. *Environ. Sci. Technol*. **45**, 2755–2760 (2011).

**SELECTED CONFERENCE PRESENTATIONS**

*Presenting author(s)

*Dawson, M.L., Riemer, N., Dabdub, D. "Aerosol Mixing State Impacts on Aqueous-Phase Chemistry." *The AMS 96th Annual Meeting*. Ernest N. Morial Convention Center, New Orleans, LA. Jan. 10 – 14, 2016. Conference Presentation.

*Dawson, M.L., Xu, J., Griffin, R.J., Dabdub, D. "Dynamics of Aromatic-Derived SOA in the South Coast Air Basin of California." *American Association for Aerosol Research: 34th Annual Conference*. Hyatt Regency, Minneapolis, MN. Oct. 12 – 16, 2015. Conference Presentation.

*Dawson, M.L. "Improved Techniques to Model Secondary Organic Aerosol from Aromatic Precursors in Regional Models." *ACCESS XIII: Thirteenth Atmospheric Chemistry Colloquium for Emerging Senior Scientists.* Brookhaven National Laboratory, NY. Jul. 30 – Aug. 1, 2015. Conference Presentation.

*Dawson, M.L. "Improved Techniques to Model Secondary Organic Aerosol from Aromatic Precursors in Regional Models." *Gordon Conference: Atmospheric Chemistry Waterville Valley Resort*, Waterville Valley, NH. Aug. 2 – 7, 2015. Poster Presentation.

*Chen, H., *Varner, M.E., *Dawson, M.L., *Martinez, A.S., Perraud, V., Arquero, K. D., Gomez, A., Gerber, R.B., Dabdub, D., Finlayson-Pitts, B.J. "Particles and Their Precursors: From the Angstrom to Regional Scales." *Collaborative Workshop in Chemistry at the Interfaces*. AirUCI. Surf and Sand Hotel, Laguna Beach, CA. Jan. 22-23, 2014. Conference Presentation.

*Dawson, M.L., Gomez, A.L., Arquero, K.D., Perraud, V., Finlayson-Pitts, B.J. "A New Method for Measurement of Gas-Phase Ammonia and Amines in Air." *AGU Fall Meeting.* American Geophysical Union. Moscone Convention Center, San Francisco, CA. December 9-13, 2013. Poster Presentation.

*Dawson, M.L., Perraud, V., Ezell, M.J., Finlayson-Pitts, B.J. "Accurately Predicting Particle Formation and Growth from Gas-Phase Precursors." *Pittcon 2013*. Pennsylvania Convention Center, Philadelphia, PA. March 19, 2013. Poster Presentation.

*Dawson, M.L., Varner, M.E., Perraud, V., Ezell, M.J., Gerber, R.B., Zelenyuk, A., Finlayson-Pitts, B.J. "A Novel Kinetics Mechanism for Particle Formation from Methanesul- fonic Acid, Amines, and Water." *AAAR 2012 Annual Conference*. American Association for Aerosol Research. Hyatt Regency, Minneapolis, MN. Oct. 8-12, 2012. Poster Presentation.

*Dawson, M.L., Varner, M.E., Perraud, V., Ezell, M.J., Wingen, L.M., Bruns, E.A., Kleinman, M.T., Gerber, R.B., Finlayson-Pitts, B.J. "Atmospheric Particle Formation and Growth from Methanesulfonic Acid and Amines." *Spring 2012 National Meeting and Exhibition*. American Chemical Society. San Diego Convention Center, San Diego, CA. March 25-29, 2012. Poster Presentation.

*Dawson, M.L., Varner, M.E., Perraud, V., Ezell, M.J., Gerber, M.J., Zelenyuk, A., Finlayson-Pitts, B.J. "Formation and Growth of Atmospheric Aerosol Particles from Methanesulfonic Acid, Amines and Water." *2012 Science Team Meeting. Atmospheric System Research.* Department of Energy. Hyatt Regency Crystal City, Arlington, VA. March 12-16, 2012. Poster Presentation.

*Dawson, M.L., Varner, M.E., Perraud, V., Ezell, M.J., Wingen, L.M., Bruns, E.A., Kleinman, M.T., Gerber, R.B., Finlayson-Pitts, B.J. "Particle Nucleation and Growth from Methanesulfonic Acid and Amines." *AAAR 2011 Annual Conference. American Association for Aerosol Research*. Rosen Shingle Creek Resort, Orlando, FL. October 3-7, 2011. Poster Presentation.

*Dawson, M.L., Perraud, V., Ezell, M.J., Wingen, L.M., Bruns, E.A., Kleinman, M.T., Varner, M.E., Gerber, R.B., Finlayson-Pitts, B.J. "Methanesulfonic Acid as a Source of New Particles in the Atmosphere." *241st ACS National Meeting and Exposition.* American Chemical Society. Anaheim Convention Center, Anaheim, CA. March 27-31, 2011. Poster Presentation.

*Dawson, M.L., Perraud, V., Ezell, M.J., Wingen, L.M., Bruns, E.A., Kleinman, M.T., Finlayson-Pitts, B.J. "New Particle Formation from Methanesulfonic Acid in Air." *Chemical Sciences Roundtable: Challenges in Characterizing Small Particles: Exploring Particles from the Nano- to Micro-scales.* National Academy of Sciences. The Washington Plaza Hotel, Washington, D.C. Oct. 25-26, 2010. Poster Presentation.

**OTHER PRESENTATIONS**

*Dawson, M.L. A Random Walk to Graduate School. *ACS High School Awards Dinner*. American Chemical Society. UCI Student Center, Irvine, CA. May 3, 2013. Invited Speaker.

# 5. Capacity of the Participating Organisations

| **Beneficiary: Barcelona Supercomputing Center (BSC)** | |
|---|---|
| **General Description** | The Barcelona Supercomputing Center (BSC) was established in 2005 and serves as the national supercomputing facility. Currently, it is hosting 1 of the 6 European Tier-0 supercomputers and is among the best supercomputing centers in the world. The mission of BSC, as a unique fusion of a classic national scientific support structure and a cutting-edge research institute, is to research, develop and manage information technologies in order to facilitate scientific progress. During the period 2011-2015, the BSC has recruited 75 pre-doctoral students, 51 Postdocs and Senior Scientist, 83 technical support staff members and 31 management staff, 146 from Spain, 39 coming from EU countries and 55 from outside Europe, being currently more than 380 staff members, from around 40 countries. Recruitment procedures are based on principles of merit, transparency, competition and gender balance and the center has been awarded with the badge of Human Resources Excellence in Research (HRS4R) in April 2015. The applicant will be enrolled at the Department of Earth Sciences (ES). |
| **Role and Commitment of key persons (supervisor)** | Dr. Oriol Jorba is an expert in the development of air quality (AQ) modeling systems to provide AQ forecasts and perform advanced research on atmospheric chemistry. As co-leader of the Atmospheric Composition group at BSC-ES, he has been involved in the deployment of the CALIOPE AQ forecasting system and is currently coordinating development of the NMMB/BSC-CTM an online multi-scale non-hydrostatic chemical weather prediction. With his experience in model development, he will supervise the Fellow during the project by providing guidance on efficient use of advanced numerical models in high performance computing environments. |
| **Key Research Facilities, Infrastructure and Equipment** | The BSC manages supercomputing facilities, notably MareNostrum, currently one of the 5 largest computers in Europe, with more than 1 PFlop. Additionally, BSC manages Minotauro, a Sandy Bridge's cluster with NVIDIA GPUs, providing more than 100 TFlops. There are also a range of purpose-built fat nodes and a storage facility that facilitates research on Big Data issues. |
| **Independent research premises?** | All BSC's departments have their own research premises. The infrastructure, equipment and key research facilities will be available for the fellow during the entire duration of the project. |
| **Previous Involvement in Research and Training Programmes** | The BSC has a successful record of national and international fellowships: since 2008 BSC hosted several Marie-Curie Individual Fellowhips (e.g. EEPPIBM, FP7-PEOPLE-2012-IEF-327899; MDRAF, FP7-PEOPLE-2013-IEF-622662; Noteworthy, that one of the MSC IF has been awarded under Dr. Oriol Jorba supervision in 2015 (INAQUA, H2020-MSCA-IF-2015-707515)) and three ITNs (SCALUS, FP7-PEOPLE-ITN-2008-238808; NEMOH, PF7-PEOPLE-2011-ITN-289976, COPA-GT, FP7-PEOPLE-ITN-2011-290042). BSC also hosts national fellowships, both for early-stage and senior postdoctoral positions: approximately 30 post-docs were awarded since 2006. |
| **Current involvement in Research and Training Programmes** | Collaboration with universities: within BSC, there is a large record of collaboration with Universidad Politècnica de Catalunya (UPC) including the Master degree in Environmental Engineering (UPC), associated with BSC Earth Science department. Excellence Programs and Networks: A number of training activities are organized under the framework of: Severo Ochoa Excellence Program (Research seminars series); RES (RES training sessions); NVIDIA CUDA/GPU excellence center (PUMPS summer school); PRACE (PRACE Advanced Training Center); HiPEAC (ACACES summer school, Computing system weeks and HiPEAC conferences) and H2020-EINFRA-Centers of Excellence for computing applications (PoP, Grant Agreement (GA) number: 676553; ESiWACE, GA number: 675191; BioExcel: GA number: 675728; NoMaD, GA number: 676580; MaX, GA number: 676598; EoCoE, GA number: 676629). Research Fellowships: BSC is currently awarded with 9 early-stage postdoc (7 Juan de la Cierva and 2 Beatriu de Pinós), 12 senior (5 Ramón y Cajal, 3 I3 and 6 ICREA) and is supporting 4 ITN, 2 RISE and 4 Marie-Curie Individual Fellowships. Noteworthy, two of these Marie-Curie actions (DPETNA, H2020-MSCA-IF-2014-655339; NeTNPPAO, H2020-MSCA-IF-2015-708063) are currently developed in BSC-ES, which will host the present Marie-Curie proposal.<br>Current involvement in Research Programs: **ACTRIS-2 (Aerosols, Clouds, and Trace gases Research InfraStructure) is a European Project supported by the European Commission Horizon 2020 Research and Innovation Framework Programme (H2020-INFRAIA-2014-2015) from 1 May 2015 to 30 April 2019. The BSC is a partner for this project. Project website: http://www.actris.eu/** |
| **Relevant Publications and/or research/ innovation products** | 1.Badia, A. et al., Gas-phase chemistry in the online multiscale NMMB/BSC Chemical Transport Model: Description and evaluation at global scale, *Geosci. Model Dev. Discuss.*, doi:10.5194/gmd-2016-141, in review (2016)<br>2. Spada, M. et al., On the evaluation of global sea-salt aerosol models at coastal/orographic sites. *Atmos. Environ*. **101**, 41-48 (2015)<br>3. Pandolfi, M. et al., Effects of sources and meteorology on particulate matter in the Western Mediterranean Basin: An overview of the DAURE campaign. *J. Geophys. Res*. **119**, 4978-5010 (2014)<br>4. Badia, A.; Jorba, O. Gas-phase evaluation of the online NMMB/BSC-CTM model over Europe for 2010 in the framework of the AQMEII-Phase2 project. *Atmos. Environ.* **115**, 657-669 (2015)<br>5. Spada, M. et al., Modeling and evaluation of the global sea-salt aerosol distribution: sensitivity to size-resolved and sea-surface temperature dependent emission schemes. *Atmos. Chem. Phys.* **13**, 11735-11755 (2013) |

| **Partner Organisation Spanish Council for Scientific Research (IDAEA-CSIC)** | |
|---|---|
| **General description** | The Agencia Estatal Consejo Superior de Investigaciones Cientificas (CSIC) (Spanish National Research Council) is the main public research organization in Spain, with 132 Institutes and Joint Research Units. The purpose of the CSIC is the development, coordination and diffusion of multidisciplinary scientific research with the purpose of contributing to the advancement of knowledge and economic, social and cultural issues. Recent international statistics recognize the CSIC as the 8th research organization in the world in terms of scientific production. The Institute of Environmental Assessment and Water Research (IDAEA), within CSIC, is a research institute devoted to atmospheric chemistry and the study of particulate and gaseous pollutants in the atmosphere. Specifically, the IDAEA-CSIC research team specializes in air quality monitoring and assessment, with broad expertise in field work. IDAEA-CSIC is well known within the European scientific community in the field of regulatory air quality monitoring and sensor technologies. |
| **Key Persons and Expertise (supervisor)** | Prof. Xavier Querol (10% FTE), Supervisor and participant in campaigns and data interpretation<br>Prof. Andrés Alastuey (10% FTE), Supervisor and participant in campaigns and data interpretation |
| **Key Research facilities, infrastructure and equipment** | Our research group is part of the Institute of Environmental Assessment and Water Research (IDAEA), within CSIC. Our competences include aerosol sampling, aerosol chemical characterisation, and receptor modelling. Our group has a network of 3 air quality monitoring sites (urban, regional background, remote), equipped with different instrumentation, including high volume particulate matter samplers, real-time PM monitors, SMPS, CPC, BC monitors, surface area monitors, ACSM, low-cost sensors for gases and PM. Moreover, we have receptor modelling tools, and off-line chemical analysis instrumentation such as ICPMS, ICP-AES, ion chromatography, and ECOC analysers. (http://contaminacion-atmosferica.es/es/) |
| **Previous and Current Involvement in Research and Training Programmes** | The IDAEA-CSIC team has substantial experience in training: X. Querol and A. Alastuey are frequent lecturers in Spanish MSc university courses (e.g., Universidad Internacional de Andalucía, Universidad Internacional Menénez Pelayo, Universidad A Coruña). The CSIC team has hosted >25 PhD Theses in the field of aerosol science. The team has participated as partners and external advisors in several EU projects such as APHEKOM, AirMonTech, GRACCIE, BREATHE, EUSAAR.<br><br>Current Research:<br>• H2020 Captor (Collective Awareness Platform for Tropospheric Ozone Pollution), 2016-2018<br>• COST Action EuNetAir<br>• H2020 ACTRIS2<br>• European Topic Center<br>• AIRUSE-LIFE+Project<br>• IMPROVE-LIFE+Project |
| **Relevant Publications and/or research/innovation product** | 1. ALASTUEY, A., QUEROL, X., et al. Geochemistry of $PM_{10}$ over Europe during the EMEP intensive measurement periods in summer 2012 and winter 2013, Atmos. Chem. Phys., 16, 6107-6129, doi:10.5194/acp-16-6107-2016, 2016.<br>2. QUEROL X., ALASTUEY A., et al.; 2001-2012 trends on air quality in Spain. Science of the Total Environment, 490, 15 (2014), 957-969.<br>3. QUEROL X., ALASTUEY A., et al., Variability of carbonaceous aerosols in remote, rural, urban and industrial environments in Spain: Implications for air quality policy. Atmos. Chem. Phys., 13, 6185-6206, doi:10.5194/acp-13-6185-2013, 2013.<br>Both Alastuey A and Querol X. are included in the 2014 and 2015 list of the 1% most cited authors in Geosciences |

# 6. Ethical Issues

No ethics issues are present in this project.

# 7. Letters of Commitment.

MINISTERIO
DE ECONOMÍA Y
COMPETITIVIDAD

CONSEJO SUPERIOR
DE INVESTIGACIONES
CIENTÍFICAS
Instituto de Diagnóstico Ambiental y Estudios
del Agua (IDAEA-CSIC)

## To whom it may concern,

September 1, 2016

On behalf of the laboratory of Atmospheric Geochemistry from the Institute Environmental Assessment and Water Research (IDAEA), from the Spanish Research Council (CSIC), I am pleased to express my strong support for the MARIE Skłodowska-CURIE Individual Fellowship proposal of Dr. Matt Dawson for the Call H2020-MSCA-IF-2016. The proposed work is an exciting scientific collaboration that will advance our understanding of the atmosphere in significant and profound ways.

The IDAEA-CSIC hosts complete laboratories and instrumentation to characterize compositional features of atmospheric aerosols. Especially relevant is a project we are starting now, and will last 3 years, on the characterization of the aerosol and O3 following the pollution plume of Barcelona Metropolitan Area towards the northern regions, where very high atmospheric levels of NH3 are also recorded due to intensive farming emission. Given the potential synergy between IDAEA-CSIC and BSC, we believe that the intellectual merits of this project are outstanding: our collaborations will yield to better understanding of the secondary formation of organic aerosols in high O3 and NH3 areas.

Our lab has and extended experience on the field of aerosol sciences, source apportionment and urban and regional background UFP. In the last 5 years our team produced around 35-40 SCI papers/year on aerosol sciences and two members of the team are in the 1% most cited scientists in the 2014 and 2015 Essencial Science Indicators, by Thomson Reuters. We believe that the secondment planned by Dr. Matt Dawson at IDAEA-CSIC will strength the formation of the candidate and will strongly contribute to the study of secondary organic aerosols formation.

I look forward to an active collaboration on this exciting and highly innovative initiative.

Xavier Querol
Research Professor
Instituto de Diagnóstico Ambiental y Estudios del Agua (IDÆA)
Consejo Superior de Investigaciones Científicas (CSIC)
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# 8. Letters of support.

UNIVERSITY OF CALIFORNIA, IRVINE

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August, 2016

Dear Sir/Madam:

I have known Matt Dawson for the better part of 5 years, first as a graduate student in the Chemistry Dept. and occasional collaborator, then as a student in my air pollution modeling class, and later as a post-doctoral researcher in my research group. From the beginning, I was impressed by his ability to work collaboratively with not just other experimentalists, but with those in other fields, including computational chemists and air quality modelers. His primary graduate project involved a combination of laboratory experiments coupled with quantum chemical calculations performed by collaborators in the Gerber group at UCI that resulted in new insights to atmospheric aerosol particle formation and a novel kinetics mechanism that will be of use to air quality and climate modelers. When asked, he always ascribes any ability to work so well collaboratively to his unique educational background, having worked for many years in a variety of industries and with an equally varied group of individuals. He has really managed to use this unique experience to benefit his research career, both in his interactions with coworkers and collaborators, as well as in bringing non-typical mechanical and computer programming skills to the table. Part of his doctoral work has been published in the *Proceeding of the National Academy of Sciences*.

While doing research as a graduate student in chemistry, Matt took on the additional challenge of enrolling in MAE261, a graduate level engineering class that I teach on air quality modeling. As the developer of this class, I can attest to the highly demanding character of its homework assignments, including the development of a complete chemically and spatially resolved air quality model. Despite never having taken a fluid dynamics class and never having programmed in FORTRAN before, Matt obtained (by far) the highest grade in the class.

After graduation, Matt jumped at the opportunity to join my group as a post-doctoral researcher, and has really 'hit the ground running.' In a few months, he has become involved in several projects, some of which he is the lead researcher on. His work is well on the way to inclusion in several publications, including first-author papers, and all indications are that his post-doctoral experience was both highly productive and valuable for his ongoing scholarship. Particularly, I believe that adding this experience in air quality modeling to his existing laboratory-based experimental background, offers a unique and highly desirable skill set that will set him up for a productive research career. As a result of his previous and current experiences, **Matt is one of the few people in the world with in-depth knowledge of experimental, theoretical and computational aspects of atmospheric chemistry.**

Matt's research area focus on the dynamics of Secondary Organic Aerosol. This is a highly visible and timely topic with ties to air pollution, energy issues and climate change. His background in chemistry and his affiliation to engineering is the *ideal* combination for this type of work.

Matt is quite skilled using state-of-the-art massively parallel computing facilities. The computing resources available to Matt comprise 32 exclusive private computing processors which are part of the High Performance Cluster (HPC) computing system managed by the University of California, Irvine. In addition, Matt will have access to additional resources in HPC, which add up to over 1300 computational cores. Matt's computational skills are superb.

In addition to Matt's research abilities, I would like to comment on his personal qualities as well. He is a sharp, pleasant, and outgoing individual with an enormous drive and energy for scholarly work. He can work harmoniously with other people and would cooperate with any faculty group. Excellence through diversity is an important element on Matt's interest. Matt has great appreciation and skills to work with people with unique backgrounds.

There is no question in my mind that he will be an excellent team member in Barcelona. The experience will be of tremendous benefit for Matt and for the Barcelona Super Computing Research Team.

Overall, **Matt is a truly exceptional individual who comes only once every few decades**. He certainly would rank on the top five among all the students and all postdocs that I have encountered in the past 20 years. He is the ideal recipient of the Marie Skłodowska-Curie Research Fellowship.

Cordially,

Donald Dabdub
Associate Dean of Undergraduate Education
Professor, Mechanical and Aerospace Engineering
Professor, Advanced Power and Energy Program

RICE

Department of Civil and Environmental Engineering
George R. Brown School of Engineering

September 9, 2016

Letter of Support for Matthew Dawson for the Marie Skłodowska-Curie Actions Individual Fellowship Application

To Whom It May Concern:

I am extremely happy to write this letter in support of the application of Dr. Matthew Dawson for his application to the Curie Fellowship. I am currently Chair of Civil and Environmental Engineering at Rice University and have over twenty years of experience in research and teaching focused on atmospheric chemistry. Therefore, I feel particularly qualified to provide this reference.

I first met Dr. Dawson when he joined the research group of my close collaborator Professor Donald Dabdub at the University of California-Irvine as a post-doctoral scholar. While Dr. Dawson was in this position, I had the pleasure of collaborating with him extensively. The results of our collaboration include presentations at scientific conferences, one published manuscript in *Geophysical Model Development*, and a second manuscript in preparation for submission to *Aerosol Science and Technology* (submission planned for October 2016).

Dr. Dawson exhibits tremendous technical strength. When he began work with Professor Dabdub and me, Dr. Dawson needed to come up to speed quickly in a new area of atmospheric chemistry (secondary organic aerosol formation). Dr. Dawson did so both efficiently and effectively; his ability to grasp topics both difficult and new to him was impressive – among the very best I have experienced in my time as a faculty member. In addition, Dr. Dawson essentially had to teach himself how to program, a daunting task. Dr. Dawson became incredibly proficient in coding in a highly independent manner. These achievements underscore Dr. Dawson's intelligence and chemical intuition, as well as his motivation and strong work ethic. In these regards, Dr. Dawson truly is one of a kind.

Perhaps even more impressive than Dr. Dawson's technical skills are his personal attributes. His oral and written communication skills are excellent, as is his dedication to following through on commitments (for example, contributing to our planed manuscript while no longer employed by Professor Dabdub). He is hard working, professional, mature, and highly collaborative. Dr. Dawson also is both engaging and engaged. He can provide constructive feedback in an appropriate manner. To summarize, Dr. Dawson is the ideal member for almost any team. I am honored to also call him friend.

In short, due to the quality and strengths of the proposed work and the individual applying, I encourage you wholeheartedly and without reservation to provide support for Dr. Dawson's application. When I write letters such as this, I always ask myself if I would hire the individual for my own research group. In this case, the answer is undoubtedly and unequivocally yes; in

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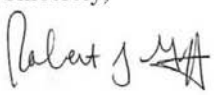
fact, I would consider myself incredibly lucky if Dr. Dawson were to join my group. I am confident you will have the same opinion once you have awarded him this Fellowship. If I can be of any further assistance, please do not hesitate to contact me.

Sincerely,



Robert J. Griffin, Ph.D.
Professor and Chair, Department of Civil and Environmental Engineering

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# ENDPAGE

MARIE SKŁODOWSKA-CURIE ACTIONS

## Individual Fellowships (IF)
## Call: H2020-MSCA-IF-2016

PART B

"ACRoNNIM"

**This proposal is to be evaluated as:**

**Standard EF**


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