

Proposal to ISSI (2013 call):
International Teams in Space and Earth Sciences

Study group on the added-value of chemical data assimilation in the stratosphere and upper-troposphere

Abstract

The past two decades, 1990-2010, have been something of a “golden age” for stratospheric chemical observations. The Odin satellite from SNBN, the ENVISAT mission from ESA and NASA missions UARS and EOS-Aura have provided an unprecedented coverage (spatial, temporal) of the stratosphere chemistry and dynamics. These missions were designated with a focus on addressing the effect of man-made changes in atmospheric composition and its implication to climate change. These missions have provided measurements of a large number of chemical species, both long-lived and short-lived, that are critical to conduct scientific studies. The integration of measurements and atmospheric predictive models can be done through a technique known as data assimilation. It is quite remarkable that although data assimilation has been applied to a wide range of geophysical problems, the assimilation of those observations into chemical transport models has been rather scarce and has hindered the additional value those observations could provide. As we have seen lately a change in research priorities of the principal funding agencies towards moving to troposphere chemistry, the necessity to facilitate the research and gathering of scientists in the field becomes even more pressing.

We propose to form a multidisciplinary team of scientist in observation studies, chemical modeling and processes (all of which are familiar with data assimilation) to work with a team of chemical data assimilation experts. One of the host Institute, the Belgium Institute for Space Aeronomy (BIRA), have developed one of the best stratospheric chemical data assimilation system known, and which can handle the assimilation of both long-lived and short-lived species. The assimilation system implemented at BIRA is based on the most advanced techniques in the field, namely 4D Var and the ensemble Kalman filter. These systems can not only assimilate long-lived species, but also provide error estimates, and be adapted to improve knowledge of parameter of the model. Several scientific areas of research have been identified in this proposal, which are either promising or have shown already scientific value with less comprehensive assimilation systems. Overall, this is a timely proposal that will help reduce the gap of uncertainties and enhance our knowledge of the stratosphere.

Scientific rationale, Goals

Data assimilation has been developed originally by the meteorological community to provide initial conditions to atmospheric models for weather forecasting. It is based on a statistical optimal method of combining observations and model of the atmosphere to find the best estimate of the atmospheric state. This optimal state or *analysis* has in principle uncertainties that are lower than the model or the observations taken separately. Data assimilation provides an estimated state that is closer to the truth, yet with a physical, spatial and temporal consistency. The success of data assimilation has triggered its application to a wide range of geophysical problems, and in the late 90's we started to see some developments of chemical data assimilation in the stratosphere, but then the focus turned onto tropospheric chemistry motivated primarily by air quality monitoring and forecasting. Chemical data assimilation can lead as well to chemical consistency, having the ability for example to reduce the model uncertainty of non-observed species, provided the necessary coupling in the assimilation system are established (yet this issue have received little attention so far). In the stratosphere, ozone forecasting and having an accurate representation of the chemical state of the atmosphere are important issues, but there is additionally a focus on processes and improving models, and this requires a dedicated assimilation effort.

There are several tasks that have been identified for the proposed study:

1. Development of a multi-year analysis of the stratosphere.

Data assimilation provides a tool to integrate observation data consistently into an atmospheric model. The Odin mission has started in 2001, the ENVISAT mission in 2002 and the Aura mission in 2004. ENVISAT end in 2012 while both other instruments are continuing. These three missions together have provides observations of dozen chemical species, including long lived (e.g. N₂O) and short lived (e.g. BrO). As done in meteorology, a chemical reanalysis of the stratosphere would be a useful product for the community. For example, it would provide initial conditions to trajectory models or boundary conditions for regional models. We have identified two challenges for such a reanalysis: (1) the day to day consistency of the reanalysis with respect to the operation of the instruments and (2) the biases between the different datasets. For example, for the first case, how the MIPAS data gaps between 2004 and 2006 would affect the quality of the reanalysis? For the second case, the situation is less clear. The meteorological community has developed methods to correct biases between different assimilated datasets but there are less experiences with bias correction schemes in chemistry. For example, in the ERA-Interim reanalysis, Dee et al. (2011) use radiosonde temperature measurements to anchor the radiance satellite observations. Development of bias correction scheme for stratospheric chemical datasets is then on of the expected output of this ISSI international team.

2. Estimation of the impact of high energy particles in the upper stratosphere

It has been known for a long time that the main source of global stratospheric NO_x is the oxidation of N₂O from the troposphere. However, energetic particle precipitation (EPP)

is considered as the most important secondary source. These particles are either high energetic electrons or protons that can produce NO directly in the stratosphere if their energies are respectively greater than 300 keV and 30MeV (Randall et al., 2006). EPP, solar and galactic cosmic rays which penetrate into the polar middle atmosphere at high latitudes give rise to ionization, dissociation, dissociative ionization and excitation processes (Brasseur and Solomon, 2005; Jackman et al., 2008). Evidence of high amounts of upper stratospheric and mesospheric polar NO₂ and anomalous values of HNO₃ as measured by the MIPAS/ENVISAT mission (Fischer and Oelhaf, 1996; ESA, 2000; Fischer et al., 2008) have been documented in the recent literature (Funke et al., 2005; Orsolini et al., 2005; Stiller et al., 2005; Verronen et al., 2008). Anomalous but continuous downward transport of these chemical constituents from the mesosphere and lower thermosphere (MLT) region into the upper stratosphere has been analysed with a 3D Var chemical data assimilation system by Robichaud et al. (2010). Here we propose to continue this study with an advanced data assimilation system. This might be also true to study the effect of PSC during polar winter of by the descent of mesospheric NO_x. With assimilation, it would be possible to optimize the source of mesospheric NO_x which might be useful by other models like CCMs.

3. Inferring information about unobserved chemical species.

Multivariate chemical assimilation can provide information about non-observed species from the chemical consistency provided by the chemical assimilation system. So far, there has been little studies on this subject, primarily because the assimilation systems used so far were tailored towards the assimilation of long-lived species which are not directly chemically related. It is practically not possible in this context to infer information about unobserved species. However, we have seen application in other geophysical fields using ensemble Kalman filtering where unobserved parameters were retrieved. The application of the ensemble Kalman filter methodology to atmospheric chemistry, and in particular the stratosphere where there is a vast number of chemical species observed, both long-lived and short-lived offers a unique ground to develop this new capability. This is a promising area of development which could bridge important chemical information and optimize the information content between models and observations. The expertise developed in the stratosphere where the number of chemical species observed is significant, would benefit troposphere problems where the number of species observed is lot more restricted.

4. Optimizing model parameters

Satellite observations in conjunction with an advanced data assimilation scheme such as the ensemble Kalman filter is useful to optimize model parameters, and not only the model states. For example, the production of N and NO during SPE is usually parameterized using commonly cited values of 0.55 N atoms and 0.7 NO molecules per ion pair (e.g., Jackman et al., 2005). Using this parameterization, ECHAM5/Messy model (Baumgaertner et al., 2010) failed to reproduce accurately MIPAS nitrogen observations during the 2003 Halloween SPE. In order to improve their simulation, they were able to tuned the parameterization of N/NO production based on chemical box model results. Assimilation methods would be very useful to use nitrogen observations (e.g. from MIPAS) to adjust, in addition to the model state, (some) model parameters like those

used to simulated nitrogen production during SPE. This is possible with both 4D-Var and EnKF method, although the implementation in 4D-Var is more complex due to the adaptation of the adjoint model. We have provided here the example of N/NO production by SPE but there are other cases where model parameter estimations would be very useful. For example, we also plan to conduct parameter estimates to determine the sulfate aerosols in the polar vortex. The surface area density of sulfate aerosols is inputs of several heterogeneous reactions include in the model. With an improved estimate of sulfate aerosol densities, a more precise evaluation of the ozone loss in the polar vortex can be performed.

5. Ozone predictability and radiative impact

The UTLS is a region where the atmosphere cools to space and so knowledge of the distribution of the radiative gases is important (e.g., PREMIER: Reports for Assessment, ESA SP-1313(5), ISSN 0379-6566, 121pp. In the tropical tropopause layer (TTL) while the net radiative heating is quite small it is nevertheless made up of several small terms which are important (Liou, 2002). In such conditions, the radiative feedback from the assimilation of ozone, methane, nitrous oxide and aerosols can be significant and can contribute to the improvement of medium range temperature forecasting. Species radiative feedback occurs through absorption and emissions processes in both solar and IR spectral regions and through other indirect mechanisms such as methane oxidation which contributes ~ 50% to the water vapour distribution in the upper stratosphere. These complex interactions need to be evaluated in detail to better understand the coupling between Greenhouse gases and the meteorology throughout the region. The radiative impact of ozone is particularly significant throughout the UTLS and has been investigated in several NWP centres. Several studies (Ménard et al., 2007 ;de Grandpré et al.,2009 and Rochon et al., 2011) show that the incorporation of the ozone radiative feedback in the EC NWP system has a significant impact on medium range temperature forecast which maximizes around 50 hPa. The impact is beneficial throughout the lower stratosphere but poor ozone values can contribute to the deterioration of the results at the tropopause where temperature biases in the forecast are significant (Charron et al., 2012). Such results suggest that the incorporation of species radiative feedback in NWP systems require a new evaluation of the model so that existing model biases in parameterization schemes do not counteract the potential benefits associated with the assimilation of composition information. Of course, the quality of the assimilation process is also limited by the quality of the measurements being ingested which are often sparse and sometimes restricted to integrated quantities such as total column ozone. Indeed, nadir viewing instruments which generally represent the main source of chemical observations within present operational data assimilation systems do not provide the necessary information to resolve species gradient at the tropopause where radiative heating is, while small, nevertheless important. Such analysis shows that further understanding of processes in the stratosphere and UTLS regions is needed before implementing the radiative feedback from ozone in operational NWP systems

The Modus Operandi of the study group can be envisioned as follows. We have gathered experts that can be divided into closely interacting sub-groups: an observation group, a modeling and process group, and an assimilation group. The Belgium Institute for Space

Aeronomy currently possesses one of the most advanced chemical data assimilation systems in the world, consisting in a four-dimensional variational system (4D Var) and a Monte Carlo assimilation system (Ensemble Kalman filter) that uses the same chemical transport model, and that can be used either in tandem or in a complementary way. The scientific user group will provide the insight and evaluation of the assimilation products. They will guide the assimilation experiments in the context of adding value to the observations. The synergy provided by these groups should be able to advance the field of chemical data assimilation and address scientific objectives.

Timeliness

The last few decades represent something of a “golden age” of stratospheric composition measurements. And now the funding agencies have turned their priorities to tropospheric chemistry. A wealth of observational data is available and it is time to capture knowledge on atmospheric composition and processes by using the most sophisticated method - data assimilation. Chemical data assimilation has now reached a maturity where it can now deliver chemically consistent estimates, of both long- and short-lived species, provide error bars to those estimates, and adjust model parameters so as to improve our knowledge of the processes that affect the stratosphere. This is a timely proposal and will further provide further momentum to build scientific collaborations towards this goal.

Expected outputs

The main goal of the project is to publish a special issue in a scientific journal – probably ACP (Atmospheric Chemistry and Physics). The plan is to establish the anticipated papers very early in the project so that the research can go in a timely fashion. Results of the proposed project will also be presented at multiple national and international conferences such as EGU, AGU, and SPARC Data Assimilation workshop.

The ultimate goal of this project is to provide momentum to the stratospheric chemical data assimilation community to develop its full capability to deliver science to the community. This is something we have seen in other geophysical areas, but has been lacking in this field because of a lack of concerted effort. This actually leads us to the next topic.

Added value of ISSI

At this time, where the funding agencies are turning their priorities lower down into the troposphere, this proposed project can't be more timely. ISSI offers a real opportunity to make a change to this situation, by providing a well structured environment where a team of multidisciplinary experts can collaborate with chemical data assimilation experts, and data assimilation experts would tailor their experiments so as to yield relevant information to the scientific community. Both communities would actually benefit from this close collaboration.

List of confirmed participants and their area of expertise

- Richard Ménard (EC), Coordinator. Expert in data assimilation theory and in chemical data assimilation. Has lead or been involved in several international research project. He is also responsible for operational implementation in NWP systems
- Quentin Errera (BIRA-IASB) , co-leader, expert in 4D-Var chemical data assimilation and PI of the BASCOE system
- Simon Chabrilat (BIRA-IASB), expert in CTM modeling
- Jean de Grandpré (EC), expert in radiative effect, assimilation of stratospheric ozone
- Michaela Hegglin (Univ. of Reading), expert in observational data. She also lead an ISSI project on trace gas intercomparison
- Yvan Orsolini (NILU), Expert in middle atmosphere dynamics and chemistry,
- Sergey Skachko (BIRA-IASB), responsible of the BASCOE EnKF version
- Michiel van Weele (KNMI), expert in radiation modeling, chemistry-climate interaction. Currently involved in the implementation of C-IFS in the MACC project

Schedule of the project

September 2013.	First teleconference to assign responsibilities and further define the tasks
End of fall 2013.	First meeting at ISSI. Presentations of preliminary studies. Establish a definite plan of research, and assimilation tasks to be performed.
Winter-Spring 2014. Fall 2014	Regular teleconferences on the progress of assimilation runs. Second meeting at ISSI. Status report on each task, discussion on the next steps, outlining the publications, writing report.
June 2015	Final report to ISSI / Submission of papers towards the special issue (if not earlier)

Facilities required

For the two meetings at ISSI we will require a room large enough to accommodate around 10 people, preferentially in U-shaped seating. It would be helpful if the tables could be rearranged so as to allow for discussions in smaller groups. While participants will bring their own laptops, a computer projector and a screen will be needed for presentations. Wireless internet connection will be needed for all participants to allow access to data bases and electronically available literature. Water/coffee/tea for refreshment during the meeting would be highly appreciated.

Financial support requested of ISSI

We request from ISSI per diem for each of the participants for 5-7 days to cover living expenses during the two meetings in Bern. We also request coverage of the travel costs

(plane and ground transportation) for the team leader. If possible, we would also like to invite one additional expert (from the modeling or data analyses community) per meeting, for whom we would ask for a per diem as well. His/her attendance however cannot be guaranteed in advance.

Contact of all participants (included in the CV)

CVs

CURRICULUM VITAE - Richard Ménard (Coordinator)

Senior Research Scientist

Air Quality Research Division, Environment Canada

Tel: 514 421-4613, Fax: 514 421-2106

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Education

Ph.D. Atmospheric and Oceanic Sciences. Mc Gill University (1994)

M.Sc. Meteorology, Mc Gill University (1985)

B.Sc. Physics. Université du Québec à Montréal (1983)

Professional experience

2000 – present. Senior research scientist, Environment Canada

Lead the effort in chemical data assimilation in Canada, both at the government and in collaboration with the Universities.

Principal investigator of a ESA study on dynamical-chemical coupling in modelling and data assimilation.

Member of the Stratospheric Dynamic Mission Advisory Group and currently of Mission Assessment Group of TRAQ.

1997-2000 Assistant Research Professor, NASA Data Assimilation Office and JCET/University of Maryland Baltimore County. Development of Kalman filter algorithms for the assimilation of stratospheric tracers observations. Assimilation of stratospheric winds from HRDI/UARS.

1994-1997 USRA Goddard visiting scientist. Implementation of Kalman filter algorithms. Error characterization in assimilation of retrievals.

Selected publications

Skachko, S., Q. Errera, R. Menard, S. Chabrillat, and Y. Christophe, 2013: Comparison of ensemble Kalman filter and 4D Var methods in the context of stratospheric chemistry data assimilation. *Submitted to Geophys. Model Devel.*

Errera, Q, and R. Ménard, 2012: Technical Note: Spectral Representation of Spatial Correlations in Variational Assimilation with Grid Point Models and Application to the Belgian Assimilation System for Chemical Observations (BASCOE), *Atmos. Chem. Phys.*, **12**, 10015-10031, doi:10.5194/acp-12-10015-2012.

R. Lindenmaier, et al., 2011: A Study of NO_y budget above Eureka, Canada, *J. Geophys. Res.*, **116**, D23302, 17 pp, doi:10.1029/2011JD016207

Co-editor of the Book *Data Assimilation: Making sense of observations*. (eds. Lahoz, W, Khattatov, B, and R. Menard) 2010, Springer-Verlag, 728 pp.

Ménard, R., 2010: Bias estimation. In *Data Assimilation: Making Sense of Observations* (eds. Lahoz, W., B. Khattatov, and R. Ménard), Springer, New York, 113-136.

deGrandPre, J., R. Menard, S. Chabrillat, C. Charette, Y. Rochon, and A. Robichaud, 2008: Radiative impact of ozone on temperature predictability in a coupled chemistry-dynamics data assimilation system. *Mon. Wea. Rev.*, **137**, 679-692.

Khattatov B.V., J.-F. Lamarque, L.V. Lyjak, R. Ménard, P. Levelt, X. Tie, G.P. Brasseur, and J.C. Gille, 2000: Assimilation of satellite observations of chemical species in global chemistry-transport models. *J. Geophys. Res.*, **105**, 29,135-29,144.

Ménard R., S.E. Cohn, L.-P. Chang, and P.M. Lyster, 2000: Assimilation of stratospheric chemical tracer observations using a Kalman filter. Part I: Formulation. *Mon. Wea. Rev.*, **128**, 2654-2671.

Ménard R., and L.-P. Chang, 2000: Assimilation of stratospheric chemical tracer observations using a Kalman filter. Part II: Chi-square validated results and analysis of variance and correlation dynamics. *Mon. Wea. Rev.*, **128**, 2672-2686.

Quentin ERRERA (co-Coordinator)

Staff Scientist at the

“ Belgisch Instituut voor Ruimte-Aeronomie - Institut d’Aéronomie Spatiale de Belgique”

BIRA-IASB

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Male

Belgian Citizenship

Born in Uccle, Belgium on 6 March 1970

Research at BIRA-IASB since 1995

1995-1998: Development of an inversion algorithm for stratospheric aerosol balloon measurements

1998-2002: PhD thesis: development of a 4D-Var data assimilation system for stratospheric chemical observations.

2002-2003: Contribute to the development of the Belgian Assimilation System for Chemical Observations (BASCOE) which was based on the system presented in my PhD thesis.

2003-2005: Member of the European FP6 ASSET project (ASSimilation of Envisat daTa).

2006-present: PI of the BASCOE project at BIRA-IASB

Education

2002: PhD in Atmospheric Physics at the Université Libre de Bruxelles.

« Assimilation des observations chimiques stratosphériques CRISTA suivant la méthode variationnelle à quatre dimensions. » supervised by R. Colin and P. C. Simon.

2001: Master in Atmospheric Sciences, Université Libre de Bruxelles.

1994: Master in Physics, Université Libre de Bruxelles.

Most relevant Publications

- **Q. Errera** and R. Ménard, “Technical Note: Spectral representation of spatial correlations in variational assimilation with grid point models and application to the Belgian Assimilation System for Chemical Observations (BASCOE)”, *Atmos. Chem. Phys. Discuss.*, 12, 16763-16809, 2012
- W.A. Lahoz and **Q. Errera**, “Constituent assimilation”, Invited chapter in *Data Assimilation: Making sense of observations*, Eds. W. A. Lahoz, B. V. Khatatov and R. Ménard. Springer, 449 – 490, 2010.
- **Q. Errera**, F. Daerden, S. Chabrilat, J. C. Lambert, W. A. Lahoz, S. Viscardy, S. Bonjean, and D. Fonteyn, “4D-Var Assimilation of MIPAS Chemical Observations: Ozone and Nitrogen Dioxide Analyses”, *Atmos. Chem. Phys.*, 8, 8009-8057, 2008.
- Geer, A. J., W. A. Lahoz, S. Bekki, N. Bormann, **Q. Errera**, H. J. Eskes, D. Fonteyn, D. R. Jackson, M.N. Juckes, S. Massart, V.-H. Peuch, S. Rharmili, and A. Segers, “*The ASSET intercomparison of ozone analyses : method and first results*”, *Atmos. Chem. Phys.*, 6, 5445-5474, 2006.
- **Errera, Q.** and D. Fonteyn, “*Four-dimensional variational chemical assimilation of CRISTA stratospheric measurements*”, *J. Geophys. Res.*, 106, 12,253–12,265, 2001.

Simon CHABRILLAT

Staff Scientist at the

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Male

French Citizenship

Born in Uccle, Belgium on 26 June 1970

Research experience

1995-1997: Graduate student at NCAR (Boulder, U.S.A.). Interactive modelling of dynamics and chemistry in the middle atmosphere (SOCRATES).

1997-2005: Research assistant at the Belgium Institute for Space Aeronomy (BIRA-IASB). Further development of SOCRATES. Modelling and 4D-VAR assimilation of stratospheric chemistry (BASCOE).

2005-2006: Long-term mission at the Meteorological Service of Canada. Extension of the Numerical Weather Prediction system to modelling and assimilation of atmospheric chemistry (GEM-BACH).

2006-now: Permanent position at BIRA-IASB as head of Chemical Weather Services. In charge for the GMES stratospheric ozone service within EU project MACC.

Education

2001: PhD PhD thesis: « Modelling global change in the middle atmosphere »
Delivered with greatest honors by Université Libre de Bruxelles (ULB).
Supervised by A. Fontana, G. Kockarts and G. Brasseur

1994: Master in Atmospheric Sciences, delivered with great honors by ULB.

1993: Engineer in mechanics and electricity. Specialization in fluid dynamics,
delivered with honors by ULB.

Most relevant Publications

Muncaster, R., Bourqui, M. S., **Chabrillat, S.**, Viscardy, S., Melo, S., and Charbonneau, P. Modelling the effects of (short-term) solar variability on stratospheric chemistry. *Atmos. Chem. Phys.*, 12, 7707-7724, doi:10.5194/acp-12-7707-2012, 2012.

de Grandpré J., Ménard R., Rochon Y., Charette C., **Chabrillat S.** and Robichaud A.
Radiative impact of ozone on temperature predictability in a coupled chemistry-dynamics data assimilation system. *Mon. Wea. Rev.*, 137, 679-692, doi:10.1175/2008MWR2572.1, 2009.

Robichaud A., Ménard R., **Chabrillat S.**, de Grandpré J., Rochon Y. J., Yang Y. and Charette C. Impact of energetic particle precipitation on stratospheric polar constituents: an assessment using monitoring and assimilation of operational MIPAS data . *Atmos. Chem. Phys.* 10, 1739-1757, 2010.

Chabrillat, S., G. Kockarts, D. Fonteyn and G. Brasseur. Impact of molecular diffusion on the CO₂ distribution and the temperature in the mesosphere. *AGU publication of the month*. *Geophys. Res. Lett.*, 29, 15, doi :10.1029/2002GL015309, 2002

Curriculum vitae – Jean de Grandpré

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Academic Qualifications

<i>B. Sc. in Physics</i>	<i>Université de Montréal (1984)</i>
<i>Graduate certificate in Meteorology</i>	<i>Université du Québec à Montréal (1988)</i>
<i>M. Sc. in Atmospheric Sciences</i>	<i>Université du Québec à Montréal (1991)</i>
<i>Ph. D. in Earth and Space Sciences</i>	<i>York University, Toronto (2005)</i>

Employment History

<i>Since 2009</i>	<i>Research Scientist in Chemical Data Assimilation Location: Centre Météorologique Canadien Modelling and Integration Section (ARQI) Air Quality Research Division (AQRD) Environment Canada</i>
<i>2006 – 2009</i>	<i>Post Doctoral visiting fellowship Location: Centre Météorologique Canadien Air Quality Research Division (AQRD) Environment Canada</i>
<i>1991 - 2006</i>	<i>Research Scientist York and McGill University</i>

Research Activities

2006 – 2013 *Contributed to the development and evaluation of a chemical data assimilation system at Environment Canada (EC) in the framework of research projects sponsored by the European (ESA) and the Canadian (CSA) Space Agency. Currently working on the development of a new operational Air Quality Forecasting system with comprehensive chemical boundary conditions and UV index forecasting capabilities.*

Selected Publications

- de Grandpré, J., R. Ménard, Y.J. Rochon, C. Charette, S. Chabrilat and A. Robichaud, Radiative impact of ozone on temperature predictability in a coupled chemistry-dynamics data assimilation system, *Monthly Weather Review*, 137, 679-692, 2009.
- Robichaud, A., R. Ménard, S. Chabrilat, J. de Grandpré, Y.J. Rochon, Y. Yang and C. Charette, Impact of energetic particle precipitation on stratospheric polar constituents: an assessment using satellite data assimilation. *Atmos. Chem. Phys.*, 10, 1739-1757, 2010.
- Fomichev, V.I., A.I. Jonsson, J. de Grandpré, S.R. Beagley, C. McLandress, K. Semeniuk and T.G. Shepherd, Response of the middle atmosphere to CO₂ doubling: Results from the Canadian Middle Atmosphere Model, *Journal of Climate*, 20, 1121-1144, 2007.
- de Grandpré, J., S.R. Beagley, V.I. Fomichev, E. Griffioen, J.C. McConnell, A.S. Medvedev and T.G. Shepherd, Ozone Climatology Using Interactive Chemistry: Results from the Canadian Middle Atmosphere Model, *J. Geophys. Res.*, (105) 26475-26491, 2000.
- Jonsson, A., J. de Grandpré, V.I. Fomichev, J.C. McConnell and S.R. Beagley, Doubled CO₂-induced cooling of the Middle Atmosphere: Photochemical analysis of the ozone radiative feedback, *J. Geophys. Res.*, 109(D24103), doi:10.1029/2004JD005093, 2004.

CURRICULUM VITAE – Michaela Imelda Hegglin

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EDUCATION

May 2004 Ph.D. (Dr. Sc. ETH), ETH Zurich, Switzerland
Oct 2000 M.Sc. in Environmental Sciences (Dipl. Umwelt-Natw. ETH), ETH Zurich, Switzerland

CAREER OUTLINE

2012-present Senior Research Fellow, Department of Meteorology, University of Reading, United Kingdom
2006-2012 Research Associate, Department of Physics, University of Toronto, Toronto, Canada
2005-2006 Postdoctoral Associate, Department of Physics, University of Toronto, Toronto, Canada
2004-2005 Postdoctoral Associate, Institute for Atmospheric and Climate Science, ETH Zurich, Switzerland
2001-2004 Ph.D. student, Institute for Atmospheric and Climate Science, ETH Zurich, Switzerland

RELEVANT EXPERIENCE

- Member of the SPARC CCM1 Steering Committee (Leads: V. Eyring and J.-F. Lamarque) (from April 2013)
- Member of scientific advisory board for the ATMO research programme at KIT Karlsruhe, Germany (from Jan 2013)
- Co-lead of SPARC Data Initiative (with S. Tegtmeier, IFM-GEOMAR, from Oct 2009)
- Co-lead author (with A. Gettelman, NCAR) of chapter 7 'The UTLS' of the SPARC CCMVal Report (Chemistry-Climate Model Validation, Eds.: V. Eyring, T. G. Shepherd, D. Waugh, 2007-2010)
- Member of the SPARC S-RIP Working Group (Leads: M. Fujiwara and D. Jackson) (from May 2012)
- Science team member of SPURT (trace gas transport in the tropopause region, an AFO2000 research project funded by the German Federal Ministry of Education and Research (BMBF)) (2001-2003)

MOST RECENT INVITED PRESENTATIONS

Nov 2012 The upper troposphere and lower stratosphere and its role in chemistry-climate coupling, Cambridge University, Cambridge, United Kingdom.
May 2012 Scientific questions and model evaluation for the UTLS, IGAC/SPARC Global Chemistry-Climate Modeling and Evaluation Workshop, Davos, Switzerland.
Mar 2012 The upper troposphere and lower stratosphere and its role in chemistry-climate coupling, McGill University, Montréal, Canada.
Dec 2011 Towards a one-atmosphere view of chemistry-climate coupling, Department of Physics, Imperial College, London, United Kingdom.

MOST RELEVANT PUBLICATIONS

Hegglin, M. I., S. Tegtmeier, and the SPARC Data Initiative Team, SPARC Data Initiative: Comparison of water vapour climatologies from international limb satellite sounders, *J. Geophys. Res.*, in revision.
Hegglin, M. I., A. Gettelman, P. Hoor, et al., Multi-model assessment in the upper troposphere and lower stratosphere: Extra-tropics, *J. Geophys. Res.*, 115, D00M09, doi:10.1029/2010JD013884, 2010.
Hegglin, M. I., and T. G. Shepherd, Large climate-induced changes in UV index and stratosphere-to-troposphere ozone flux, *Nature Geosci.*, 2, 687-691, 2009.
Hegglin, M. I., C. D. Boone, G. L. Manney et al., A global view of the extratropical tropopause transition layer from Atmospheric Chemistry Experiment Fourier Transform Spectrometer O3, H2O, and CO, *J. Geophys. Res.*, 114, D00B11, doi:10.1029/2008JD009984, 2009.
Hegglin, M. I., C. D. Boone, G. L. Manney et al., Validation of ACE-FTS satellite data in the upper troposphere/lower stratosphere (UTLS) using non-coincident measurements, *Atmos. Chem. Phys.*, 8, 1483-1499, 2008.
Hegglin, M. I. and T. G. Shepherd, O3-N2O correlations from the Atmospheric Chemistry Experiment: Revisiting a diagnostic of transport and chemistry in the stratosphere, *J. Geophys. Res.*, 112, D19301, doi:10.1029/2006JD008281, 2007.
Hegglin, M. I., D. Brunner, Th. Peter et al., Measurements of NO, NOy, N2O, and O3 during SPURT: Implications for transport and chemistry in the lowermost stratosphere, *Atmos. Chem. Phys.*, 6, 1331-1350, 2006.
Hegglin, M. I., D. Brunner, H. Wernli et al., Tracing troposphere to stratosphere transport within a mid-latitude deep convective system. *Atmos. Chem. Phys.*, 4, 741-756, 2004.

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RESEARCH INTERESTS *Dynamics, Chemistry and Satellite Remote Sensing of the Middle Atmosphere, Cryosphere-Climate Interactions*

EDUCATION

1983 Diplome de Sciences Physiques, Université Libre de Bruxelles, Belgium.

1986 MSc in Atmospheric Sciences, University of Illinois (Urbana), USA.

1991 PhD in Geophysics, University of Washington, Seattle, USA .

PROFESSIONAL EXPERIENCE

1984-86 Research Assistant, Dept. of Atmospheric Sciences, University of Illinois, USA.

1986-91 Research Assistant and Postdoctoral Fellow (9-12/91), Dept. of Atmospheric Sciences, U. of Washington (Seattle), USA.

1992-98 Visiting Scientist, Météo-France, Centre National de Recherches Météorologiques, Toulouse, France.

Since 03/98 Senior Research Scientist, Norwegian Institute for Air Research (NILU), Kjeller, Norway.

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Project Acquisition and Management.

Coordinator or PI for several European and national projects on middle atmosphere dynamics and chemistry, and climate dynamics. He is author or co-author of over 55 peer-reviewed publications. Citation h-index:16.

SELECTED PUBLICATIONS (out of 58: ISI Citation Index 16)

Lahoz, W.A., A.J. Geer, and Y.J. Orsolini, Northern hemisphere stratospheric summer from Envisat observations, *Quart. J. of the Roy. Meteor. Soc.* 133, 197-211, 2007.

Jackson D.R., Y. J. Orsolini, Estimation of Arctic ozone loss in winter 2004/05 based on assimilation of EOS MLS observations, *Quart. J. of the Roy. Meteor. Soc.*, 134, 1833-1841, 2008.

Lahoz, W.A., Y.J. Orsolini, A.J. Geer, W. Choi and D.R. Allen, Mesosphere-stratosphere transport during southern hemisphere autumn deduced from MIPAS observations, *Q. J. R. Meteor. Soc.*, 135:681:694, DOI: 10.1002/qj.397, 2009.

Orsolini, Y. J., A. Karpechko and G. Nikulin, Variability of the northern hemisphere polar stratospheric cloud potential: the role of North Pacific disturbances, *Q. J. R. Meteor. Soc.*, 135:1020:1029, DOI: 10.1002/qj.409, 2009.

Orsolini, Y.J., J. Urban, and D. Murtagh Nitric acid in the stratosphere based on Odin observations from 2001 to 2009- part 2: High-altitude polar enhancements, *Atmos. Chem. Phys.*, 9,7045-7052, 2009

Orsolini, Y.J., J. Urban, D. Murtagh, S. Lossow and V. Limpasuvan Descent from the polar mesosphere and anomalously high stratopause observed in 8 years of water vapor and temperature satellite observations by the Odin Submillimeter Radiometer, *J. Geophys. Res.*, 115, D12305, doi:10.1029/2009JD013501, 2010

Jackson, D. R., Y. J. Orsolini, and O. Engelsen (2011), Low-ozone events in the southern polar summer as indicated by Met Office ozone analyses, *J. Geophys. Res.*, 116, D06302, doi:10.1029/2010JD014858.

Balis, D., et al. (2011), Observed and Modelled record ozone decline over the Arctic during winter/spring 2011, *Geophys. Res. Lett.*, 38, L23801, doi:10.1029/2011GL049259, 2011.

Kvissel, O.-K., Y. J. Orsolini, F. Stordal, V. Limpasuvan, D. Marsh and J. H. Richter, 2012: Mesospheric intrusion and anomalous chemistry during and after a major stratospheric sudden warming, *J. Atmos. Sol. Terr. Phys*, Special Issue on Mesosphere-Lower Thermosphere, doi:10.1016/j.jastp.2011.08.015.

Kvissel, O.-K., Orsolini, Y.J., Stordal, F., Isaksen, I.S.A., Santee, M.L. (2012) Formation of stratospheric nitric acid by a hydrated ion cluster reaction: Implications for the effect of energetic particle precipitation on the middle atmosphere. *J. Geophys. Res.*, 117, D16301, doi:10.1029/2011JD017257.

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PROFESSIONAL EXPERIENCE

09.2011 – present time **Research scientist**, Belgium Institute for Space Aeronomy (BIRA-IASB)
11.2010- 08.2011 **Research scientist** at University of Quebec in Montreal, Department of Earth and Atmospheric Sciences
03.2010-10.2010 **Research scientist** at Fisheries and Oceans Canada (DFO)
01.2008-02.2010 **Research scientist** at University of Quebec in Montreal, Department of Earth and Atmospheric Sciences
09.2006-12.2007 **Research scientist** at Alfred-Wegener Institute for Polar and Marine Research, Bremerhaven, Germany
09.2004-08.2006 **Post-Doctoral Research Associate** at Laboratoire des Ecoulements Géophysiques et Industriels (LEGI), MEOM team (Équipe de Modélisation des Écoulements Océaniques à Moyenne et grande échelle), Grenoble, France

UNIVERSITY BACKGROUND

2000-2003 **PhD** in Physics and Mathematics (**Physics of Atmosphere and Hydrosphere**) at Moscow State University, Faculty of Physics, Department of Physics of Sea and Inland Waters, Moscow, Russia
2000 **MSc in Physics at Moscow State University**, Faculty of Physics, Moscow, Russia.

RESEARCH TOPICS

- 8 years of experience in data assimilation (sequential and variational methods);
- 6.5 years of experience in atmospheric and oceanic numerical weather prediction (NWP) modelling;
- 1.5 year of experience with chemical transport models (CTM)

SELECTED PUBLICATIONS

1. Skachko S., Errera Q., Ménard R., Christophe Y. and Chabrilat S. Comparison of EnKF and 4DVar methods in the context of stratospheric chemistry data assimilation. In preparation to submit to GMD;
2. Skachko, S., Danilov, S., Janjić, T., Schröter, J., Sidorenko, D., Savcenko, R., and Bosch, W. Sequential assimilation of multi-mission dynamical topography into a global finite-element ocean model, *Ocean Sci.*, 4, 307-318, 2008;
3. Janjić T., Nerger L., Albertella A., Schröter J. and Skachko S. On domain localization in ensemble based Kalman filter algorithms. *Monthly Weather Review*, Vol. 139, Nr. 7, pp 2046-2060, DOI: 10.1175/2011MWR3552.1, 2011
4. S. Skachko, J.-M. Brankart, F. Castruccio, P. Brasseur and J. Verron Improved turbulent air-sea flux bulk parameters for the control of the ocean mixed layer: a sequential data assimilation approach, *Journal of Atmospheric and Oceanic Technology*, Vol. 26, No. 3., pp. 538—555, 2009;
5. P. Brasseur, P. Bahurel, L. Bertino, F. Birol, J.-M. Brankart, N. Ferry, S. Loza, E. Remy, J. Schröter, S. Skachko, C.-E. Testut, B. Tranchant, P.J. van Leeuwen, J. Verron Data assimilation in operational ocean forecasting systems: the MERCATOR and MERSEA developments. *Quart.J.R.Met.Soc.*, 131, pp3561-3582, 2005, doi:10.1256/qj.05.142;
6. Nosov M.A., Skachko S.N. Nonlinear Tsunami Generation Mechanism. *Natural Hazards and Earth System Sciences*, 2001, 1, pp. 251 – 253;

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Dr. Michiel van Weele has >20 years of experience in multi-disciplinary atmospheric research. From 1991 - 1996 he did his PhD research on the analysis of actinic flux, photolysis, and chemistry measurements, and their interpretation with ultraviolet radiative transfer models. Since 1997 he is employed as atmospheric research scientist at the Climate Research Department of KNMI. His expertise is in the field of chemistry-climate interactions and the interpretation of satellite and ground-based observations of atmospheric composition. Research tools include the global climate model EC Earth, the global atmospheric chemistry-transport model TM5 as well as radiative transfer codes. He has been deeply involved in the definition of satellite user and data requirements for future Operational Atmospheric Chemistry Monitoring Missions (CAPACITY, 2003-2005) and Eumetsat requirements, both in relation to Sentinel 4 and 5. He first authored the science requirements document for TROPOMI. TROPOMI is the successor of OMI and will be flown as Sentinel-5 precursor in the 2015+ timeframe. He is a member of the PREMIER Mission Advisory Group and led the definition of the scientific and data requirements for PREMIER. He has been contributing author and/or reviewer for different international scientific assessment reports and participated in many EU and national science projects. He has been guiding many students and post-docs over the years. Currently he supports the development of C-IFS within MACC(-II) as well as the inclusion of climate-composition couplings in the EC Earth general circulation model, e.g. in the framework of the ESA Ozone-CCI and the EU FP7 project SPECS.

Selected recent publications:

- Bândă, N., Krol, M., van Weele, M., van Noije, T., and Röckmann, T.: Analysis of global methane changes after the 1991 Pinatubo volcanic eruption, *Atmos. Chem. Phys.*, 13, 2267-2281, doi:10.5194/acp-13-2267-2013, 2013.
- Miyazaki, K., H. J. Eskes, K. Sudo, M. Takigawa, M. van Weele, and K. F. Boersma: Simultaneous assimilation of satellite NO₂, O₃, CO, and HNO₃ data for the analysis of tropospheric chemical composition and emissions, *Atmos. Chem. Phys.*, 12, 9545-9579, doi:10.5194/acp-12-9545-2012, 2012.
- Williams, J. E., M. van Weele, P.F.J. van Velthoven, M.P. Scheele, C. Liousse, and G.R. van der Werf, The Impact of Uncertainties in African Biomass Burning Emission Estimates on Modeling Global Air Quality, Long Range Transport and Tropospheric Chemical Lifetimes, *Atmosphere*, 3, 132-163; doi:10.3390/atmos3010132, www.mdpi.com/journal/atmosphere, 2012.
- De Laat, A.T.J. and M. van Weele, The 2010 Antarctic ozone hole: Observed reduction in ozone destruction by minor sudden stratospheric warmings, *Sci. Rep.*, 1, 38; DOI:10.1038/srep00038, 2011.
- Spahni, R., Wania, R., Neef, L., van Weele, M., Pison, I., Bousquet, P., Frankenberg, C., Foster, P. N., Joos, F., Prentice, I. C., and van Velthoven, P.: Constraining global methane emissions and uptake by ecosystems, *Biogeosciences*, 8, 1643-1665, doi:10.5194/bg-8-1643-2011, 2011.
- Huijnen, V., J.E. Williams, M. van Weele, T.P.C. van Noije, M.C. Krol, F. Dentener, A. Segers, S. Houweling, W. Peters, A.T.J. de Laat, K.F. Boersma, P. Bergamaschi, P.F.J. van Velthoven, P. Le Sager, H. Eskes, F. Alkemade, M.P. Scheele, P. Nédélec and H.-W. Pätz: The global chemistry transport model TM5: description and evaluation of the tropospheric chemistry version 3.0, *Geosci. Model Dev.*, 3, 445-473, doi:10.5194/gmdd-3-445-2010, 2010.
- De Laat, A.T.J., R.J. van der A, M.A.F. Allaart, M. van Weele, G.C. Benitez, C. Casaccia, N.M. Paes Leme, E. Quel, J. Salvador and E. Wolfram, Extreme sunbathing: three weeks of small total O₃ columns and high UV radiation over the Southern tip of South America during the 2009 Antarctic O₃ hole season, *Geophys. Res. Lett.*, vol. 37, L14805, 6 PP., doi:10.1029/2010GL043699, 2010.