

# Chemical forecasts

D. Fonteyn (@oma.be)  
Belgisch Instituut voor Ruimte-Aëronomie (BIRA-IASB)

---

1

# OUTLINE

- Introduction: stratospheric chemistry overview
- Diagnostic capability of chemical data assimilation
- Operational set-up & forecasts
- Scientific issues

---

2

## Operational implementation

Operational chemical data assimilation



Daily best estimate of chemical composition

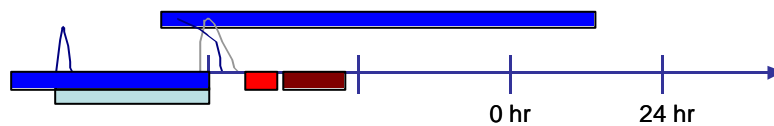






Chemical forecasts *based on dynamical forecasts*

3

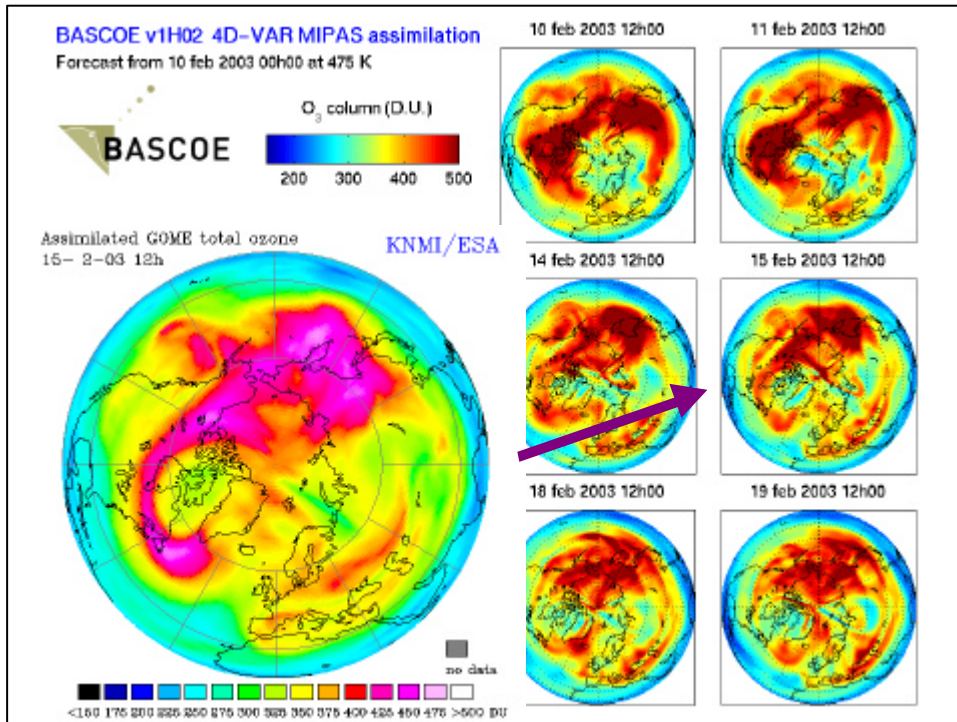
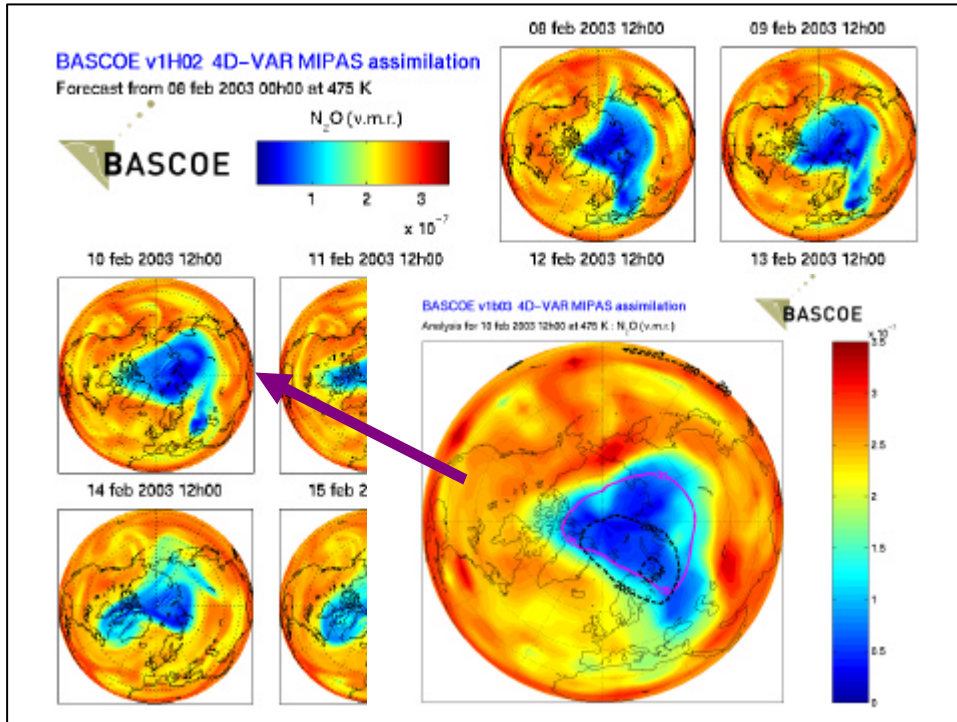
## Operational implementation

Forecast



-  ECMWF fields
-  MIPAS NRT observations
-  24 hr Chemical analysis
-  10 day Chemical forecast

4

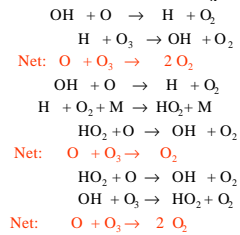


## Stratospheric chemistry

Gas phase chemistry

1. Chapman Cycle
2. Catalytic cycles

1. Hydrogen radicals ( $\text{HO}_x$ )



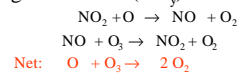
Hydrogen Source Gases:  $\text{H}_2\text{O}$ ,  $\text{CH}_4$

- Long term trends
- $\text{HO}_x$  chemistry in the upper stratosphere and mesosphere

7

## Stratospheric chemistry

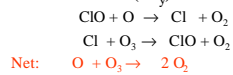
2. Nitrogen radicals ( $\text{NO}_y$ )



Nitrogen Source Gas:  $\text{N}_2\text{O}$  (and ...)

- Long term trends
- $\text{NO}_y$  partitioning (in the lower stratosphere: aerosols)

3. Chlorine radicals ( $\text{Cl}_y$ )



Chlorine Source Gases: Organic Chlorine

- Long term trends
- $\text{Cl}_y$  partitioning (in the lower stratosphere: aerosols)

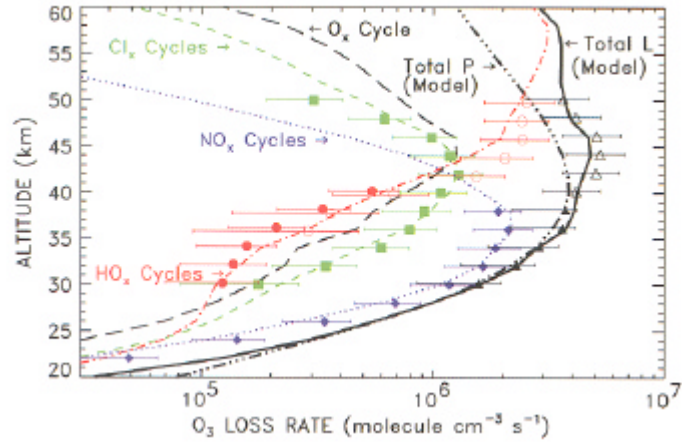
8

## Ozone loss

35°N, September 1993

24 hour average

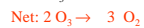
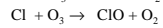
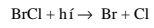
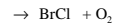
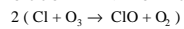
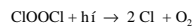
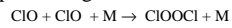
WMO, 1998



9

## Lower Stratosphere

Gas phase chemistry triggered by heterogeneous processing



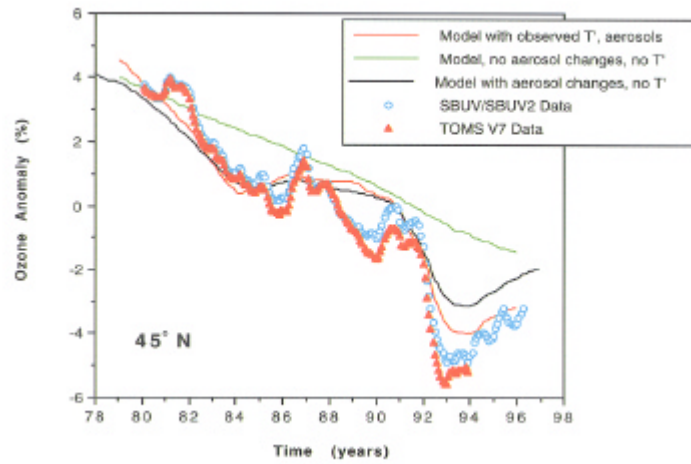
ClO<sub>x</sub>/Cl<sub>x</sub> & NO<sub>x</sub>/NO<sub>y</sub>

Polar Stratospheric Clouds

Aerosols (Pinatubo)

10

## Lower Stratosphere Ozone Loss



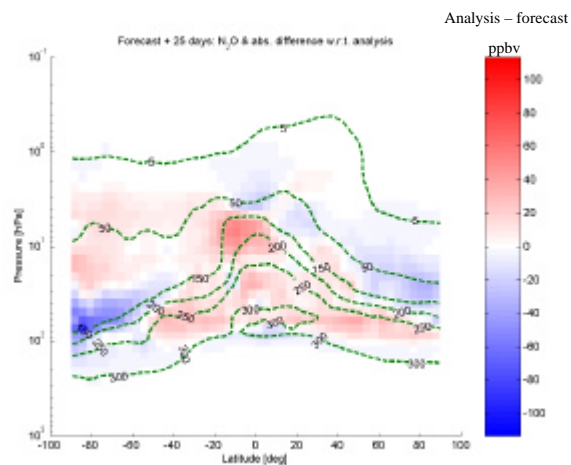
11

## Why CDA & Forecast?

Dispersion of tracer advection  
 (Schoeberl et al., JGR 2003)

25 Day free model run: N<sub>2</sub>O  
 and comparison with  
 analyses

“Chemical species drift”



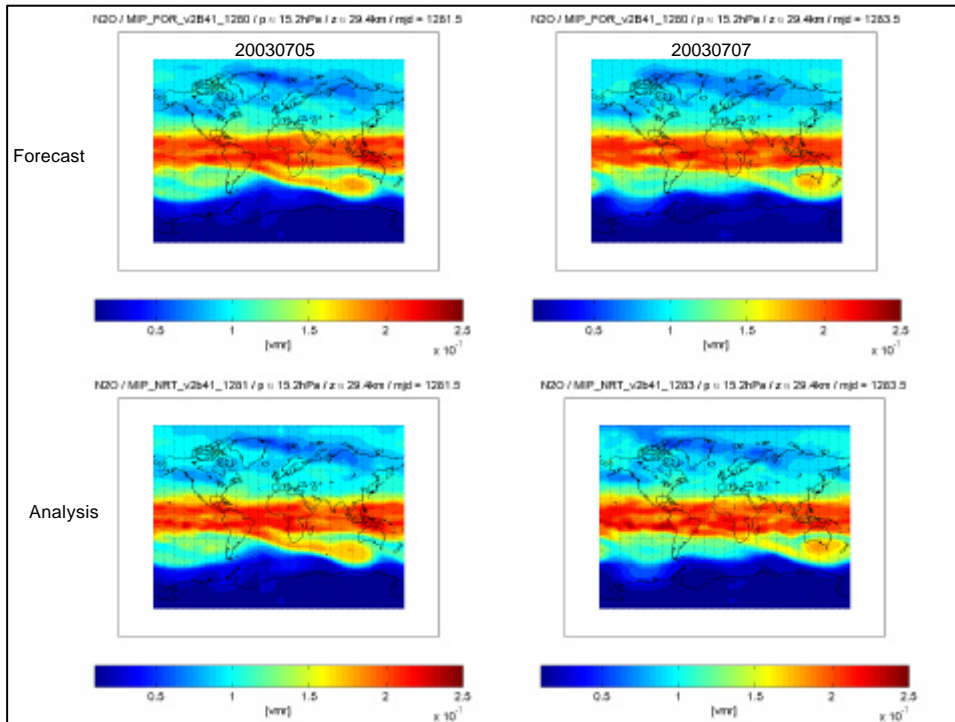
12

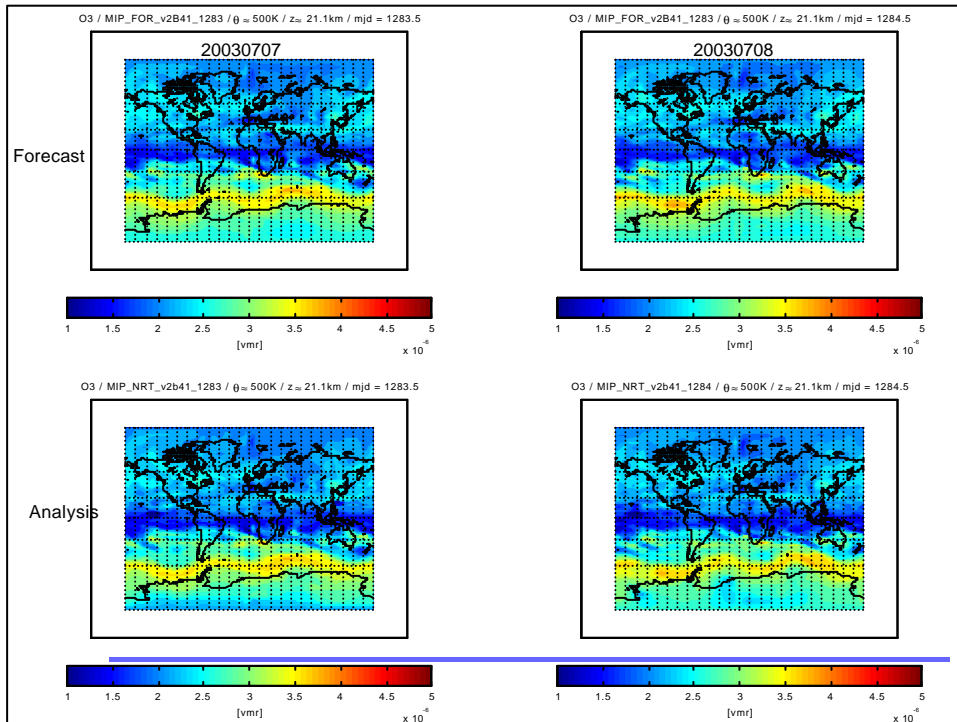
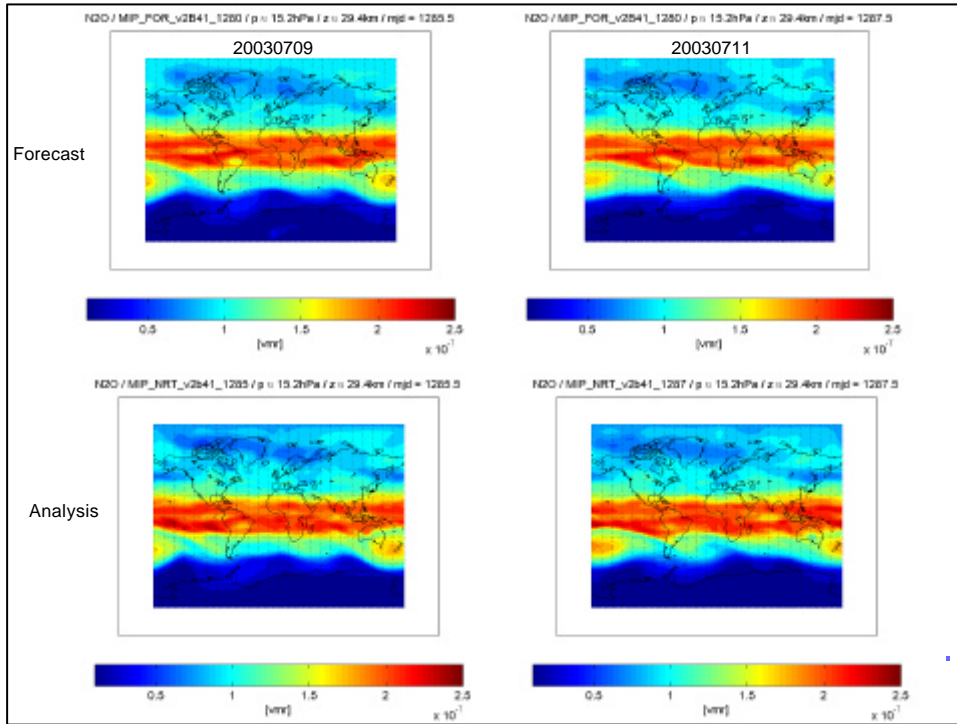
## Operational forecasts

- Operational chemical data assimilation: (BASCOE)
  - CTM, 57 species, PSCs, ECMWF dynamics
  - 4D-VAR, MIPAS NRT data
- Chemical analyses: initial state for forecast
- CTM must be driven by dynamical forecast
  
- Now mainly winter periods
  
- This course:
  - Examples to get a feeling
    - N<sub>2</sub>O, O<sub>3</sub>, HNO<sub>3</sub>, NAT particles, ClO
  - Quantitative “forecast skill”?

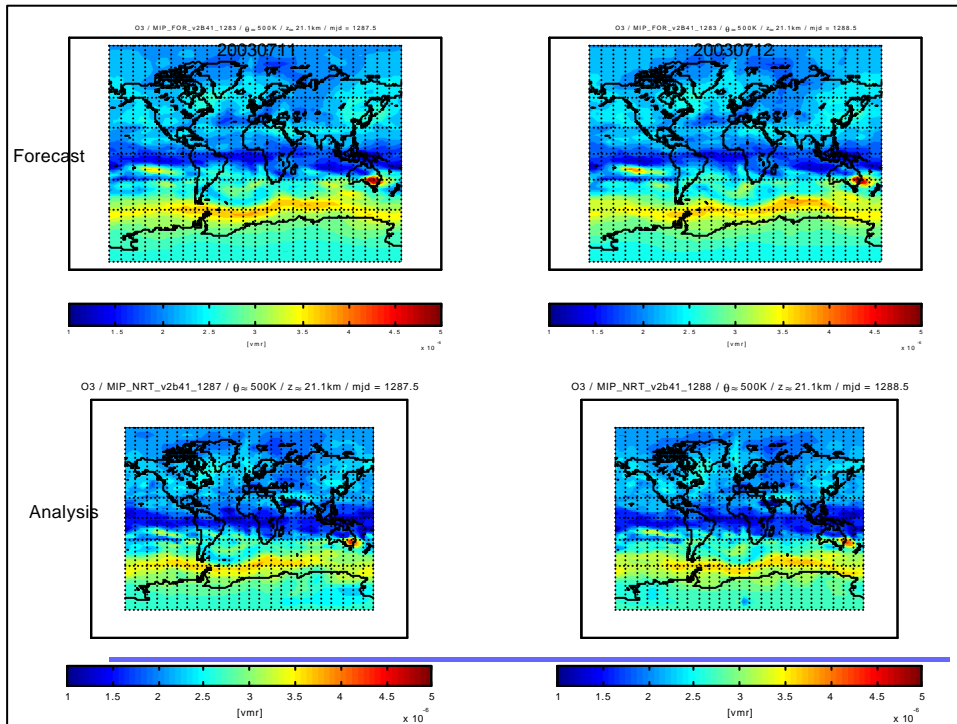
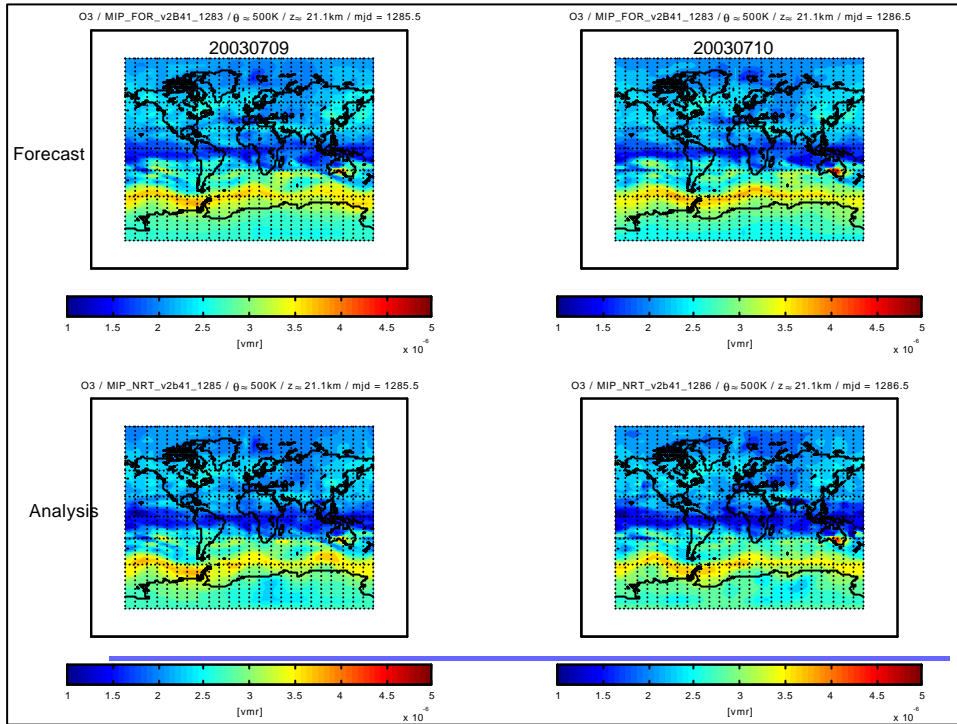


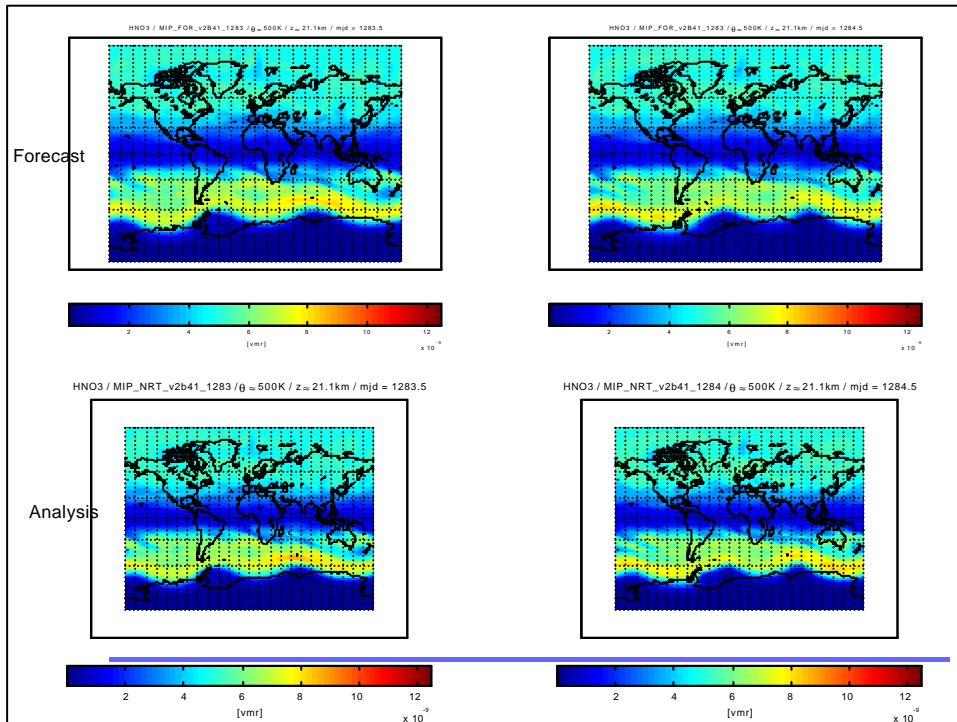
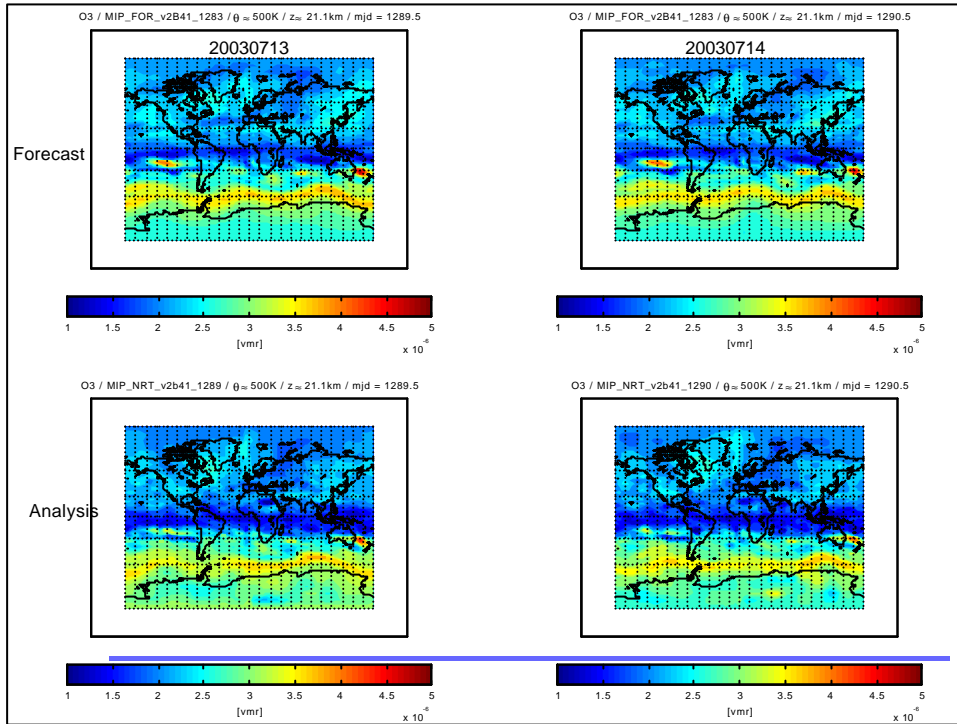
13

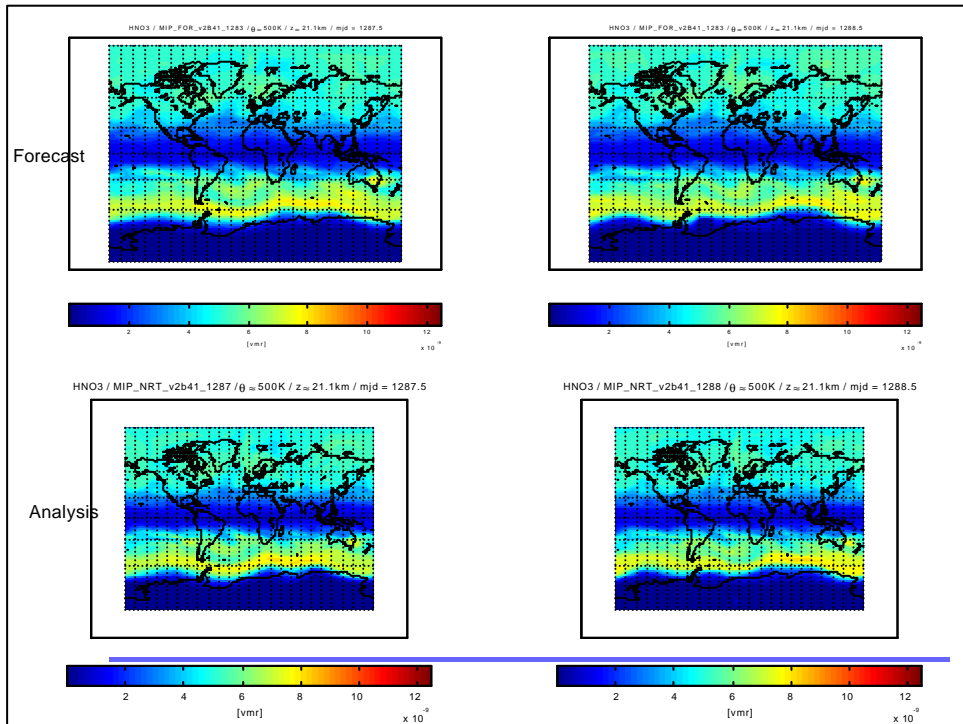
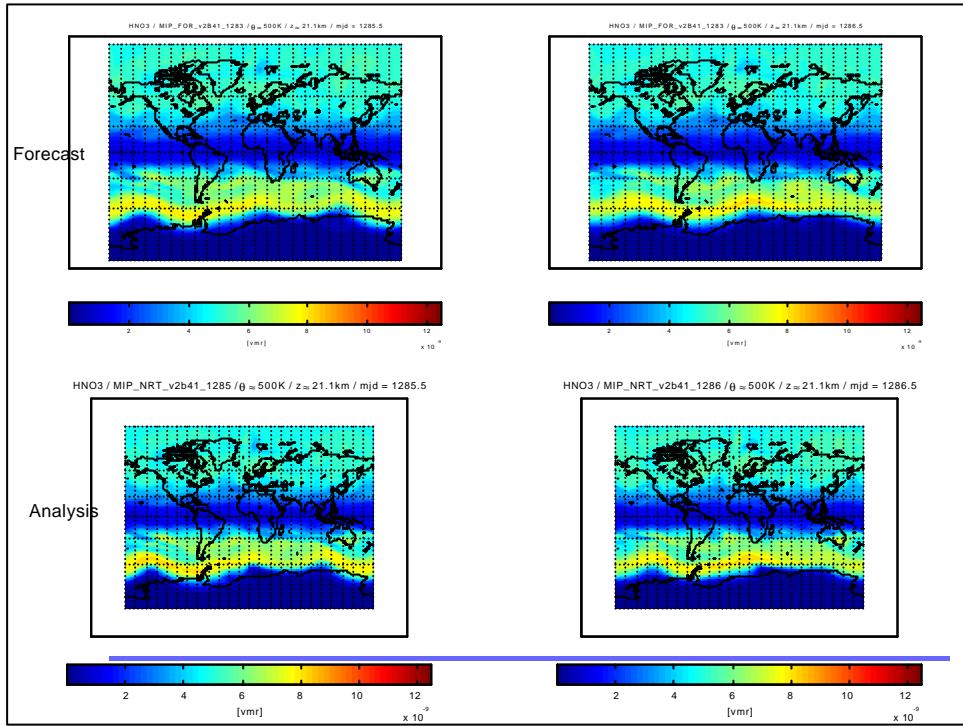


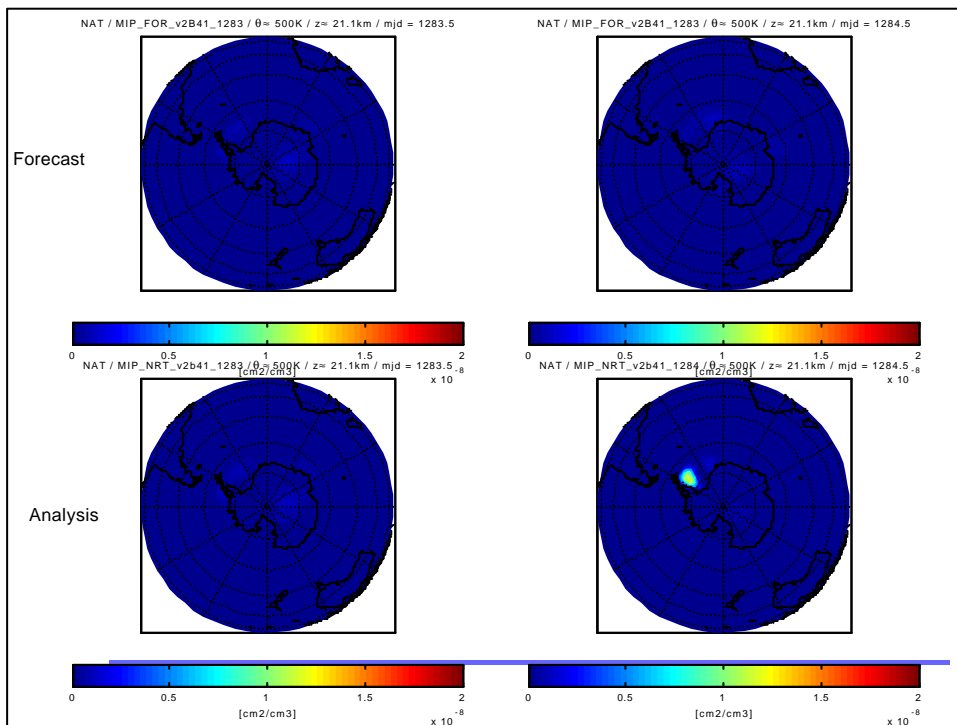
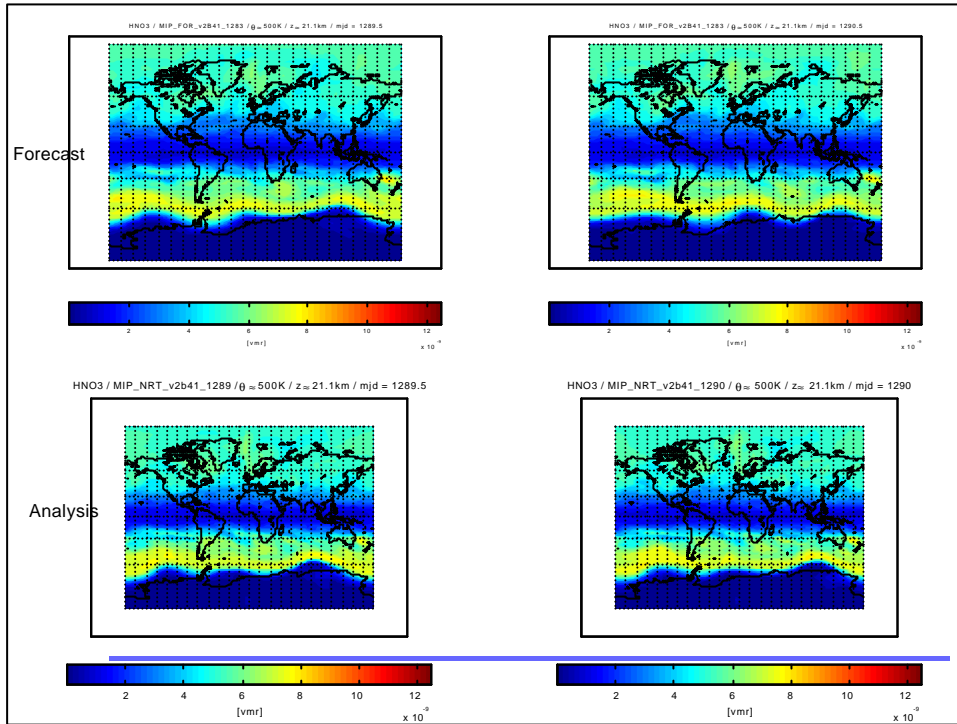


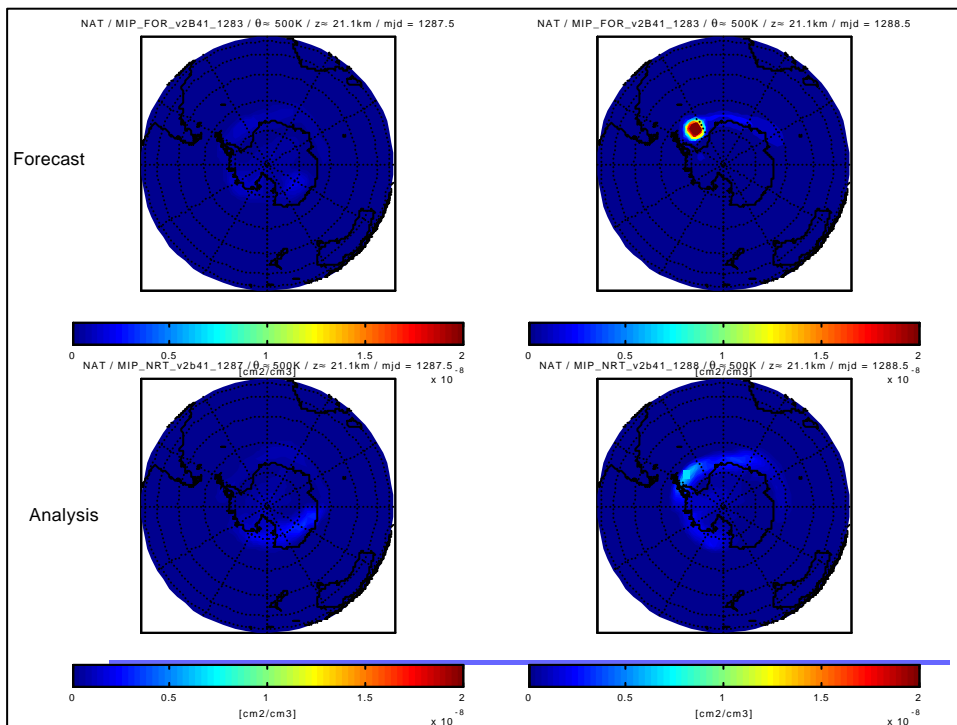
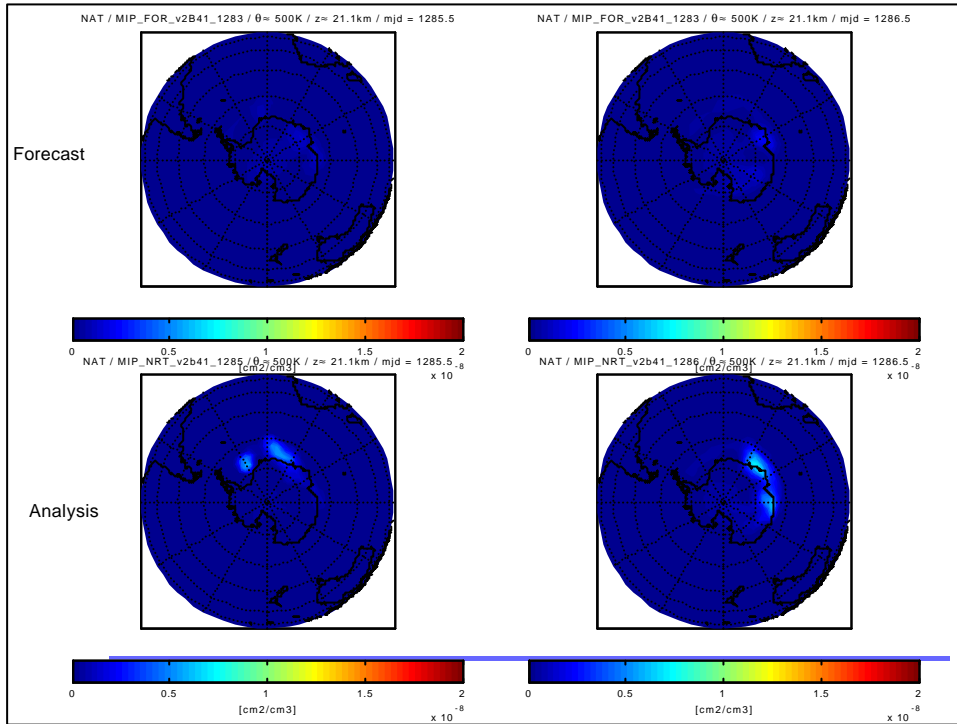


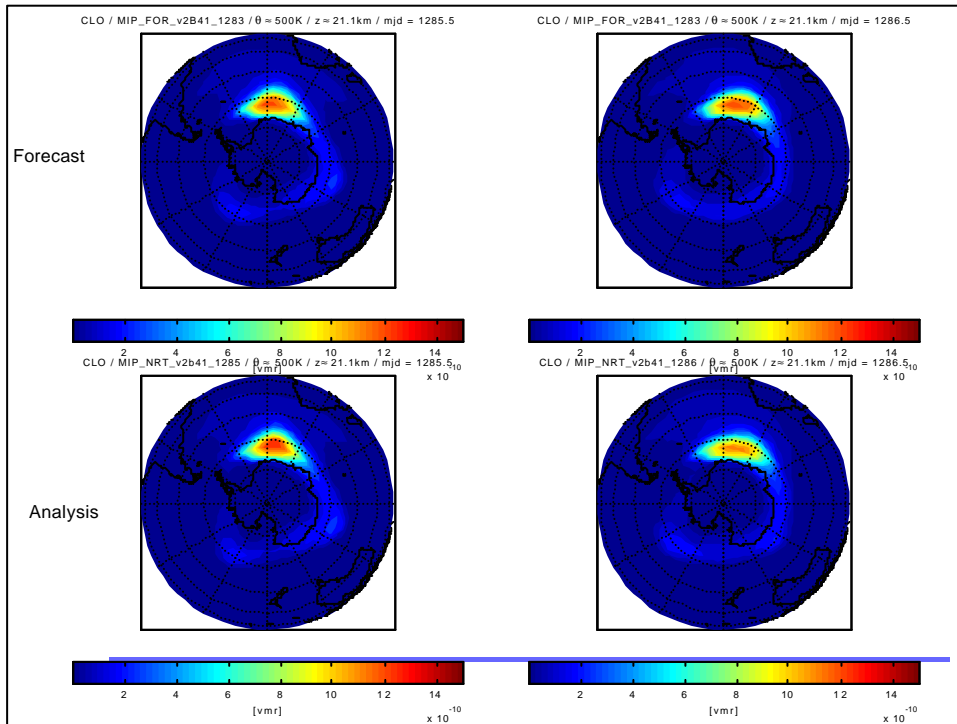
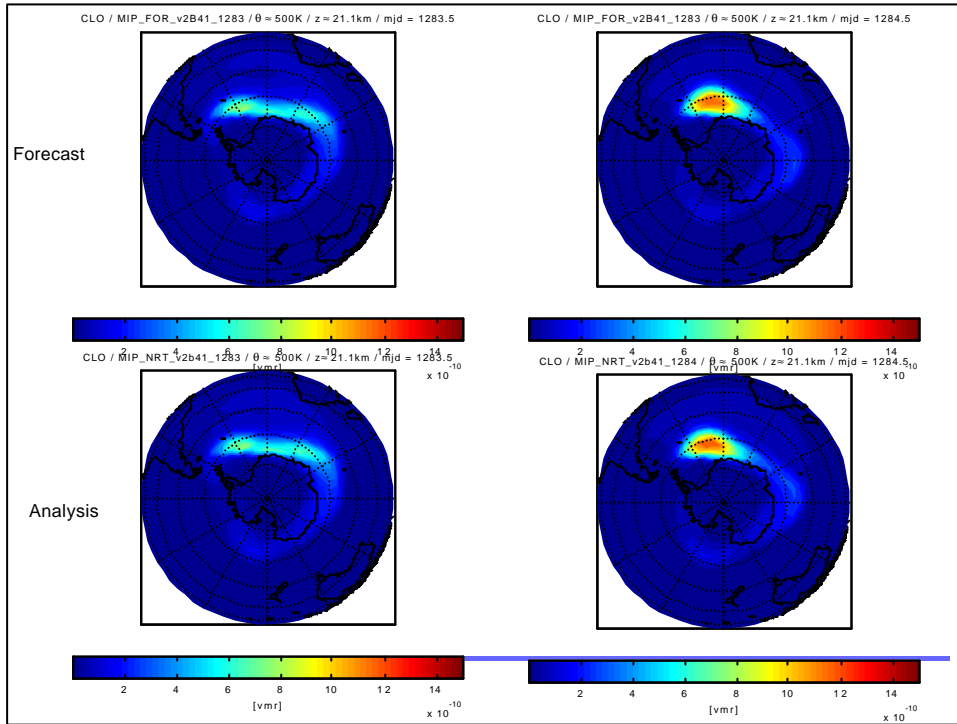


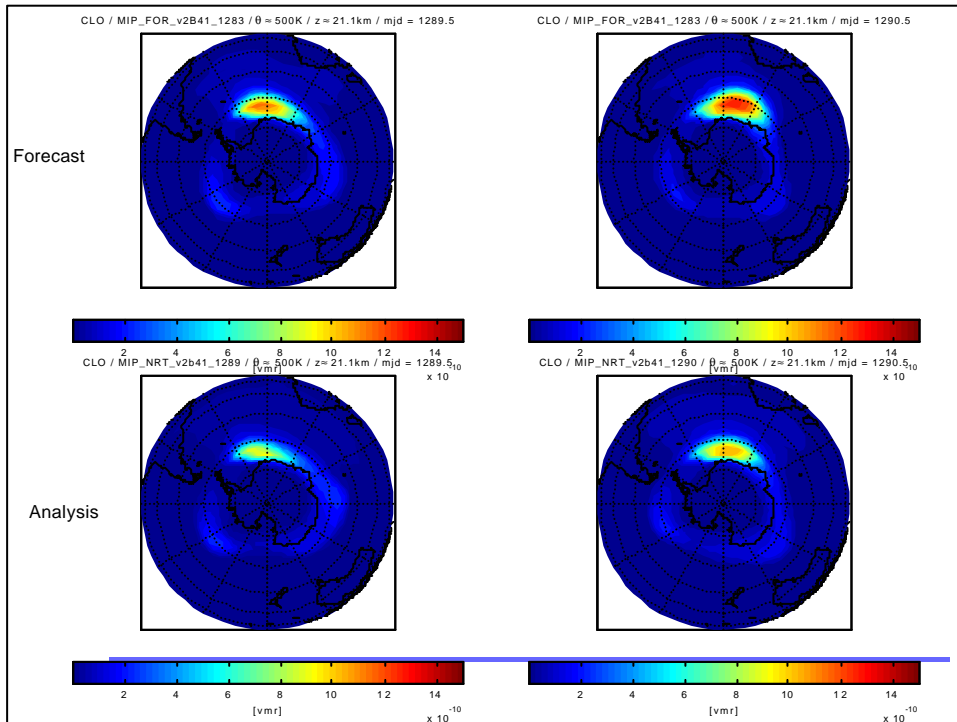
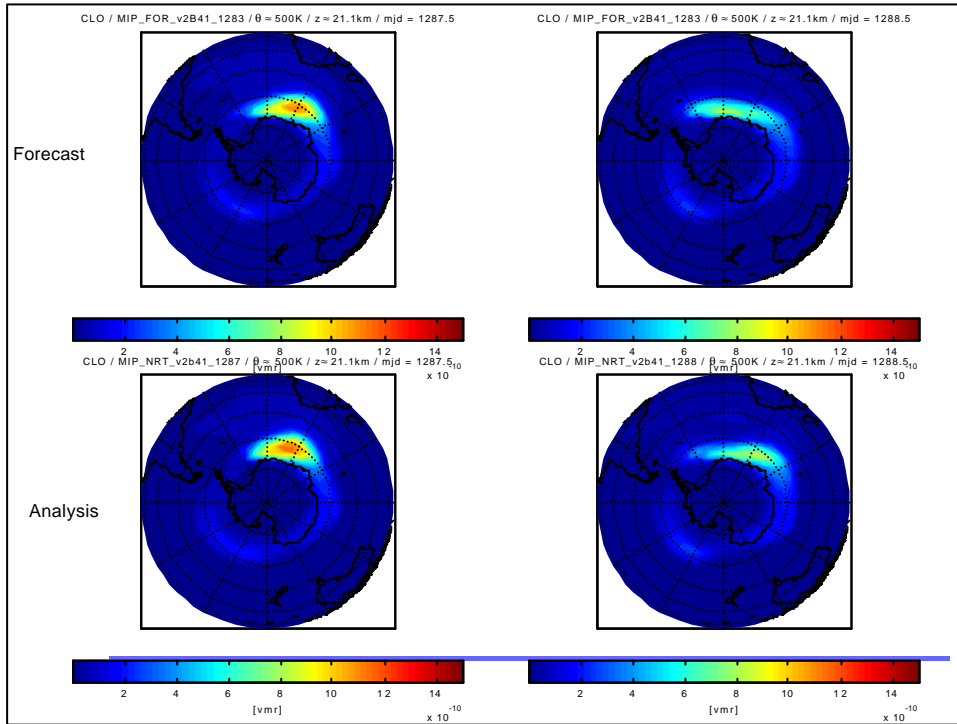


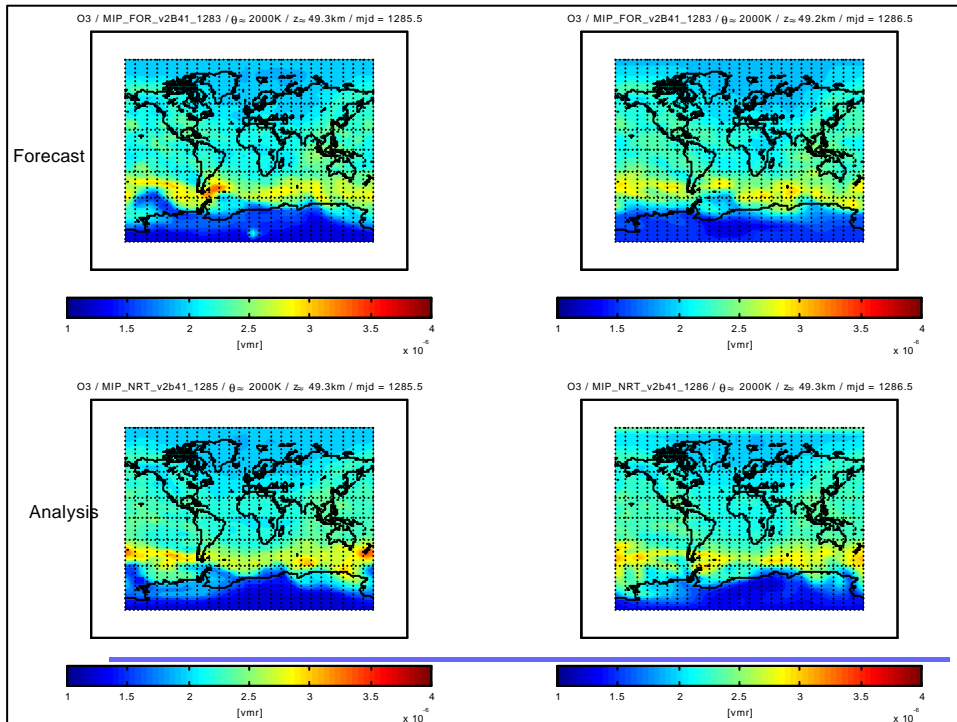
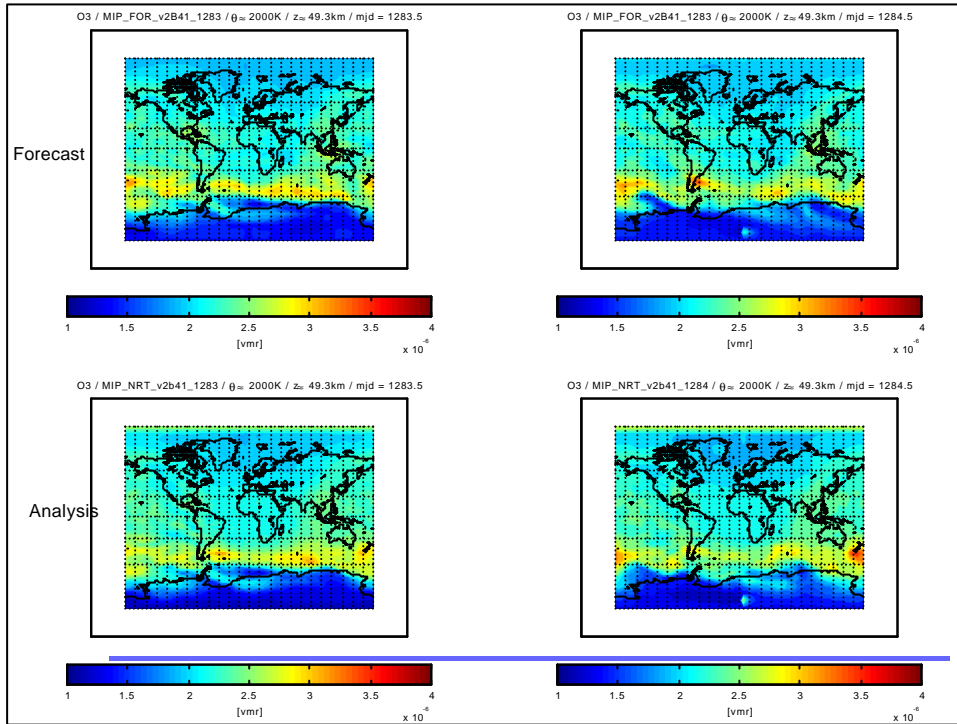




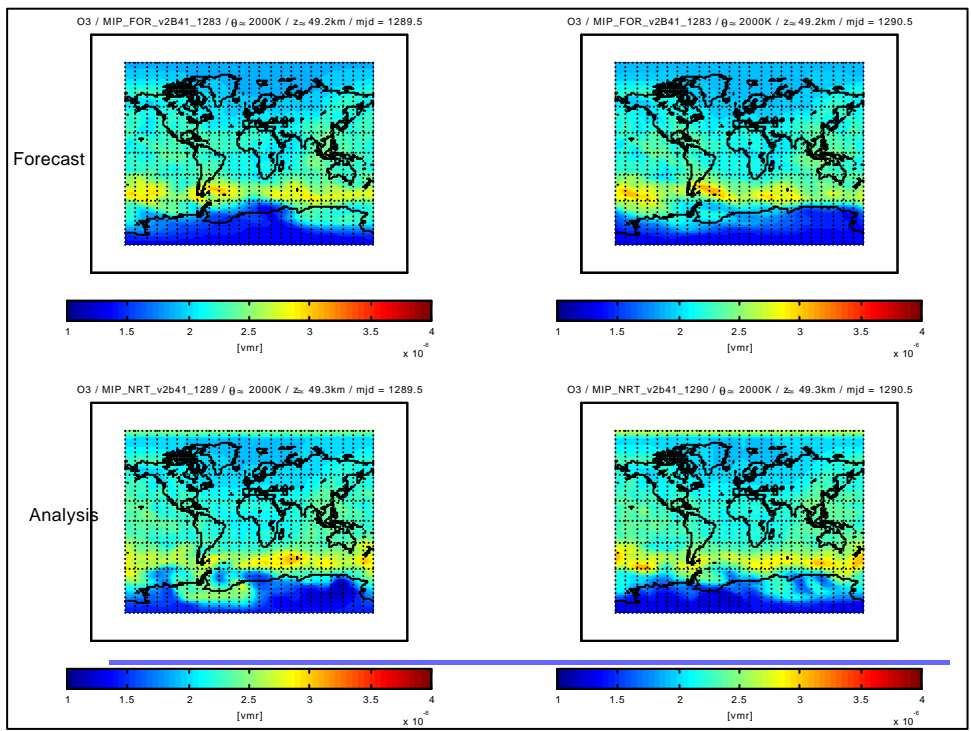
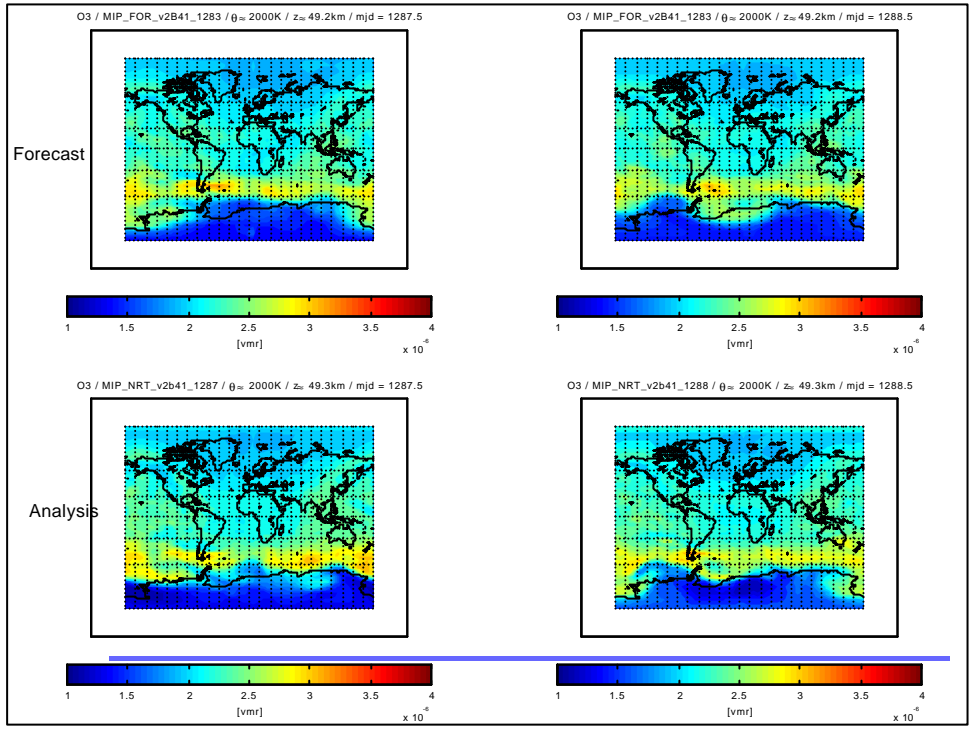












## Forecast skill: first estimate ILLUSTRATIVE

- H. Eskes Atmos.Chem.Phys., 2, 271-278, 2002
- Root Mean Square Error; f=forecast,a=analysis,c=climatology

$$RMSE = \frac{\sqrt{(f - a)^2}}{\sqrt{(a - c)^2}}$$

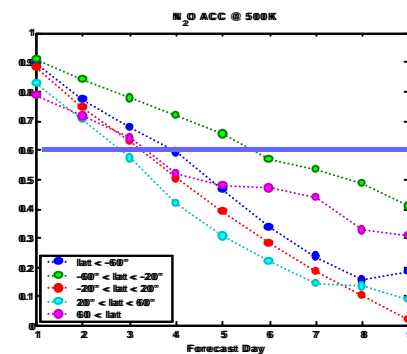
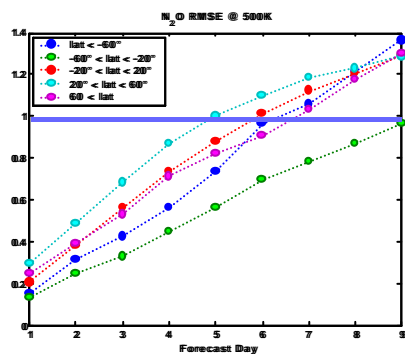
- Anomaly correlation coefficient:

$$ACC = \frac{(f - a)(a - c)}{\sqrt{(f - c)^2(a - c)^2}}$$

- Climatology: H. Eskes; modified climatology (running monthly mean)

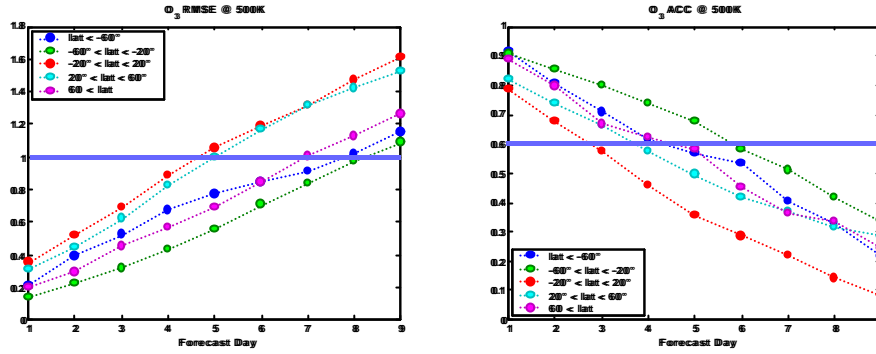
35

## Forecast skill N<sub>2</sub>O, Lower Strat. SH winter



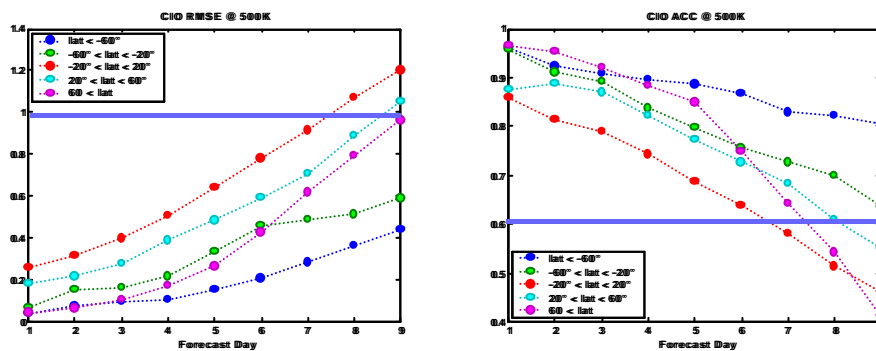
36

### Forecast skill O<sub>3</sub>, Lower Strat. SH winter



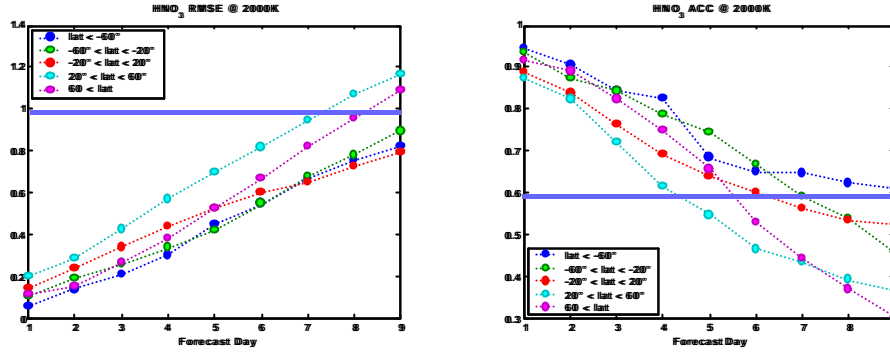
37

### Forecast skill ClO, Lower Strat. SH winter



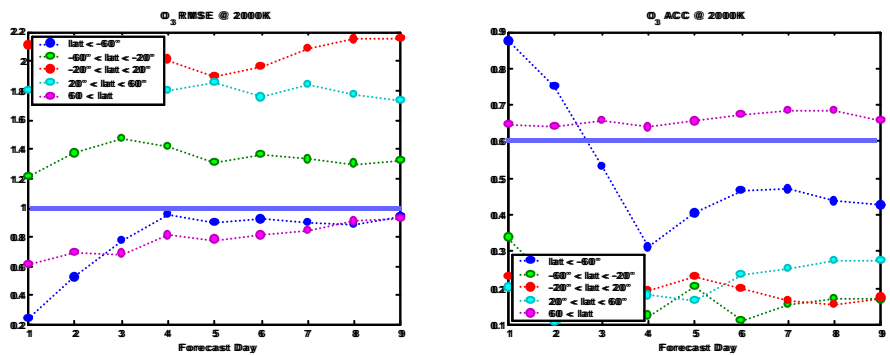
38

### Forecast skill $\text{HNO}_3$ , Lower Strat. SH winter



39

### Forecast skill $\text{O}_3$ , Lower Strat. SH winter



40

## Forecast skill: first estimate conclusion

- H. Eskes Atmos.Chem.Phys., 2, 271-278, 2002
- RMSE & ACC give similar picture
- ClO non-observed species: very good forecast skill?
- HNO<sub>3</sub> better than O<sub>3</sub>, N<sub>2</sub>O (tracer)
- Latitudinal & species dependence:
  - Assimilation & observational quality (biases, noise)
  - Effect of photo-chemistry
- A larger number of forecasts, investigation on modified climatology
- First illustration of stratospheric chemical forecast skill
- **STILL A LONG WAY TO GO**

---

41

## Chemical stratospheric forecasts conclusion

- Chemical forecasts set-up like NWP set-up
- “More expensive” (computer time) than NWP (3-5 times)
- First set-up for Cal/Val
- Scientific value
- Other domains:
  - A priori information for retrieval
  - Precursor of chemical weather

---

42