ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

FARPOCC – Atmospheric Chemistry Modelling

Leif, Laura, Sanna-Maria

3rd FARPOCC Meeting

Nov 21-22, 2007

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

FARPOCC – Atmospheric Chemistry Modelling

- **Model development**
  - FinROSE-ctm
    - FinROSE box model
  - HAMMONIA CCM
- **Long-term modelling studies**
  - ECMWF, ERA-40
  - CCM data
- **Model validation**
  - Ozone, NO_2, BrO, H_2O, … (NOx, HOx, Clx)
- **Polar ozone loss**
  - IPY Match campaigns
- **Water vapour**
  - COST0604 – WAVACS

FinROSE-ctm: Model description

- A global 3-D grid point model based on the NCAR-ROSE-model
- Flux-form Semi-Lagrange Transport-scheme (Lin & Rood)
- Typical resolution: Lon:10°× Lat:5°
  32 levels, up to 0.1hPa (ca. 65km)
  45 levels, up to 0.01hPa (ca. 80km)
- Meteorological data: ECMWF, ERA-40 and Operational analyses
- 27 long-lived species/families and 14 species in photochemical equilibrium
- Chemistry (Updated 'JPL-2006' chemical kinetics)
- Around 110 gas-phase reactions
  - 37 photodissociation processes
  - 10 heterogeneous reactions (liq, NAT, ICE)
- Photodissociation coefficients through look-up table
  - compiled using PHODIS radiative transfer model
- PSC and aerosol processing
  - LBA, TER, NAT, NAT-rock and ICE- particles, and sedimentation

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

Climate Chemistry Model - HAMMONIA

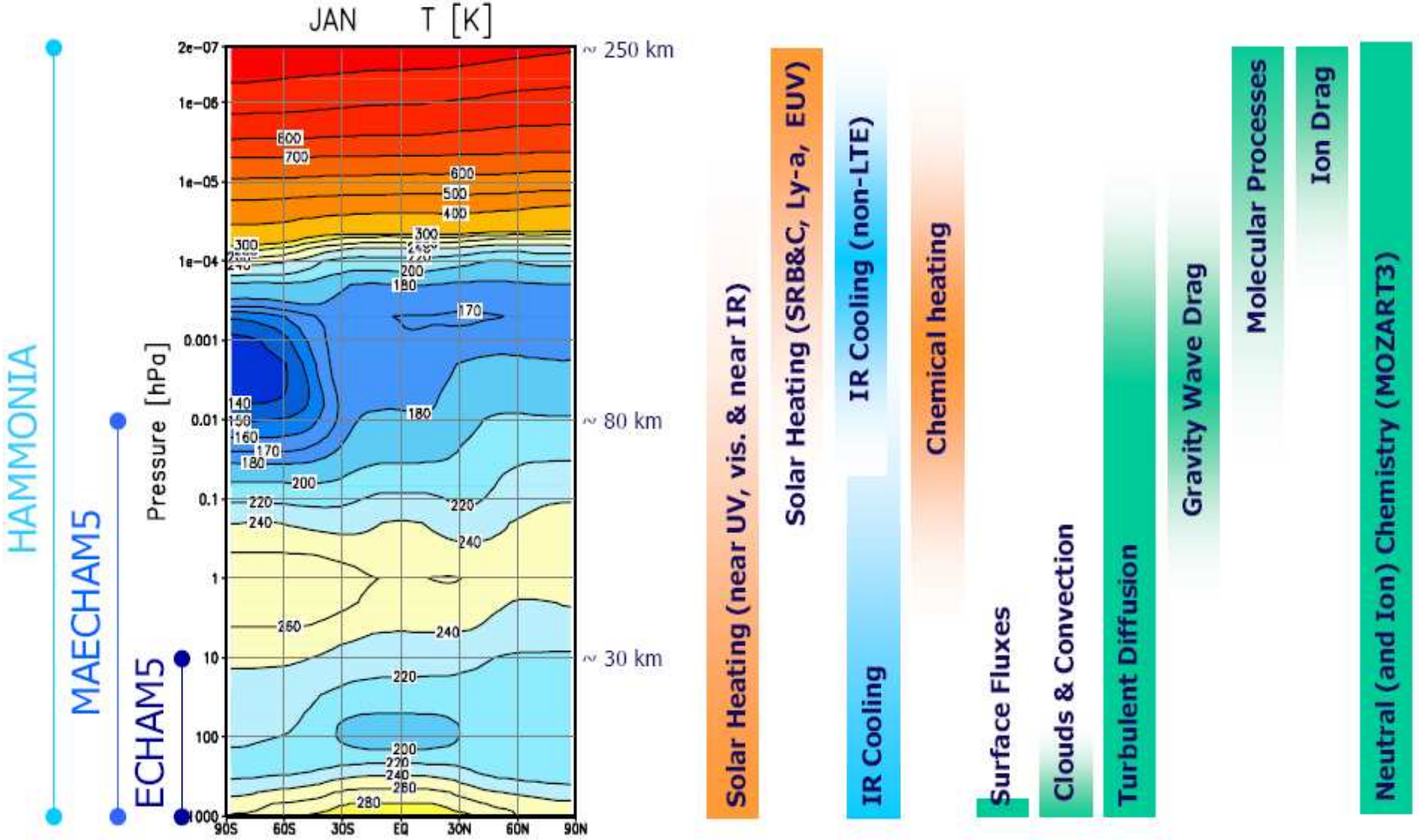
- **HAMMONIA - Hamburg Model of the Neutral and Ionized Atmosphere,** Schmidt *et al.* (2006) J.Climate 19(16), 3903.
- **Vertical extension to the thermosphere of the MAECHAM5 GCM,** Giorgetta *et al.* (2006) Geophys.Res.Lett. 29, 1245.
- **Condensed version of MOZART-3 CTM chemistry,** Kinnison *et al.* (2007) J.Geophys.Res.
- **Max Planck Institute for Meteorology, Hamburg, Germany**
  - FMI - MPI Cooperation within COSMOS

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

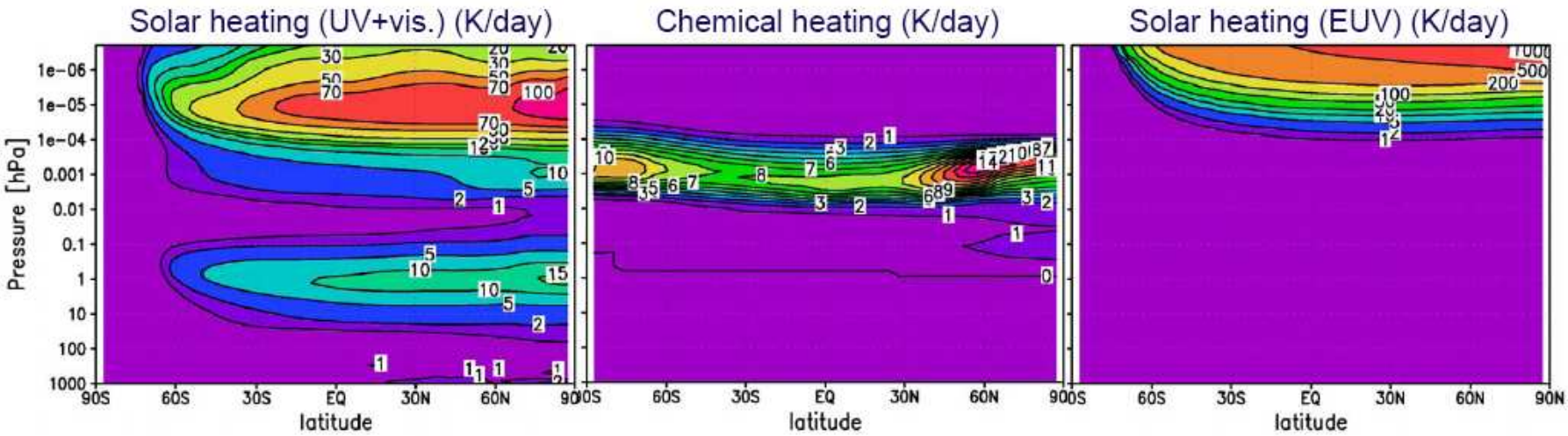
HAMMONIA at FMI

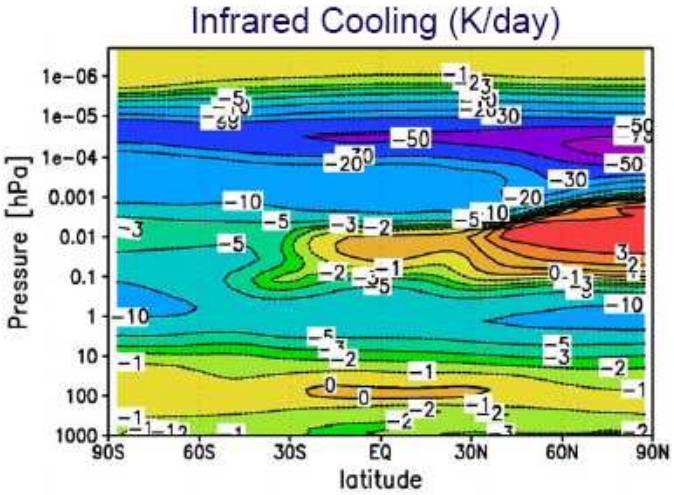
- **Chemistry climate modelling**
  - Started up in spring 2007
  - Implemented to local super computing environment
  - MPI – Summer School on Earth System Modelling
- **Planned model development**
  - Ozone loss chemistry and PSC processes
  - Ion-chemistry
  - Aerosols, Sulphur chemistry
- **First studies related to middle atmosphere**
  - Ozone and NO_x - GOMOS
- **CCMVal simulations in 2008**
  - Shared load with MPI

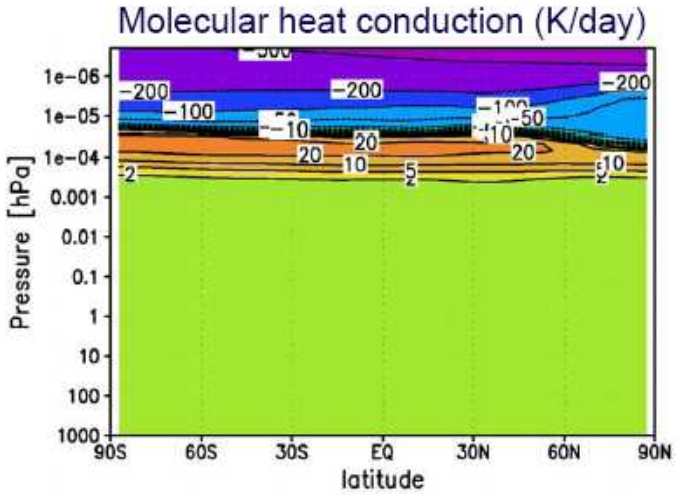
Processes – radiative, dynamics & chemistry



Climate Chemistry Model - HAMMONIA







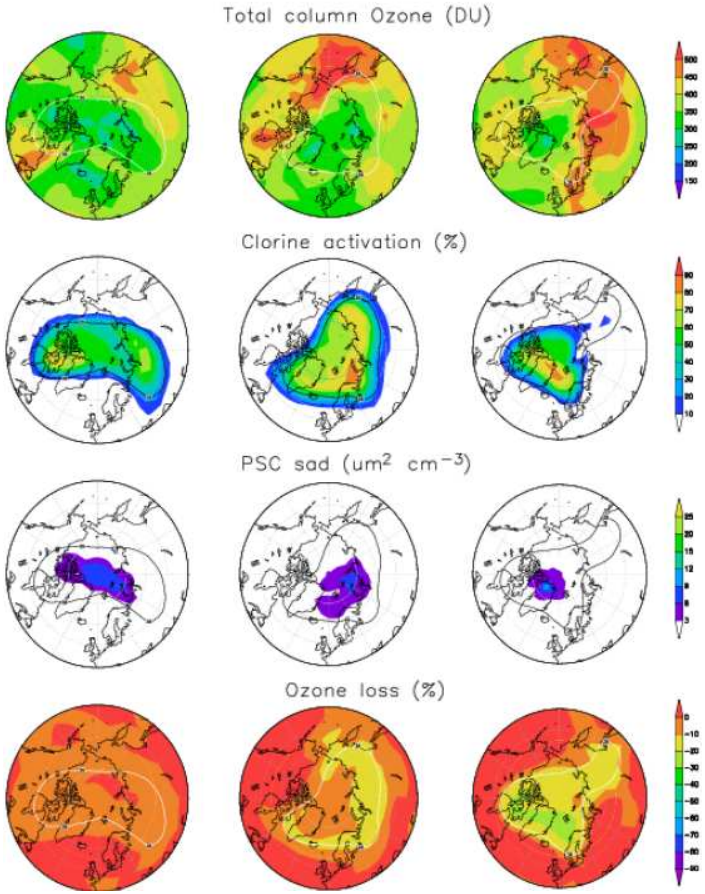
HAMMONIA CCM

- **Resolution, T31 L67 (L119)**
  - Horizontal: ~3.71°x 3.75° (Lat x Lon)
  - Vertical: Surface to 1.7e-7 hPa (ca. 250km), constant distance in logP in mesosphere and lower thermosphere, ca. 2-3 km
- **Chemical species updated on each timestep (typically 5-10min)**
  - Advection (Lin and Rood, 1996)
  - Molecular diffusion
  - Cloud processes
  - Chemistry
    - 48 compounds, 46 photolyses, 107 gas phase reactions, heterogeneous chemistry (Liq/NAT/ICE)
    - Simplified tropospheric chemistry (O_3, NOx ,HOx, CH_4)
    - Parameterized production of NO in the thermosphere + NO production in the stratosphere by cosmic rays
    - Lower boundary (surface) from MOZART2
    - Upper boundary free (except H and O^3P)
- **Radiative processes use the concentrations of**
  - O_3, O_2, O^3P, CO_2, H_2O, CH_4, N_2, N_2O, CFCs and aerosols

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

FinROSE-ctm development & updates

- **Model I/O**
- **Initialization**
- **Restart routine**
- **Boundary conditions (troposphere, top level)**
  - H_2O, Ozone
- **Dynamic tropopause**
- **Supercomputer environment**
  - parallelization
- **Scenarios, 'profiles'**
  - Aerosols, H_2SO_4
  - CH_4, N_2O, Clx, Brx
- **Chemistry**
  - Kinetics
  - Photochemistry (diss. rates, ref. atmospheres)
  - Solvers

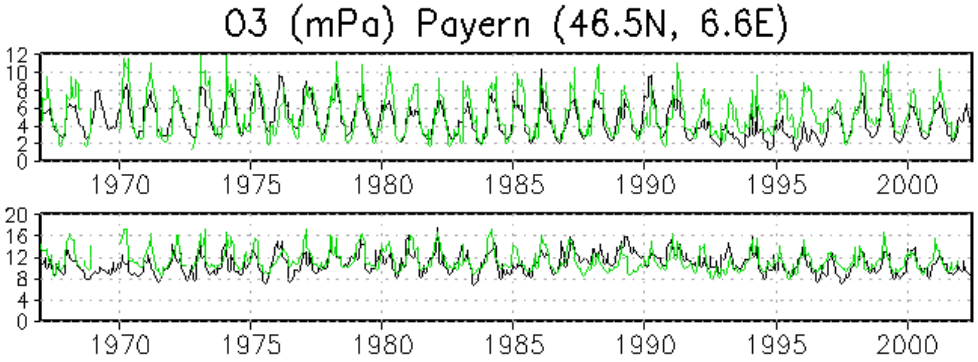


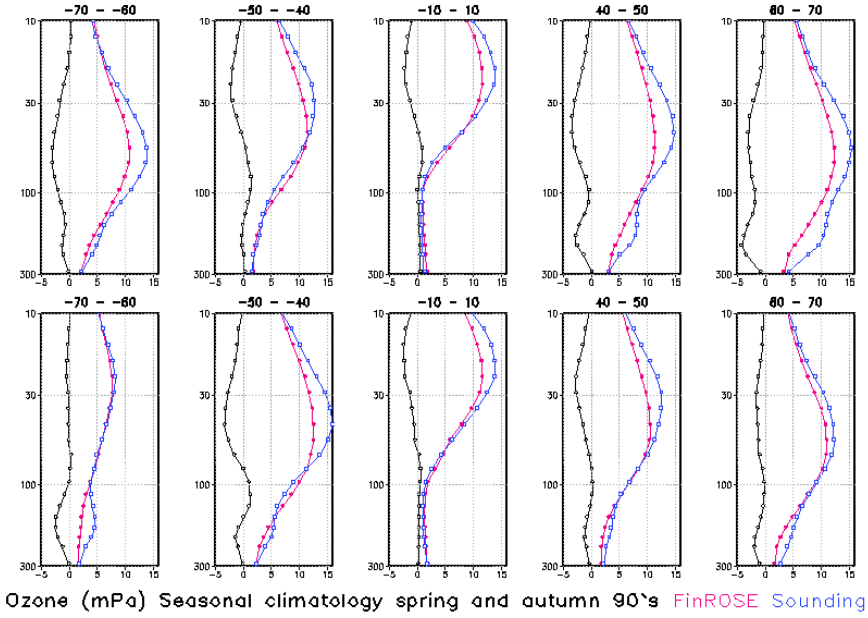
Damski, J., Thölix, L., Backman, L., Taalas, P. and Kulmala, M., FinROSE - Middle atmospheric chemistry transport model, 2007, Boreal Env. Res., 12, 535-550.

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

FinROSE-ctm: Long-term modelling studies

- **ECMWF ERA-40 Analyses**
- **Trends in ozone**
- **Polar ozone loss**

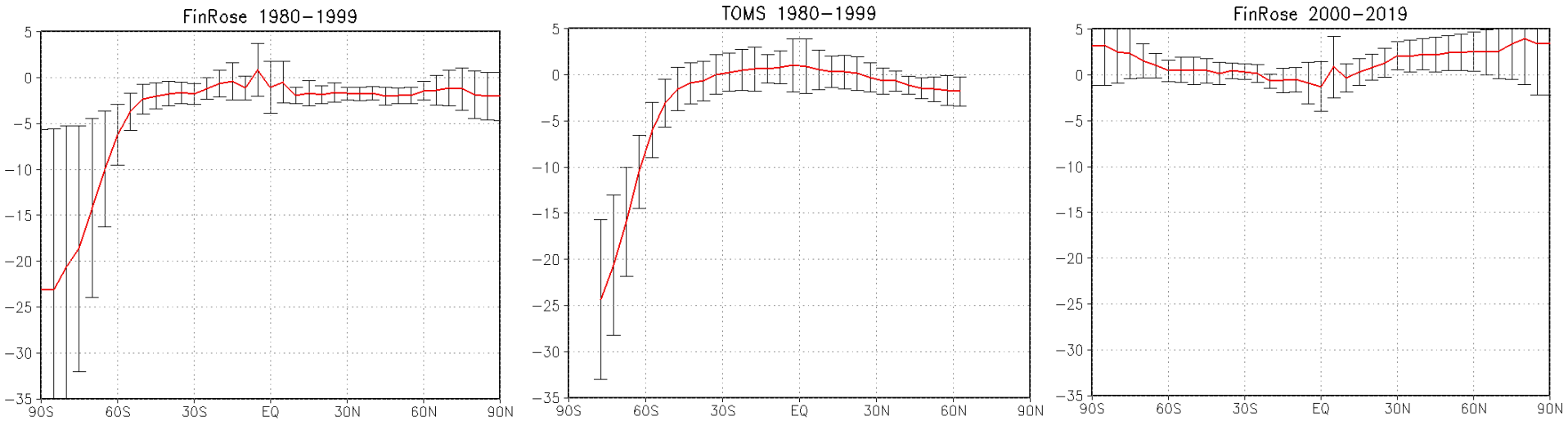




- M.G. Schultz, L. Backman, Y. Balkanski, S. Bjoerndalsaeter, R. Brand, J.P. Burrows, S. Dalsoeren, M. de Vasconcelos, B. Grodtmann, D.A. Hauglustaine, A. Heil, J.J. Hoelzemann, I.S.A. Isaksen, J. Kaurola, W. Knorr, A. Ladstaetter-Weißenmayer, B. Mota, D. Oom, J. Pacyna, D. Panasiuk, J.M.C. Pereira, T. Pulles, J. Pyle, S. Rast, A. Richter, N. Savage, C. Schnadt, M. Schulz, A. Spessa, J. Staehelin, J.K. Sundet, S. Szopa, K. Thonicke, M. van het Bolscher, T. van Noije, P. van Velthoven, A.F. Vik, F. Wittrock REanalysis of the TROpospheric chemical composition over the past 40 years (RETRO) — A long-term global modeling study of tropospheric chemistry, Final Report, Jülich/Hamburg, Germany, August 2007
- Backman, L., Thölix, L., Ojanen S-M. and Damski J., Long-term chemistry-transport model simulations of middle atmospheric ozone, Long Term Trends Workshop, Sodankylä, Finland, 4-8 Sep. 2006, Poster presentation, 2006.
- Thölix, L., Backman, L., Ojanen, S-M., and Damski, J., Analysis and validation of long-term chemistry-transport model simulations of middle atmospheric ozone, European Geosciences Union General Assembly 2006, Vienna, Austria, 2-7 April, Poster presentation, 2006.

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

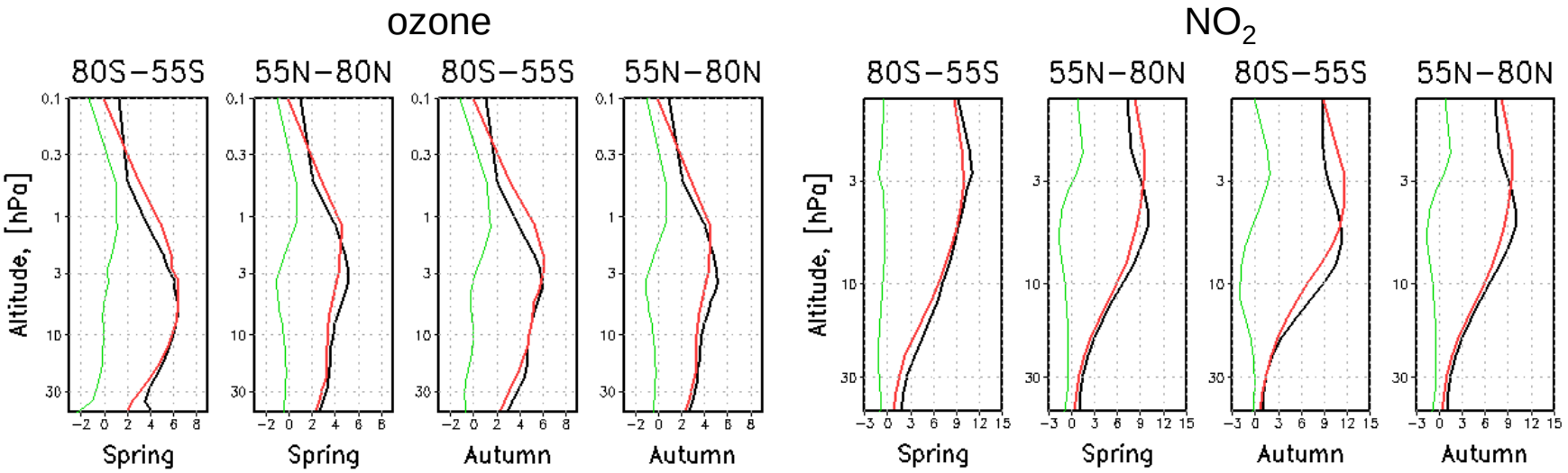
FinROSE-ctm: CCM data 1980-2019



- Backman, L., Damski, J., Thölix, L., Kaurola, J., Taalas, P., Austin, J., Butchart, N. and Kulmala, M., Polar ozone processes in a middle atmosphere CTM simulation from 1980 to 2019 forced with GCM meteorology, UKMO CCM data, Manuscript.
- Damski, J., Thölix, L., Backman, L., Kaurola, J., Taalas, P., Austin, J., Butchart, N. and Kulmala, M., 2007, A Chemistry-Transport Model Simulation of Middle Atmospheric Ozone from 1980 to 2019 Using Coupled Chemistry GCM Winds and Temperatures, Atmos. Chem. Phys., 7, 2165-2181.

FinROSE-ctm: Model validation

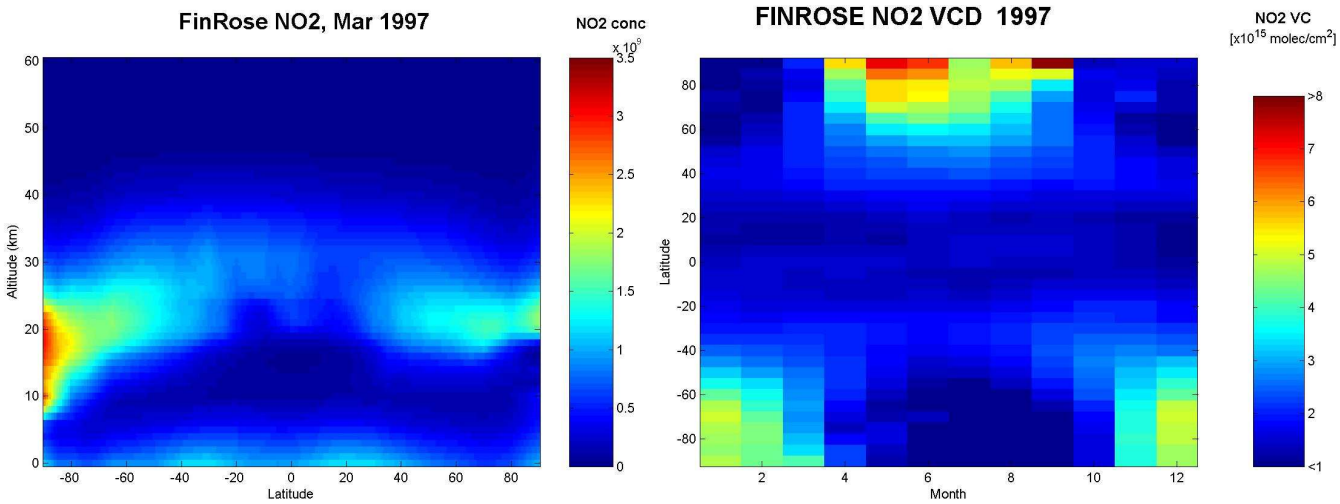
- GOMOS - O_3 and NO_2
- FinROSE ECMWF oper data



- **L. Thölix, L. Backman, S.-M. Ojanen, E. Kyrölä, J. Tamminen and S. Hassinen, Comparison of O_3 and NO_2 profiles from GOMOS and FinROSE-ctm, Envisat Symposium 2007, 23-27 April, Montreux, Switzerland, 2007.**

FinROSE-ctm: NO_2 and BrO

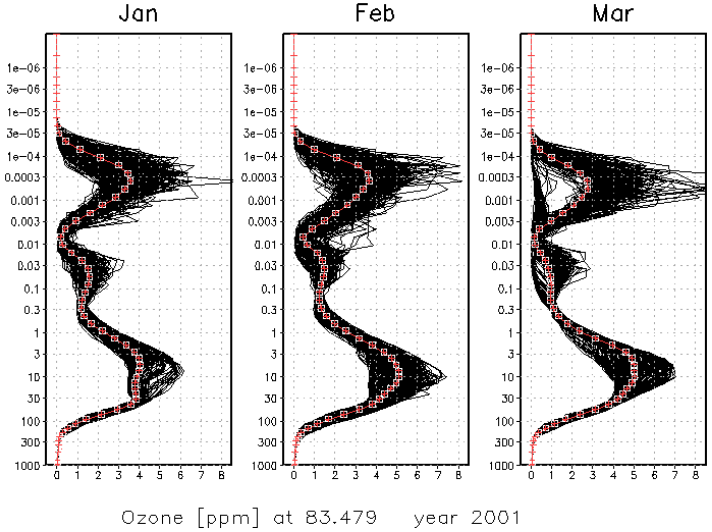
- **Ozone SAF**
- **Model validation**
  - Model data
  - Soundings
  - Satellite, GOME
- **Tropospheric BrO**

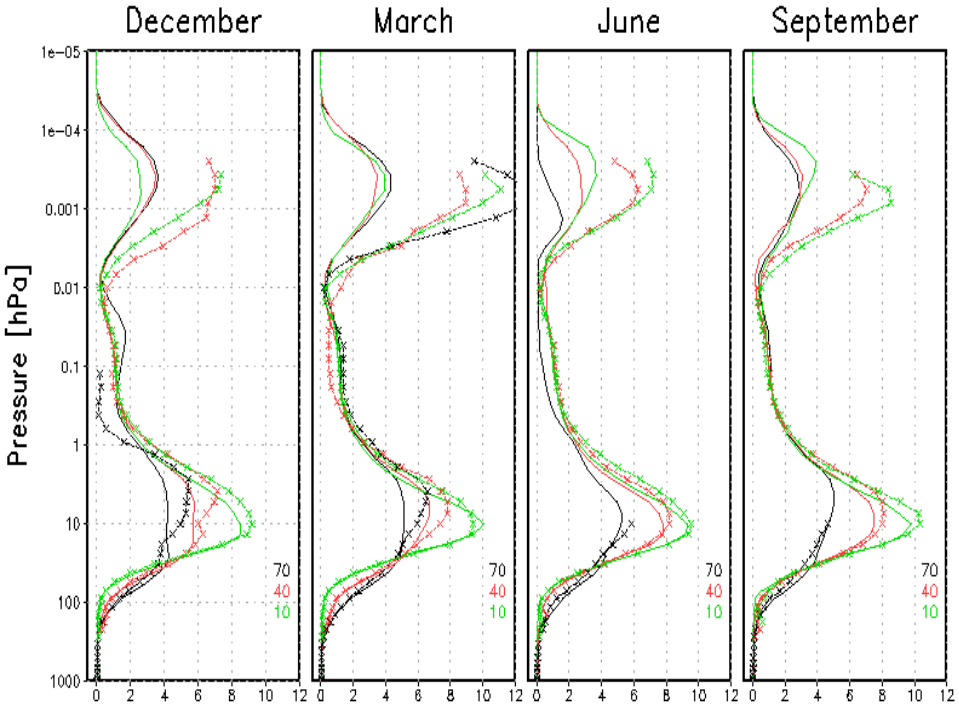


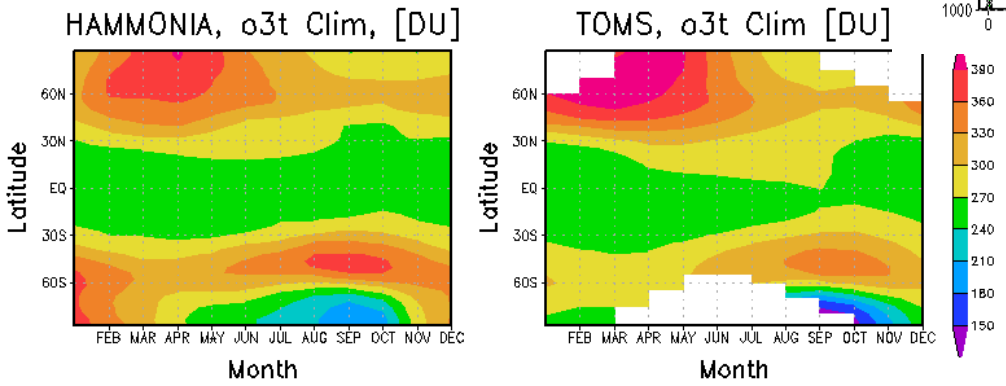
- Post, P., Backman, L., Thölix, L. Ojanen S.-M. et al., Temporal and Spatial distribution of NO_2 and BrO in the Northern Hemisphere Stratosphere. Manuscript.
- Post, P., Backman, L., Thölix, L., Van Roozendael, M. and Fayt, C., Tropospheric and stratospheric BrO and NO_2 columns derived by use of satellite observations and 3D CTM FinROSE, ESA-Atmospheric science conference, Esrin, Frascati, Italy, 8-12 May 2006, Poster presentation, 2006.

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

Ozone in HAMMONIA

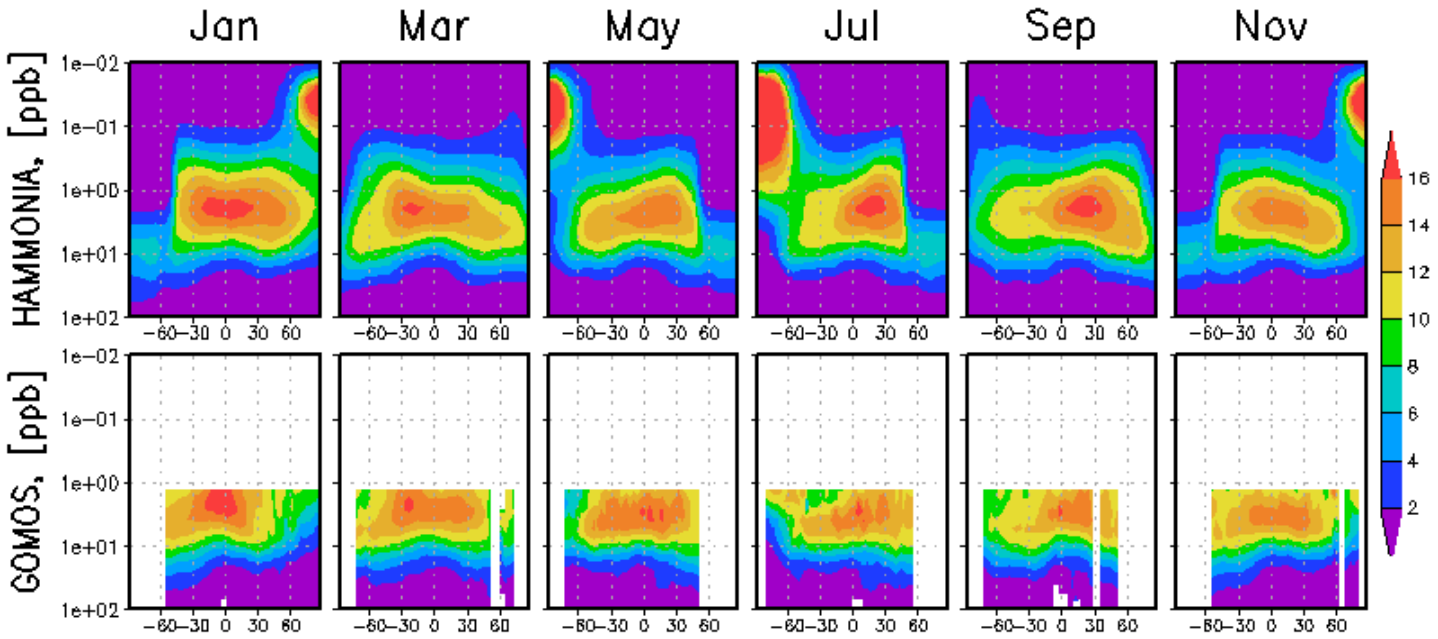






- Backman L., Thölix L., Ojanen S.-M., Kyrölä E., Tamminen J., Kyrö E., Kivi R., Schmidt H. and Giorgetta M. A., Comparison of Climatological Ozone Profiles from the HAMMONIA Climate Model with GOMOS and Ozone Sounding Data, 2nd ICESM, 27-31 August, Hamburg, Germany, 2007.

HAMMONIA NOx

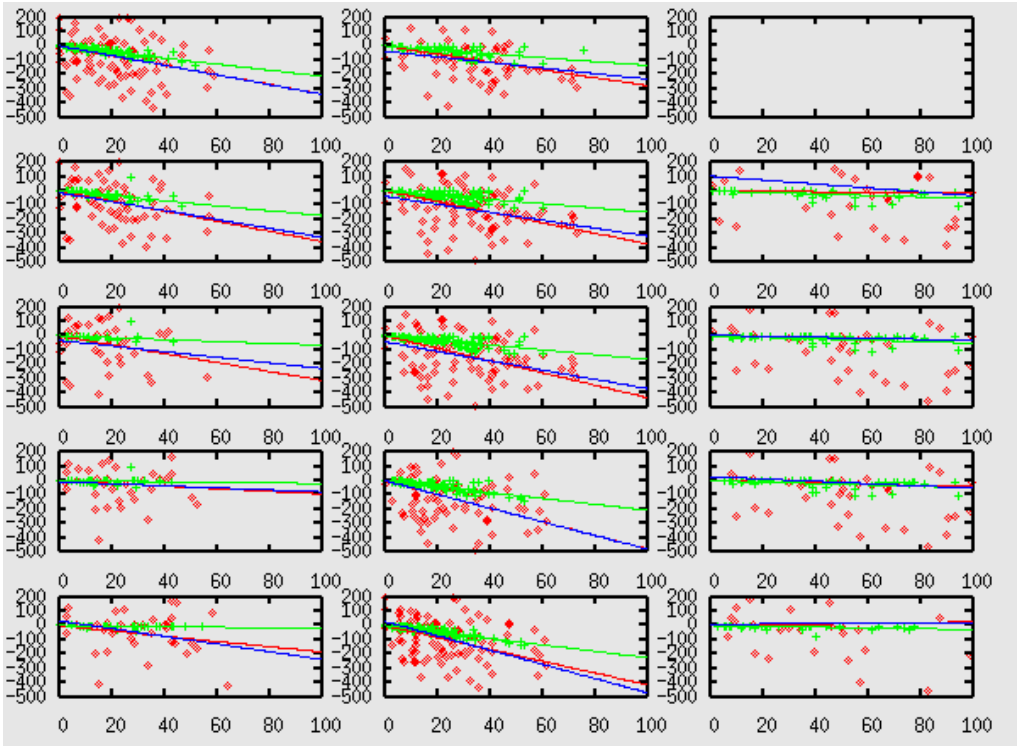


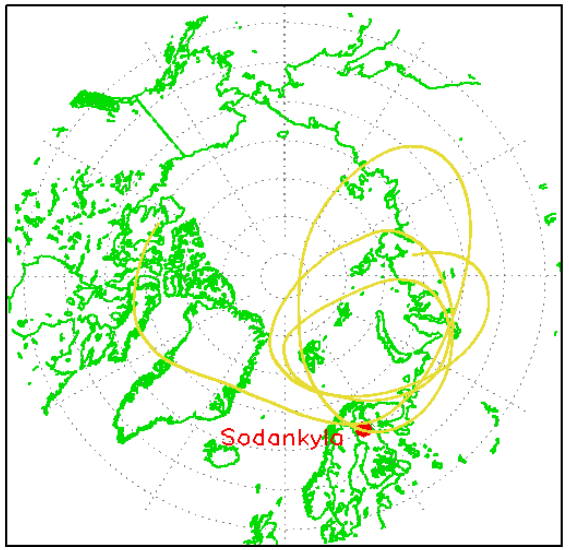
- Thölix, L,. Backman, L., Ojanen, S.-M., Seppälä, A., Tamminen, J., Kyrölä, E., Arctic NOx, ACP, Manuscript, GOMOS Special issue
- Laura, Lefa, International Summer School on Earth System Modelling, MPI Hamburg

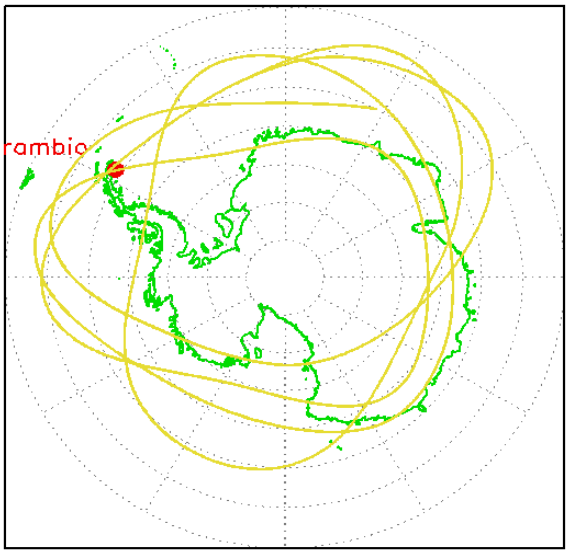
ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

Match campaigns - IPY

Sonde and Model ΔO3/sunlit time



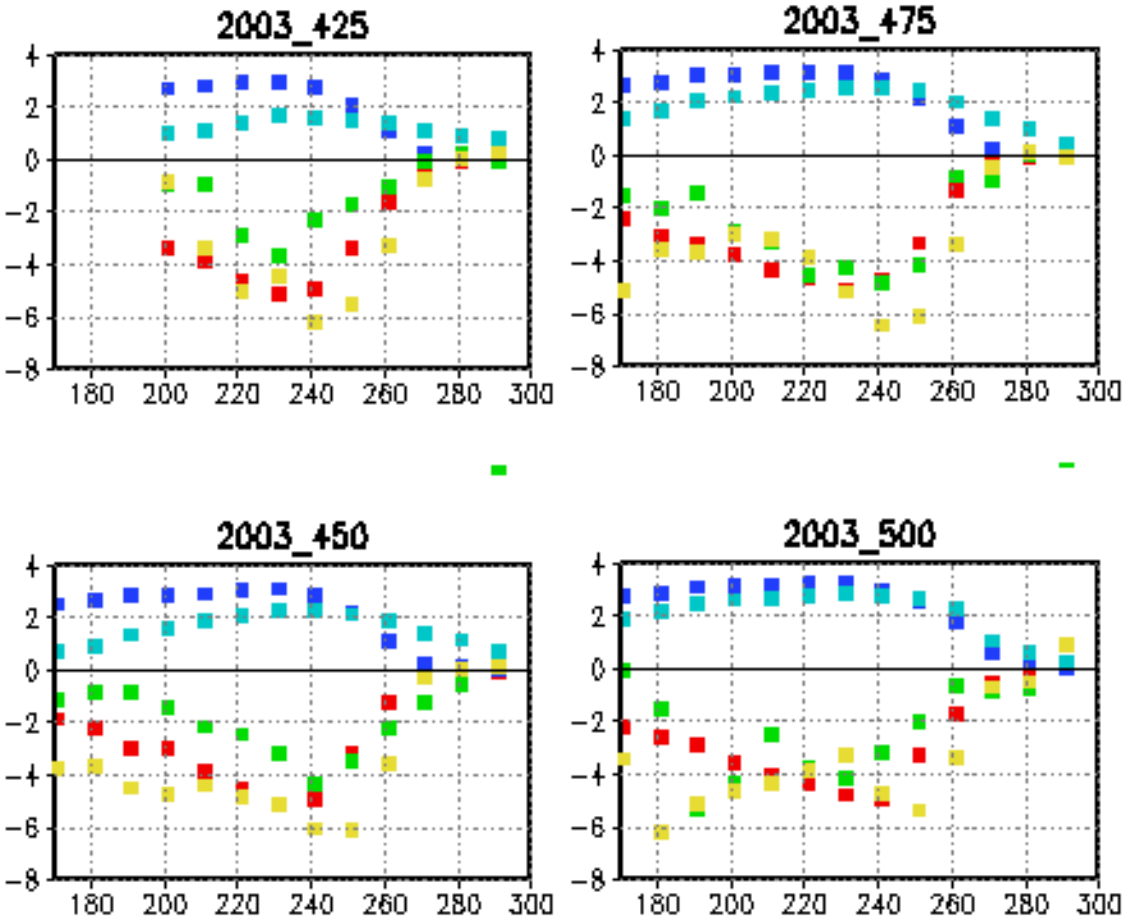




ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

Match vs. FinROSE

Ozone loss rates (ppb/sunlit hour)



Match data

Box model

3D model

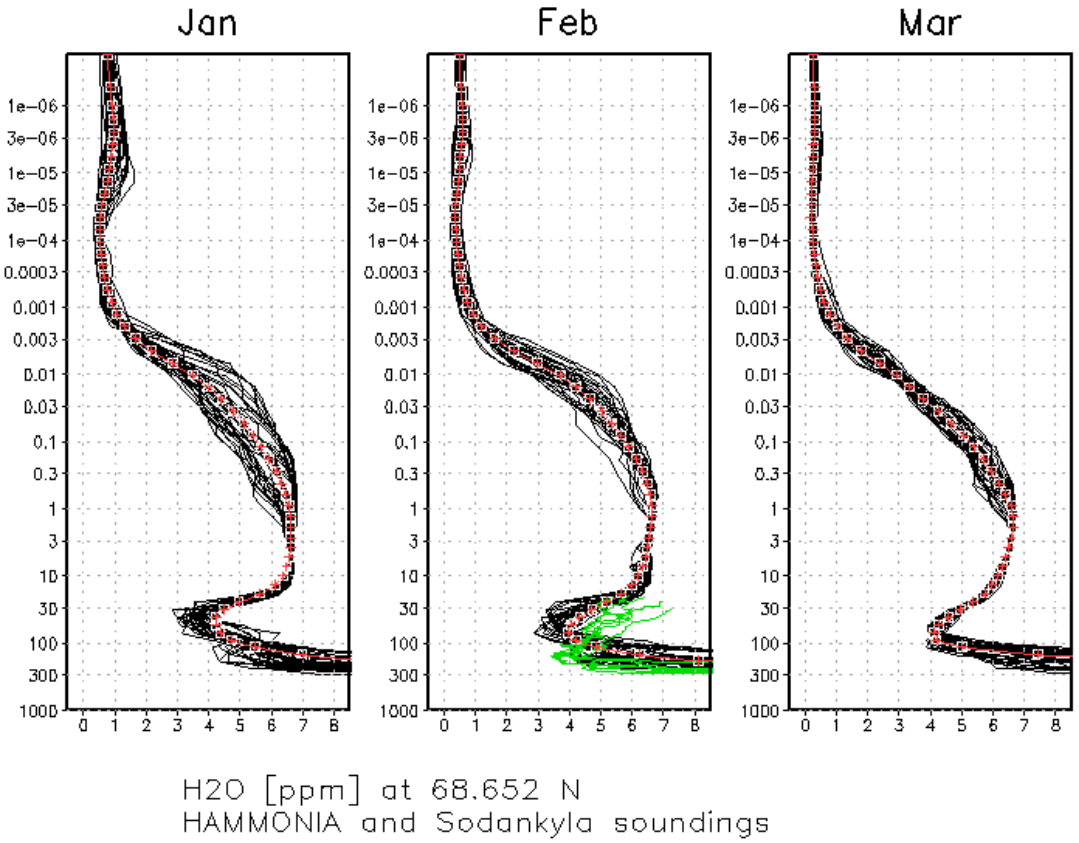
Match ozone data &
-Trajectory data, AWI

Initial values
- FinROSE 3-D
- Satellite profile data

- NOx, Clx, BrO, … (GOMOS, OSIRIS, MLS, …)

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

Water vapour



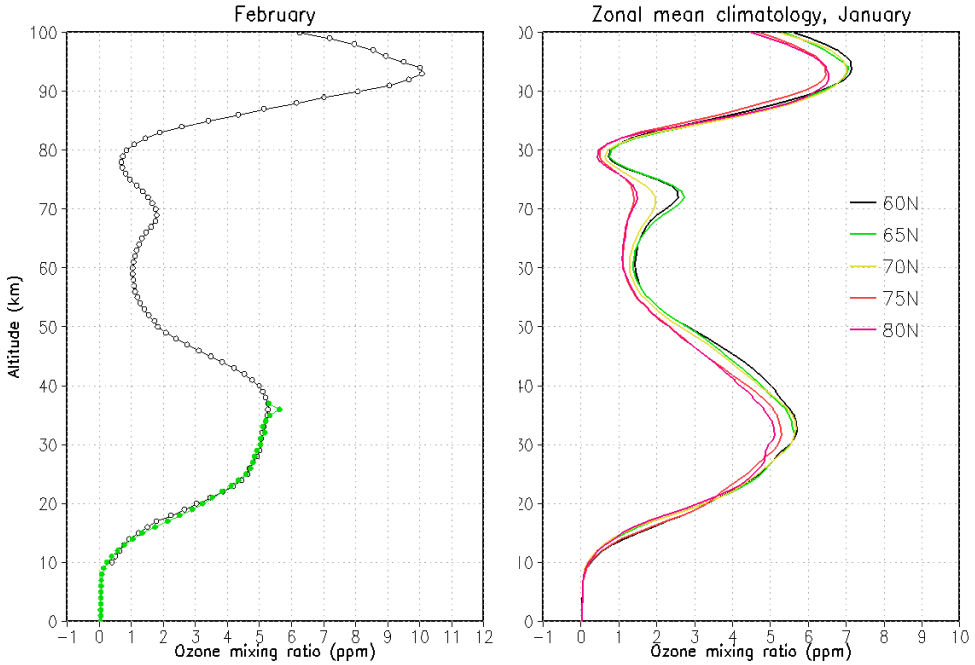
H2O [ppm] at 68.652 N
HAMMONIA and Sodankyla soundings

- **COST ES0604, Atmospheric Water Vapour in the Climate System**

ILMATIETEEN LAITOS
METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

Polar night ozone profile climatology

- **Zonal monthly profile climatology**
  - **Ozone sonde data**
  - **GOMOS proiles**
- **Tested for supplementing the ozone sonde profiles above the balloon burst point**



- Backman, L., E. Kyrö, E. Kyrölä, J. Tamminen, R. Kivi, L. Thölix, Height resolved ozone climatologies in the Arctic winter based on ozone sounding and GOMOS/Envisat profiles, Fall AGU 2007
- Backman, L., Kyrö, E., Kyrölä, E., Thölix, L., Ojanen S.-M., Hassinen, S., Kivi, R. and Heikkinen, P., Height Resolved Ozone Climatologies in the Arctic Winter from Ozone Soundings, GOMOS and FinROSE-ctm, Envisat Symposium 2007, 23-27 April, Montreux, Switzerland, 2007.

Beyond FARPOCC

- CCMVal simulations shared load with MPI Hamburg (2010 UNEP/WMO Ozone Assessment)
  - Reference data set
  - Future projections, recovery
  - Effect of greenhouse gases on temp and dynamics (circulation)
- Downward and upward couplings
  - Solar interaction
    - Ion chemistry
    - NOx, HOx chemistry
  - Gravity-waves (Model parameterization & GOMOS)
- ClO-dimer photolysis
  - MCMC
  - Implications for 3D modelling
  - Match data analysis, FinROSE-ctm and box-model
    - Satellite data, validation and “assimilation”
- Aerosols
  - Volcanic eruption and Links to Climate engineering
    - radiative coupling
    - heterogeneous chemistry, e.g. effect on ozone loss

- **Heterogeneous chemistry to HAMMONIA**
- **Heterogeneous chemistry to DLR-ROSE**
- **Ion chemistry to FinROSE**
- **FinROSE chemistry to SILAM**