REQUEST FOR A SPECIAL PROJECT 2012–2014

MEMBER STATE: …… FRANCE ………………….…………………………………………...…

Principal Investigator[1]: … Dr Virginie MARECAL ……………………………………………………………….……

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Dr H. Reide (Post-doc)
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Project Title: Modelling the impact on atmospheric chemistry of very short-lived species and volcanic emissions of halogens
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If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** _________________	
Starting year: (Each project will have a well defined duration, up to a maximum of 3 years, agreed at the beginning of the project.)		
Would you accept support for 1 year only, if necessary?	YES ☒	NO ☐

Computer resources required for 2012-2014: (The maximum project duration is 3 years, therefore a continuation project cannot request resources for 2014.)	**2012**	**2013**	**2014**
High Performance Computing Facility (units)	800 000 SBU	450 000 SBU	150 000 SBU
Data storage capacity (total archive volume) (gigabytes)	150	150	150

An electronic copy of this form ***must be sent*** *via e-mail to:* *special_projects@ecmwf.int*

Electronic copy of the form sent on (please specify date): …28/04/2011………………………… ………………

Continue overleaf

[1] The Principal Investigator will act as contact person for this Special Project and, in particular, will be asked to register the project, provide an annual progress report of the project's activities, etc.

Principal Investigator: Dr Virginie Marécal

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Project Title: Modelling the impact on atmospheric chemistry of very short-lived species and volcanic emissions of halogens

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Extended abstract

It is expected that Special Projects requesting large amounts of computing resources (500,000 SBU or more) should provide a more detailed abstract/project description (3-5 pages) including a scientific plan, a justification of the computer resources requested and the technical characteristics of the code to be used. The Scientific Advisory Committee and the Technical Advisory Committee review the scientific and technical aspects of each Special Project application. The review process takes into account the resources available, the quality of the scientific and technical proposals, the use of ECMWF software and data infrastructure, and their relevance to ECMWF's objectives. - Descriptions of all accepted projects will be published on the ECMWF website.

1. INTRODUCTION

Dr Virginie Marécal, who is the coordinator of this request for special projects, is a CNRS permanent researcher. She moved at CNRM/GAME (Météo-France) since September 2010. She has worked for the last 10 years and she is still working on the modelling of air composition using the limited-area coupled meteorological-chemistry C-CATT-BRAMS model. This model is optimized for parallel computers and is run operationally at CPTEC/INPE (Brazil) for air quality predictions over South America. The C-CATT-BRAMS was firstly implemented on the NEC Météo-France computer but its performances on this scalar computer are very poor and cannot be improved without major code modifications (as discussed with NEC user support). This is why the C-CATT-BRAMS was recently implemented on ECMWF IBM parallel computer on which it gives good performances. For these tests, we used SBUs that were attributed to Météo-France. These SBUs were not planned to be used for C-CATT-BRAMS simulations since it was not anticipated that the model will not work properly on Météo-France NEC computer. The present request, if accepted, will allow to perform the C-CATT-BRAMS simulations planned in the SHIVA and HEVA scientific projects (see below) in which CNRM/GAME is involved for the period 2012-2014. A late request form for a special project is submitted in parallel to this one to obtain SBUs for 2011. The extended abstract provided with each form is the same since it refers to the same scientific project. The difference is on the SBUs requested which depends on the year and which are detailed in Section 3.

2. SCIENTIFIC CONTEXT

Halogen reactive species from any source (anthropogenic or natural) are of particular interest for atmospheric chemistry. Their role on stratospheric ozone depletion is well established since the 1980's Reactive halogen sources were assumed so far to be long-lived natural and anthropogenic organic substances (mostly CFCs) (Wamsley et al. 1998). But recent studies have shown that additional sources (~30%) should be considered to explain bromine measurements in the stratosphere (Pfeilsticker et al. 2000, Salawitch et al. 2005, Dorf et al., 2008). These sources may come from Very Short-Lived Substances (VSLS) or volcanoes as stated in the World Meteorological Organization Scientific assessment of ozone depletion conducted in 2006 (WMO report 2007)**.** Observations show that atmospheric halogen loading is now decreasing and will carry on declining over half a century (Montzka et al., 2003; WMO, 2007), reflecting the control of CFC emissions by the Montreal Protocol and its Amendments. As a result, the contribution of VSLSs and volcanic halogens to the total halogen loading and hence to stratospheric ozone depletion is bound to become relatively more important in the future. In the troposphere, it was shown recently that halogen reactive species have an implication in the general oxidation power of the troposphere (von Glasow et al. 2004, Lary 2005, Yang et al. 2005). The contribution of volcanoes to the reactive halogen compound content at the global scale is identified to be one of the objectives to be reached in the future (von Glasow et al., 2009; HitT project of IGAC (International Global Atmospheric

Chemistry)).

The CNRM/GAME (Centre National de Recherches Météorologiques/Groupe d'étude de l'Atmoshère Metéorologique) is involved in two projects addressing these issues. The first one is the SHIVA European project devoted to the study of halogen VSLSs. The second one is on volcanic emissions (HEVA) and is funded by INSU/CNRS (Institut National des Sciences de l'Univers/ Centre National de la Recherche Scientifique). These projects will provide important results on the role of halogen VSLS and volcanic (emissions, transport and chemistry processes) on tropospheric air composition at local and regional scales. These processes will then be included in MOCAGE and C-IFS models in the frame of the MACC-2 project lead by ECMWF.

2. SCIENTIFIC PLAN

2.1 SHIVA European Project

The FP7 European project SHIVA (Stratospheric ozone: Halogen Impacts in a varying Atmosphere http://shiva.iup.uni-heidelberg.de/) is coordinated by the University of Heidelberg and funded for 3 years until June 2012. An extension of 1 year will be requested and is very likely to be accepted.

The main objectives of the project are to quantify natural emissions (mainly from oceans) of halogen VSLSs and to study their impact on stratospheric ozone. The CNRM-GAME objective in the project is to perform local and regional process studies (chemistry and transport) of the evolution of VSLS in the troposphere and in the lower stratosphere based on a modelling approach. This work will be done in link with field campaign measurements planned in November 2011 in Malaysia and Chemistry-Transport Model (CTM) studies in collaboration with Dr M. Chipperfield (Univ. Leeds, UK). More precisely, the C-CATT-BRAMS (Freitas et al. 2009) will be used to simulate several case studies of the field campaign in convective environments using a chemistry scheme (89 gaseous species) including tropospheric chemistry (RACM scheme, Stockwell et al. 1997) and chemistry for $CHBr_3$ and CH_2Br_2 (Hossaini et al. 2010) which are the most abundant halogen VSLSs. We will use the grid nesting capability of the model in order to make process studies at the local scale and comparisons at the regional scale with global CTM results for validation purposes. The model developments to include halogen VSLS chemistry in the C-CATT-BRAMS are done. A publication on first results obtained with this new scheme in an idealised framework is currently under preparation (to be submitted to Geophys. Res. Lett.).

In practice, Dr V. Marécal (permanent CNRS researcher at CNRM/GAME) is in charge of C-CATT-BRAMS modelling work which is done in collaboration with Pr M. Pirre (Laboratoire de Physique et Chimie de l'Environnement et de l'Espace, Orléans, France). A 20-month post-doc will work at CNRM/GAME on the C-CATT-BRAMS modelling under V. Marécal's supervision from September 2011.

2.2 HEVA project

The HEVA (Halogen Emissions from Volcanoes and their impact on Atmospheric chemistry) project is coordinated by V. Marécal (CNRM/GAME) and is currently funded by INSU/CNRS for 3 years until 2012. A proposal for additional funds (4 years) to continue the project was submitted to ANR (Agence Nationale pour la Recherche) in January 2011. The ANR decision should be known by June 2011.

The objectives of HEVA are to produce the first geographical inventory of halogen emissions by volcanoes and to study their impact on tropospheric chemistry and, potentially, on the ozone budget in the stratosphere including its feedback on climate. It is based on a pluri-disciplinary consortium associating specialists in volcanology and in atmospheric chemistry. Detailed studies at the local and regional scales in volcanology and atmospheric chemistry will be done for three volcanoes at different latitudes during periods for which emission fluxes and air composition of plumes close to and/or far from the crater are available: Etna (Italy), Eyjafjallajökull (Iceland) and Ambrym (Vanuatu). These local studies will be used for extrapolation at the global scale.

In this project the CNRM/GAME is in charge of the atmospheric chemistry modelling studies at the local and regional scales based on the C-CATT-BRAMS model. This model will be used to study the chemical evolution of the volcanic halogen emissions in the atmosphere for the three selected volcanoes/events. The results will be compared to those obtained by the global CTM MOCAGE (Josse et al. 2004, Bousserez et al. 2007) used operationally at CNRM/GAME. As for SHIVA, grid-nested simulations will be run for comparisons with MOCAGE.

Halogen species emitted by volcanoes are mainly in the form of inorganic hydrogen halides HCl, HBr, HI (Oppenheimer et al, 1998). Due to their high water solubility it was assumed that they were rapidly removed by precipitation and had only local effects. However, high levels of reactive halogen BrO (Bobrowski et al., 2003, Oppenheimer et al. 2006) were observed recently in volcanic plumes. 0D-modelling studies (e.g. Roberts et al. 2009) have shown that they are rapidly generated from HBr, HCl and Br emissions by heterogeneous reactions on sulphate aerosols also emitted by volcanoes. A plume chemistry module was implemented in both MOCAGE and C-CATT-BRAMS model and is currently tested. The chemistry scheme used in C-CATT-BRAMS for this project includes RACM scheme (Stockwell et al. 1997) and inorganic halogen chemistry (88 species in total).

In practice, Dr V. Marécal is in charge of the C-CATT-BRAMS modelling work which is done in collaboration with B. Josse (CNRM/GAME) and Pr M. Pirre and Dr L. Jourdain (Laboratoire de Physique et Chimie de l'Environnement et de l'Espace, Orléans, France). She will work on the C-CATT-BRAMS simulations of the Etna case study. A post-graduate student (L. Grellier) will work on the C-CATT-BRAMS modelling of the Eyjafjallajökull's eruptions in the frame of her thesis to be started in October 2011 (3 years-funds already obtained).

3. SIMULATIONS PLANNED AND COMPUTING RESOURCES NEEDED

Since detailed studies at the local and regional scales are required in SHIVA and HEVA the simulations planned in both projects will include up two to three nested grids with typically 130x130x45 grid points, ~90 gaseous species. Simulations will be run for 4 to 7 days. A reference simulation without the VSLS (resp. volcanic emissions) is required to study the impact of VSLS (resp. volcanic emissions). For SHIVA at least two case studies from the field campaign will be simulated. Sensitivity tests on the VSLS chemistry scheme which is still not fully explored will be done. For HEVA, simulations for Etna and Eyjafjallajökull will be run at CNRM/GAME, those for Ambrym being done at LPC2E. Major sources of uncertainty in HEVA are the quantification of the halogen emissions from volcanoes and the chemistry within the plume. Therefore sensitivity tests on these two aspects will be done.

The C-CATT-BRAMS model is a code developed and optimized for both operational and research applications that can be run on massively parallel computers (MPI). It is used operationally at CPTEC (http://meioambiente.cptec.inpe.br, Brazil) for air quality forecasts. It is based on the BRAMS meteorological model (Brazilian Regional Atmospheric Modeling System, Freitas et al. 2009) which can be run with horizontal resolutions spanning from a few meters to several hundreds kilometers. It is mainly coded in Fortran 90. For parallelism the model divides the geographical domain in sub-domains with a master node configuration.

The C-CATT-BRAMS model has been recently implemented on ECMWF IBM Power 6 computer. The reference simulation for HEVA project without volcanic emissions was run with 2 nested grids (130x80x44 grid points for the coarse grid and 192x142x44 grid points for the fine grid) over two days. It required 6770 SBU per 24 hours of simulation on 2 nodes of 64 processes.

For the whole SHIVA project from 2011 to 2013, it is planned to run a reference simulation without VSLS, a simulation with the VSLS and 6 sensitivity tests on the chemistry scheme and on the emissions. Each simulation will use 3 nested grids over 4 days and is estimated ~40 KSBU. It is anticipated to make simulations for two case studies. The total of these simulations leads to 640 KSBU.

For the whole HEVA project from 2011 to 2014, it is planned to run for Etna and for Eyjafjallajökull a reference simulation without volcanic emissions, 8 simulations with minimum and maximum estimates of volcanic emissions of HBr, HCl and SO_2 and with different assumptions in the plume chemistry. Each simulation will use 3 nested grids over 7 days for Etna and 5 days for Eyjafjallajökull and is estimated ~70 KSBU for Etna and ~50 KSBU for Eyjafjallajökull. The total of these simulations leads to 1080 KSBU.

The planned repartition for each year is :

2011: 320 KSBU
2012: 800 KSBU
2013: 450 KSBU
2014: 150 KSBU
We thus request here 800 KSBU for 2012, 450 KSBU for 2013 and 150 KSBU for 2014.

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