REQUEST FOR A SPECIAL PROJECT 2018–2020

MEMBER STATE: The Netherlands

This form needs to be submitted via the relevant National Meteorological Service.

Principal Investigator[1]: Vincent Huijnen

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Project Title: Chemistry and aerosol processes modelling within IFS in extension to CAMS activities (SPNLCAMS)

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** NLMACC → SPNLCAMS	
Starting year: (A project can have a duration of up to 3 years, agreed at the beginning of the project.)	2018	
Would you accept support for 1 year only, if necessary?	YES X	NO ☐

Computer resources required for 2018-2020: (To make changes to an existing project please submit an amended version of the original form.)		**2018**	**2019**	**2020**
High Performance Computing Facility	(SBU)	1500k	1700k	1900k
Accumulated data storage (total archive volume)[2]	(GB)	2TB	5TB	9TB

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):

……………………………………………

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.

[2] If e.g. you archive x GB in year one and y GB in year two and don't delete anything you need to request x + y GB for the second project year.

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Extended abstract

Within the Copernicus Atmosphere Monitoring Service (CAMS) a module for tropospheric chemistry originally based on the TM5 model (Huijnen et al., 2010), integrated in the Integrated Forecasting System (IFS), is providing routine analyses and forecasts of atmospheric chemistry (Flemming et al., 2015; Inness et al., 2015; Flemming et al., 2017). An extension of this CB05-chemistry with BASCOE for the stratosphere (Huijnen et al., 2016a) is expected to become operational in the near future, to expand the ability of the system in terms of stratospheric composition. Resulting from these efforts KNMI takes the lead within the CAMS tender on reactive gases modelling and assimilation (CAMS_42) in a consortium to support further development of the system. This concerns aspects relatively close to operations, such as support to operational upgrades, implementation and testing of mature sub-modules (on-line dry deposition, chemistry-aerosol interaction), and provision of a mini-model ensemble existing of three independent implementations of atmospheric chemistry (C-IFS-CB05BASCOE, C-IFS-MOCAGE, C-IFS-MOZART).
However, CAMS_42 does not cover any spin-offs from these 'near-operational' tasks, in terms of progress in scientific terms, e.g. investigations of the benefit of an ensemble-approach, sensitivity studies of dry deposition, or improved interaction with aerosol modelling.

This special project aims to provide us with in the computer resources needed to execute such science-related aspects. This is essential to consolidate sufficient quality of the modelling system over the long term and to exploit the availability of this advanced system for scientific purposes, as done in the past for instance for an analysis of the 2015 peatland fires in Indonesia (Huijnen et al., 2016b). Topics currently foreseen to be considered in this special project are described below.

1. Whereas a baseline version of full stratospheric chemistry has now been established within the IFS, there are important open questions remaining, deserving dedicated attention. The basic idea is to benefit from strengths of parameterizations originally developed for the troposphere (stratosphere) for application in the stratosphere (troposphere). These include:
    - Investigation of the benefits of an extension of representation of trace gases already modelled in stratosphere towards the troposphere (e.g., application of chlorine chemistry in troposphere, potentially affecting the methane lifetime)
    - Extension of parameterizations available in the tropospheric module for the stratosphere. An example here is an investigation of the benefits of cloud effects on stratospheric (NO_2) photolysis rates, and in turn composition, as available from the tropospheric chemistry module.
    - An assessment of the quality of the stratospheric water vapour, as governed by stratospheric chemistry, in comparison to existing, operational parameterizations within the IFS. Better constraints on stratospheric H_2O in operational model versions could potentially contribute to improved IFS meteorological forecasts skills on weekly to seasonal time period. In line with such a study also the quality of modelled stratospheric CH_4, together with its loss term, will be closely assessed.

2. A further integration of the chemistry module available within IFS with the existing aerosol schemes available within CAMS is foreseen:
    - Although already a closer integration within the GLOMAP representation of aerosol (Mann et al., 2010) was considered during the previous special project

(SPNLMACC), this has so far not been achieved, mainly due to delays in the integration of the GLOMAP scheme within IFS. As part of the current special project request we foresee again that efforts are needed for such testing integration. Specifically we aim to implement and evaluate a stratospheric sulfate chemistry to act as precursor for stratospheric aerosol.

- During SPNLMACC first steps have been made regarding the introduction of a module representing secondary organic aerosol (SOA). Production from biogenic and anthropogenic sources have been introduced, based on a simplification of the Tsimpidi et al. (2014) scheme. As part of this special project a further development and testing of this module is foreseen.

3. This request for computer resources also aims to support any additional scientific items to be picked up during the course of this special project, such as was the case for the Peatland Fire case (Huijnen et al., 2016b). Specifically, we plan to re-evaluate this situation, with focus on the assessment of the sensitivity to OH (and in turn methane lifetime) for different assumptions of the GFAS-emissions (specifically the NOx and VOC emissions).

Computational expenses

In the current standard model setup C-IFS-CB05BASCOE, in conjunction with the aerosol module, is run with a 0.5-hour time step on a resolution of T255L60 (which corresponds to a horizontal resolution of approx. 0.7 deg). In this setup the total billing units for a one-year hindcast simulation are estimated to be approx. 120 kSBU; producing approx. 200 GB of data on the MARS archive. Additional costs are expected with an increase in vertical resolution of the model to T255L91, upon following the standard IFS resolution in more recent model cycles. This would imply increases of billing units by 50% and higher. On the other hand, more efficient system setups (e.g. optimizing model output requirements, or switching on only specific sub-modules rather than the full-blown atmospheric composition system) can accommodate some of these expected increases.
Considering the current uncertainty of the specifications of future model runs, it is difficult to estimate the total resources required for the full period of this special project. Here we assume that about an equivalence of 20 one-year hindcasts will be executed in every year, with computational expenses of, on average, 100 kSBU per year. (In practise we foresee that there will be many more short runs executed at the expense of a few long hindcast runs.) This adds up to a total of approx. 2MSBU annually needed, and ~4 TB of data storage needs. Such annual hindcast runs are used as benchmark specific system setups, and execute various sensitivity experiments in support of the research topics as listed above. Part of these runs can be accounted for from the CAMS budget, wherever associated to developments close to operational support, therefore requesting here only for a fraction of these resources.

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