# REQUEST FOR A SPECIAL PROJECT 2015–2017


**MEMBER STATE:** Netherlands

**Principal Investigator[1]:** Dr. V. Huijnen

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**Project Title:** Inline chemistry for tropospheric and stratospheric trace gases in IFS

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|---|---|---|
| If this is a continuation of an existing project, please state the computer project account assigned previously. | **SP** NLMACC | |
| Starting year:<br>(Each project will have a well defined duration, up to a maximum of 3 years, agreed at the beginning of the project.) | 2015 | |
| Would you accept support for 1 year only, if necessary? | YES X | NO ☐ |

| **Computer resources required for 2015-2017:**<br>(The maximum project duration is 3 years, therefore a continuation project cannot request resources for 2017.) | **2015** | **2016** | **2017** |
|---|---|---|---|
| High Performance Computing Facility (units) | 700k | 800k | 900k |
| Data storage capacity (total archive volume) (gigabytes) | 250 Gb | 300Gb | 350Gb |

*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.

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# Extended abstract

Within the past EU projects MACC and MACC-II a system has been developed where chemistry schemes originating from various Chemical Transport Models (CTM's), such as from the TM5 model (Huijnen et al., 2010), have been implemented into the ECMWF's Integrated Forecasting System (IFS). This extended version of IFS is referred to as Composition-IFS (C-IFS), which has been developed in close collaboration with ECMWF staff. This has resulted in a well-tested system for providing hindcasts and forecasts of tropospheric composition (Huijnen et al., 2014; Eskes et al., 2014). During summer 2014 C-IFS will start providing semi-operational analyses and forecasts of reactive gases for MACC, replacing the predecessor system. In this earlier setup of the MACC system, CTM's, such as TM5 and MOZART, were coupled to the IFS, where both the CTM and IFS were running side-by-side, Flemming et al. (2009). In contrast to those systems, the C-IFS, where photochemistry is an integral part of the IFS, allows for enhanced computational efficiency, and numerous unexploited physical interactions. In this special project we aim to improve the current C-IFS system and explore new interactions with other physical and chemical aspects, to support the work performed in the MACC-III and forthcoming projects in the framework of the Copernicus Atmospheric Service.

1. The current version of C-IFS contains tropospheric photochemistry based on a modified version of the Carbon Bond mechanism (CB05), while for stratospheric composition it fully relies on data assimilation in combination with climatologies of trace gas distributions. To improve on this we are working on an extension of the C-IFS-CB05 model version with chemistry originating from the Belgian Assimilation System for Chemical ObsErvations (BASCOE, www.bascoe.oma.be). A first aim will be to extend the ability of the C-IFS system to forecast realistic tracer concentrations during ozone hole conditions. Similar to experiences with the development of C-IFS-CB05, we plan to benchmark the C-IFS-BASCOE system as compared to the BASCOE offline system and ensure stable, and well understood model performance. Next, we will merge the stratospheric chemistry with the existing tropospheric chemistry scheme. This implies a doubling in the amount of modelled chemical tracers, and hence a significant increase of the computational costs as compared to C-IFS-CB05 or C-IFS-BASCOE alone. We plan to investigate on efficient methods to merge tropospheric with stratospheric chemistry schemes, e.g. by calling different solvers for the tropospheric and stratospheric regions separately. Also we want to investigate the impact of including tropospheric chemistry and emissions to the stratospheric trace gas distributions, such as methane and $N_2O$ and their impact on stratospheric $H_2O$, and $NO_2$, respectively.
2. A second line of developments concerns the implementation and testing of the Kinetic PreProcessor (KPP, Sandu and Sander, 2006) wich will provide the chemical solver for C-IFS. KPP allows for a much more efficient development stream for chemical mechanisms, by providing an interface between a human-readable specification of the chemical model and the actual fortran code for the solver, as applied in the IFS. At the same time KPP can provide an adjoint of the solver, allowing for backward computations as required for data-assimilation applications. Application of the KPP framework will directly simplify an integration of the tropospheric chemistry with reactions with specific trace gases, such as chlorine and bromine, that are introduced originally for the stratospheric chemistry.
   Nevertheless, before more general use, various issues need to be resolved. First of all, the computational efficiency may need special care, e.g. by carrying through a vectorization of the solver code. Also the stability of the chemical solver needs to be ensured. Finally, the performance of the KPP solver with respect to the resulting tracer composition needs to be investigated in detail, as compared to reference C-IFS runs with the original chemical solver.

3. In earlier work the C-IFS-CB05 model has been coupled to the existing MACC aerosol model to study the impact of aerosol fields upon tropospheric composition, through modified photolysis and heterogeneous reaction rates (Huijnen et al., 2014). As part of this special project we foresee an implementation and testing of a similar coupling to the follow-up aerosol model 'GLOMAP' (Mann et al., 2010). Also we plan to consider the evaluation of a reversed interaction, where the impact of tropospheric chemistry on aerosol composition is investigated. In this respect we focus on sensitivity of aerosol composition to modelling assumption of aerosol precursors, as well as the oxidizing field. Finally, a coupling to the MACC $CH_4$ fields needs to be established and further investigated. The impact of using the CH4 analyses on reactive trace distributions will be investigated in more detail.

**Computational expenses**

In the current standard testing setup, C-IFS-CB05 is run with a 1-hour time step on a resolution of T159L60, which corresponds to a horizontal resolution of approx. 1.1 deg. In this setup the total billing units for a one-year hindcast simulation are estimated to be approx. 18 kSBU. With a doubling of the number of chemical tracers (merging CB05 chemistry with BASCOE), the costs increase accordingly to ~35 kSBU. Similar increases can be expected in runs where an aerosol model is run in conjunction with the tropospheric chemistry.

Additional costs are expected with an increase in horizontal and 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 up to 4-fold and higher. On the other hand, more efficient system setups (e.g. splitting the simulation into longer hindcast periods with nudged meteorology) 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, 40kSBU per year. This adds up to a total of 800kSBU annually needed. 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. In practise we foresee that there will be many more short runs executed at the expense of a few long hindcast runs.

**References**


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