AQ-CHEM - Air quality sensitivity to temperature variability

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Young Scientist Summer School 2011

on Integrated Modelling of Meteorological and Chemical Transport Processes / Impact of Chemical Weather on Numerical Weather Prediction and Climate Modelling

Odessa State Environmental University

Task - Motivation

- Assessing the air temperature – chemical composition interactions and feedbacks

- *temperature changes <=> chemical reaction rates*
- *temperature variations <=> photolysis rates*
- *temperature variability <=> chemical compound concentrations*
- *temperature dependence <=> gases in urban/rural areas*

1D Enviro-HIRLAM: a short overview

- 1-dimensional version of Enviro-HIRLAM for chemical studies => **no advection**
- 80 vertical levels – Sigma Coordinates
- 150 second timestep
- Simulation for 4 days – reducing the dependency on estimated initial concentrations

Input:

- Vertical profiles of T and q
- Chemical reaction temperature
- Initial chemical compounds concentration (60 gases)
- Emissions (urban/rural/marine studies)
- Geographical location and time (UV variation)
- Land cover

Air quality – Ozone

Ozone Concentration (ppm) (8-hour average, unless noted)	**Air Quality Index Values**	**Air Quality Descriptor**
0.0 to 0.064	0 to 50	Good
0.065 to 0.084	51 to 100	Moderate
0.085 to 0.104	101 to 150	Unhealthy for Sensitive Groups
0.105 to 0.124	151 to 200	Unhealthy
0.125 (8-hr.) to 0.404 (1-hr.)	201 to 300	Very Unhealthy

-> Tropospheric Ozone, as a toxic gas, is an important indicator for air quality

Air quality – Ozone
Application: Forecast USA 08.07.11

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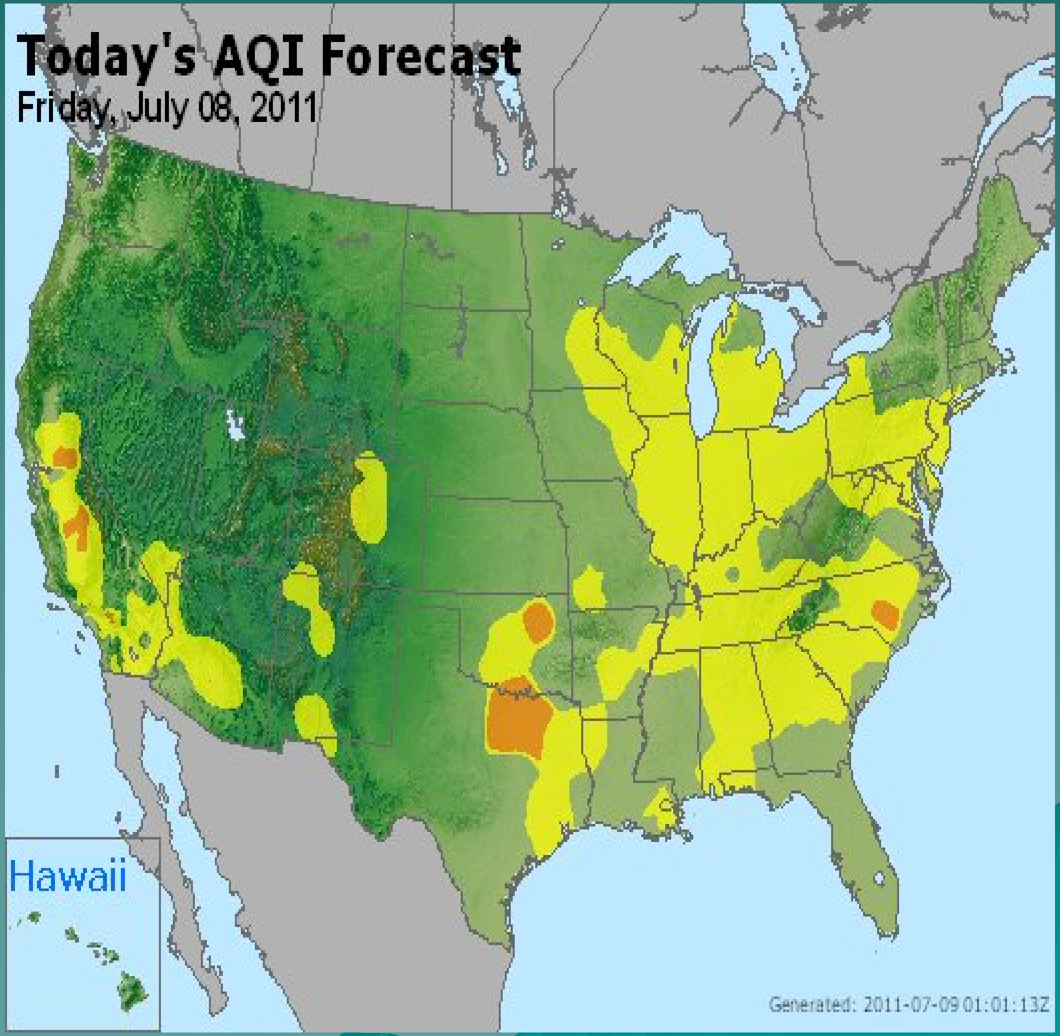


Chemical Reaction Feedback

Arrhenius Equation:

$$k = \underbrace{\pi d^2 \left(\frac{8k_B T}{\pi\mu}\right)^{1/2}}_{A} \exp\left(-\frac{E}{RT}\right)$$

k – chemical reaction rate
A – empirical constant
E – Energy of activation of reaction
R – Gas constant
T - Temperature

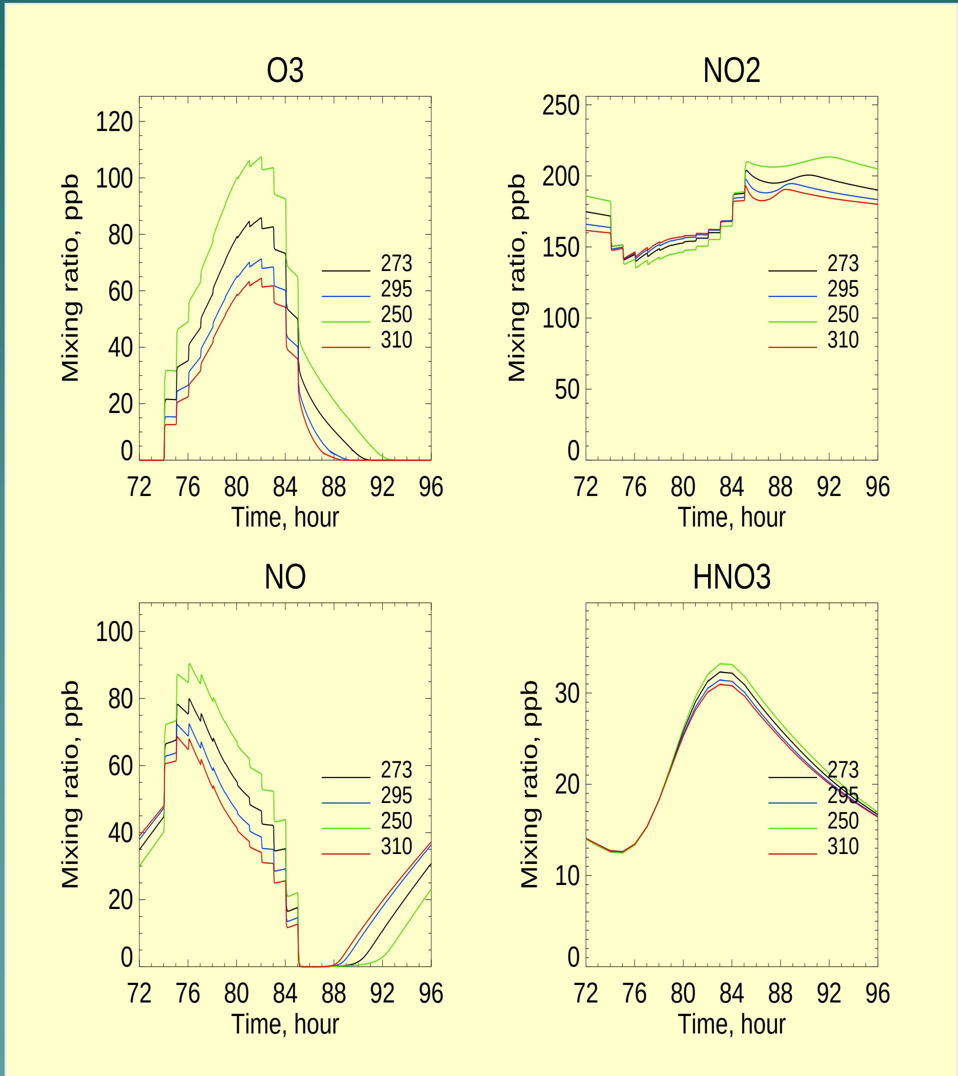
$$k(T) = \left\{\frac{k_0(T)[M]}{1 + \frac{k_0(T)[M]}{k_\infty(T)}}\right\} F^{\left\{\left(1+\left[\log_{10}\left(\frac{k_0(T)[M]}{k_\infty(T)}\right)\right]^2\right)^{-1}\right\}}$$

$$k_0(T) = k_0^{300} \quad (T/300)^{-n} \quad \mathrm{cm^6\ molecule^{-2}\ s^{-1}}$$

$$k_\infty(T) = k_\infty^{300}(T/300)^{-m} \quad \mathrm{cm^3\ molecule^{-1}\ s^{-1}}$$

- Rates of chemical reactions depend on temperature
- Heating or cooling leads to repartioning of chemical species
- With higher temperature, higher reaction rates are expected (if E is positive)

Enviro-HIRLAM simulation (urban)



- With higher temperature lower rates of Ozone are simulated

- Ozone formation is dependent on NOx and CO and hydrocarbons concentrations (this dependence has a maximum)

Photolysis Feedback

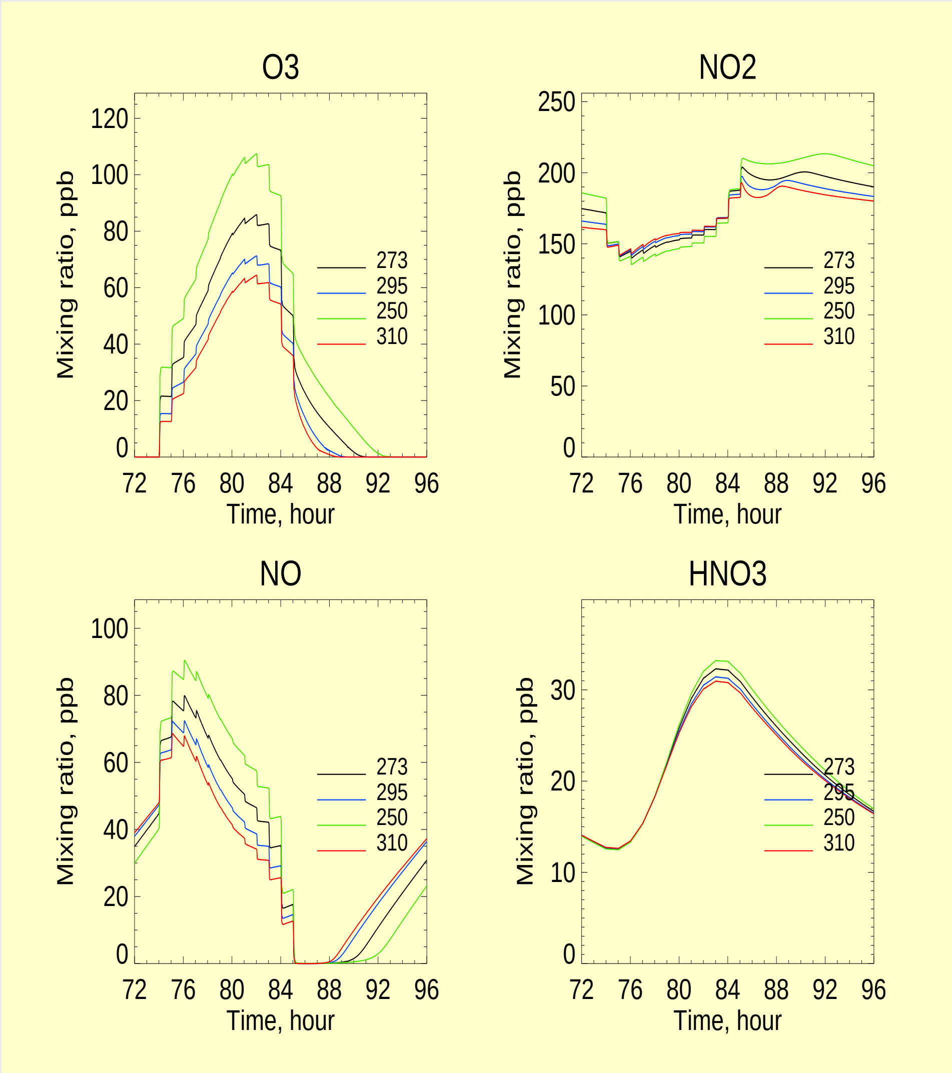
$$j_A = \int_{\lambda_1}^{\lambda_2} \sigma_A(\lambda, T)\phi_A(\lambda, T)I(\lambda)\, d\lambda$$

- Reactions which are dependent on radiation (wavelength)
- Diurnal cycle expected due to:

- Incoming short λ from the sun
- Outgoing long λ from the surface

- The model is not able to reproduce the feedback due to the absence cross-section and quantum yield –dependency of photolysis rates

Photolysis Dependence



- Reactions which are dependent on radiation (wavelength)
- Diurnal cycle expected due to:

\- Incoming short λ from the sun

\- Outgoing long λ from the surface

-> Diurnal cycle obvious

NOx concentrations in different environments

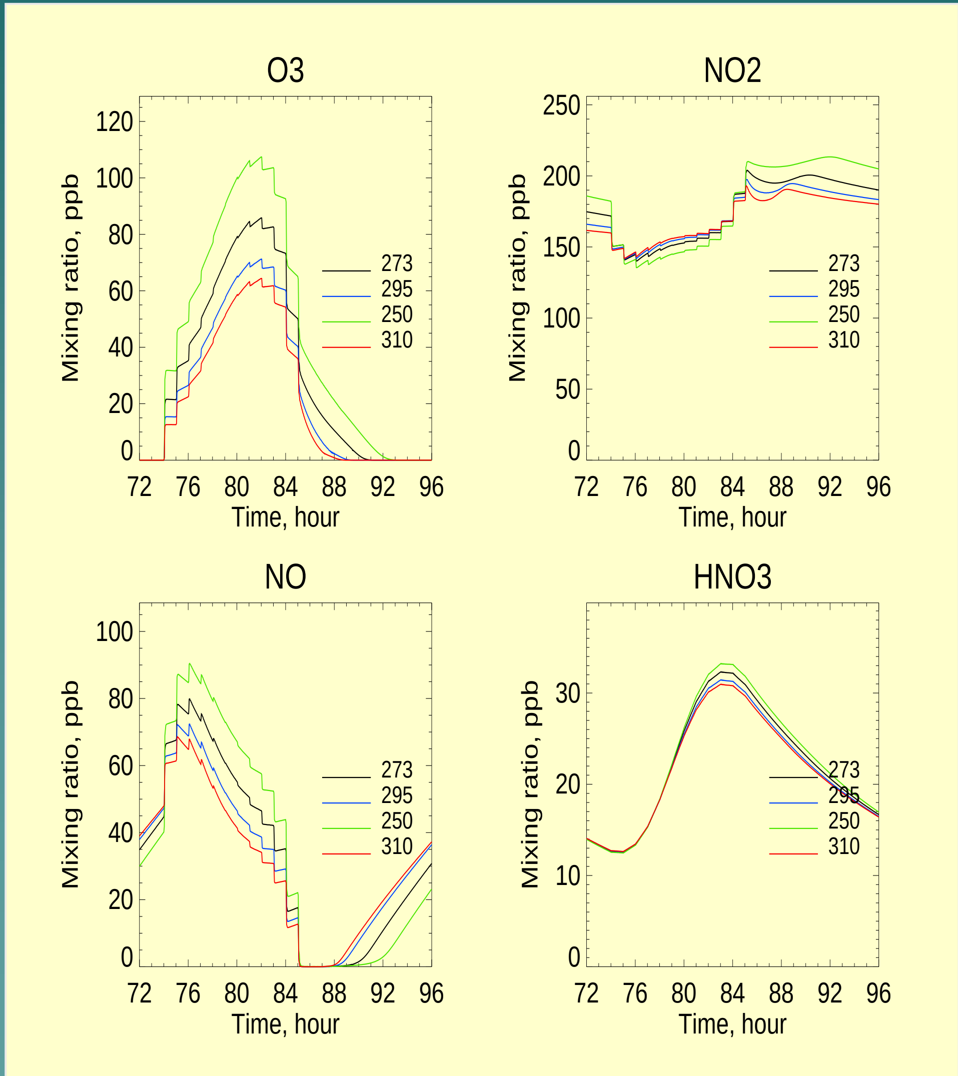
TABLE 2.7 Typical Boundary-Layer NO_x Mixing Ratios

Region	NO_x, ppb
Urban–suburban	10–1000
Rural	0.2–10
Remote tropical forest	0.02–0.08
Remote marine	0.02–0.04

Source: National Research Council (1991).

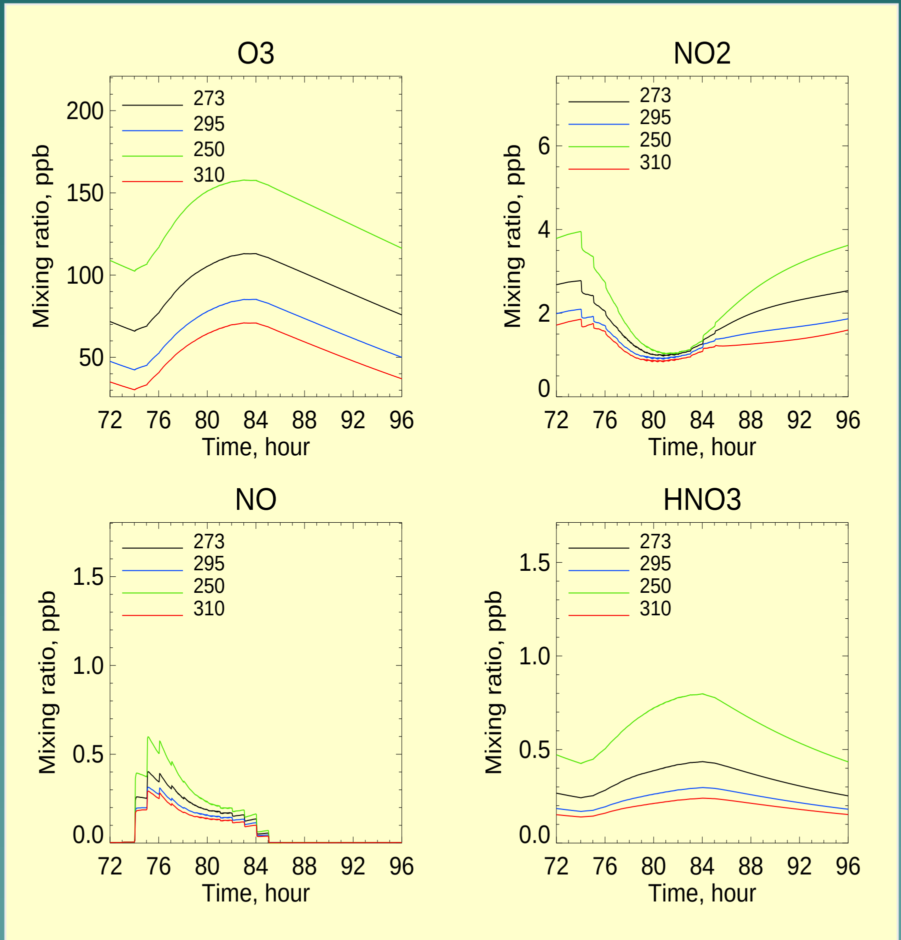
Range of NOx values vary in magnitude to a big extend dependant on the location

High NO_x emissions (urban)



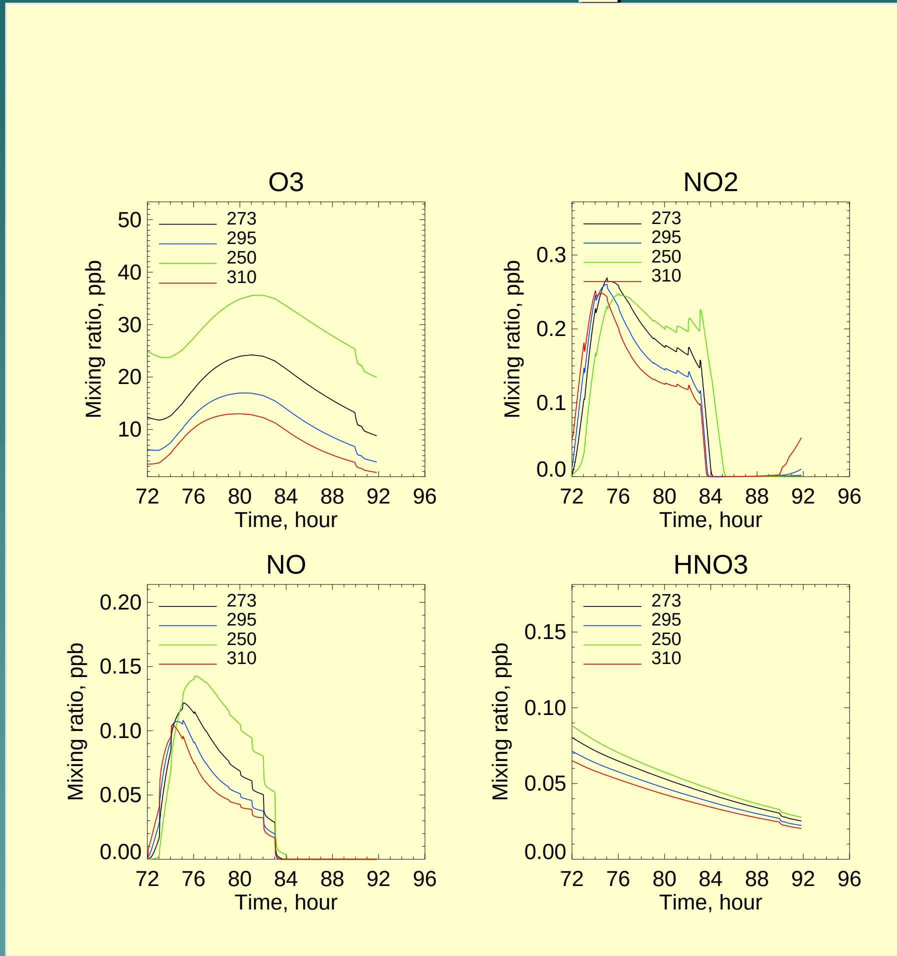
- Very high NOx values due to urban emissions
- High Ozone concentrations in the day-time
- Strong diurnal variations

Moderate NO_x emissions (rural)



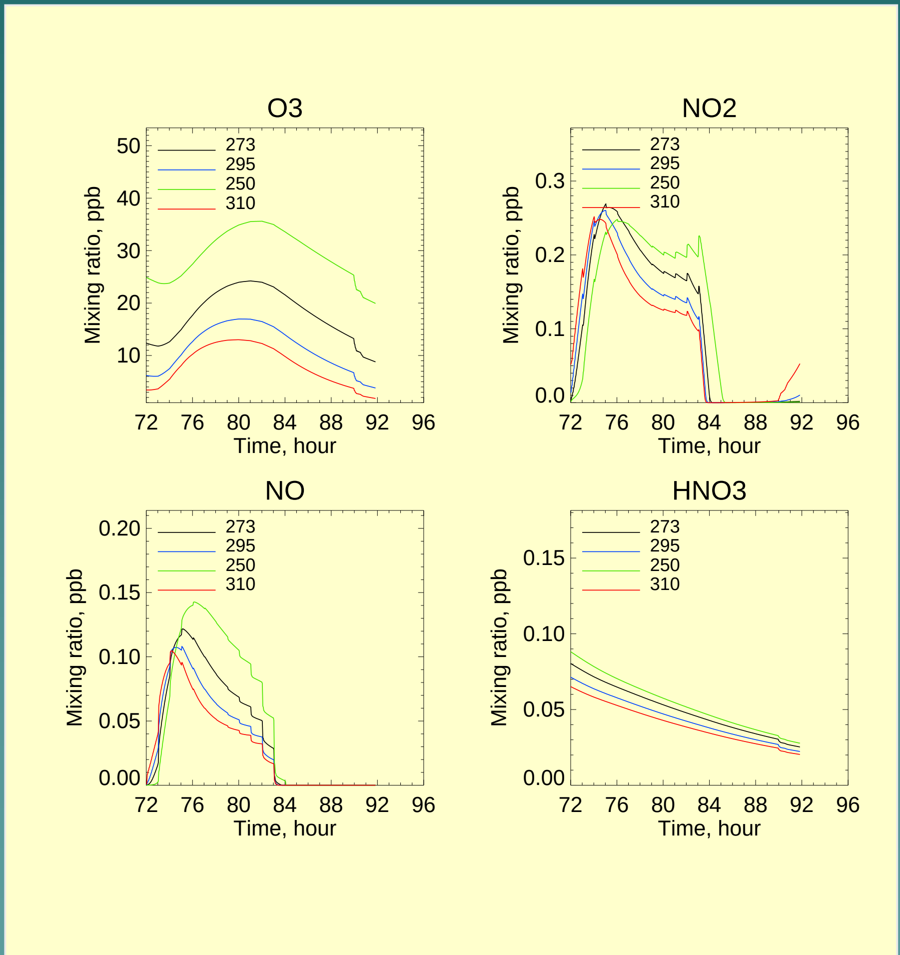
- High Ozone concentration
- Lower rural NOx emissions
- Diurnal variation lower than in urban areas

Low NO_x emissions (marine)



- Low values of Ozone and NOx
- Small diurnal variations

Low NO_x emissions (marine)



- Low values of Ozone and NOx
- Small diurnal variations

-> Urban, rural and marine regions reveal specific trace gas patters

Conclusions

- With higher temperature, lower ozone values (as an indicator of air quality) are observed
- Higher temperatures cause enhanced chemical reaction rates
- With lower temperature, the diurnal variations of all considered trace gases are more pronounced
- Characteristic patters for urban, rural and marine environments – i.e. clearly visible in the NOx concentrations

Thank you very much for your attention