Mass budget simulations of ozone in the city plume of Berlin for an episode of the BERLIOZ experiment

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Objectives

On July 20[th], 1998, an episode of the BERLIOZ Experiment, an ozone plume developed north-north-west of the City of Berlin. For this episode simulations have been carried out with the model system KAMM/DRAIS (Fig. 1). It allows calculating the individual contributions of different processes to the mass budget of an air pollutant like ozone (Fig. 2). The purpose of the modelling was to analyse the relevance of the different ozone mass budget components along the plume, especially, that of chemical transformation. Three different horizontal regions north of Berlin have been considered (Fig. 3). In order to investigate the vertical variations of the relevant processes, four layers above each area have been analysed (Tab. 1).

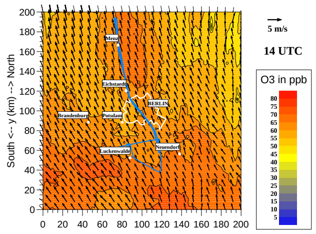

Fig. 1: Simulated ozone distribution (ppb) and wind field in 10 m above ground in the model area. Aircraft flight track is also shown.

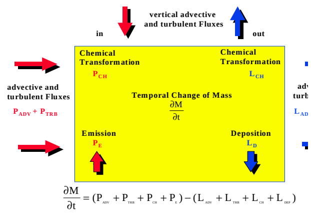

Fig. 2: Illustration of mass budget calculation

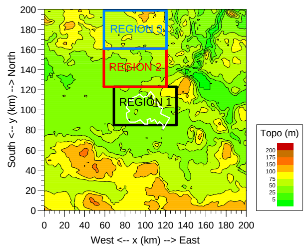

Fig. 3: Topography (m) around Berlin and locations of mass balance regions

	Vertical extension (m above ground)	Characterization
Layer 1	2000 - 5000	Free troposphere
Layer 2	1200 - 2000	Upper mixing layer
Layer 3	75 - 1200	Lower mixing layer
Layer 4	Ground - 75	Surface layer

Tab. 1: Vertical layers for mass budget calculations

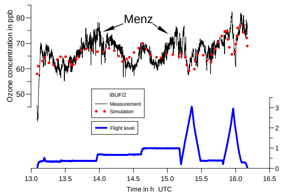

Fig. 4: Comparison of calculated ozone concentrations (ppb) and measurements onboard an aircraft flying through the plume

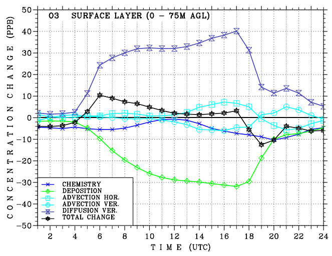

Fig. 5: Diurnal cycle of most important mass budget components in the surface layer (ground to 75 m) above region 1

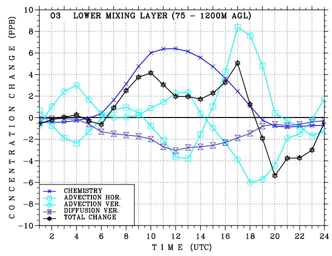

Fig. 6: Diurnal cycle of most important mass budget components in the lower mixing layer (75 m – 1200 m) above region 1

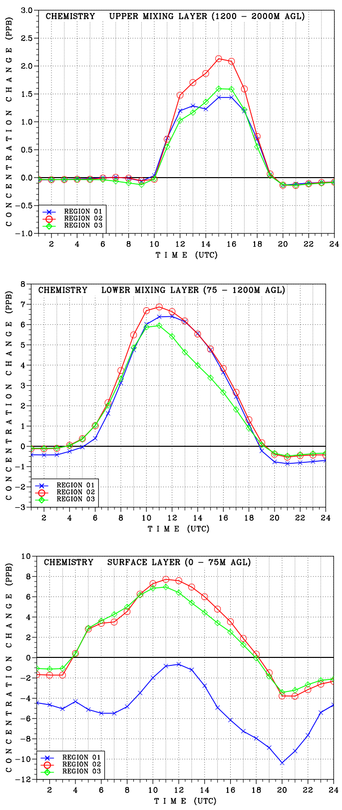

Fig. 7: Diurnal cycle of ozone formation rate due to chemical reactions in three layers above the three regions

Results and Conclusion

- **Comparison of model results with chemical measurements onboard of an aircraft flying through the plume in different levels shows acceptable agreement (Fig. 4). Maximum ozone concentration in the plume occurs about 70 km downwind of Berlin close to station Menz. The simulation underestimates this maximum by about 10 ppb.**
- **In the surface layer over the city (Region 1), chemical processes decrease the mean ozone concentration during the whole day (Fig 5, Fig. 7 bottom). Nevertheless, an increase of the ozone concentration occurs during daytime, because air from above, carrying a higher ozone load, is mixed downward. Deposition is the most dominant loss term. In the lower mixing layer (Fig. 6), chemical processes are mainly responsible for the change of the ozone concentration during daytime, independent of the considered region. In the late afternoon and the early morning, advection dominates the change of the ozone concentration in all layers because of changes in the wind field, and the decreasing influence of other processes.**
- **In contrast to Region 1, chemical production of ozone occurs in the surface layer above the regions 2 and 3 (Fig. 7, bottom).**
- **During daytime, ozone is produced chemically throughout the lower mixing layer above all regions (Fig. 7, middle). The production rate is most pronounced in region 2 (7 ppb/h at 11 UTC).**
- **The peak chemical ozone production in the upper mixing layer is remarkably reduced (Fig. 7, top), and it occurs in the afternoon. In the free atmosphere above, advective processes are dominating and the chemical production is of minor importance (not shown).**
- **In the afternoon, an ozone formation rate in the urban plume of about (6.5 ± 1.0) ppb/h have been derived from aircraft measurements in the lower mixing layer over the regions 2 and 3. Averaging the modelled ozone production rates over corresponding periods leads to values of 5.1 ppb/h for regions 2 and 3.5 ppb/h for region 3 (Fig. 7, middle). The last value is obviously too low, a result reflecting the underestimation of the ozone concentration in the plume at farther downwind distances. A corresponding comparison for the city provides the values (4.5 ±1.0) ppb/h and 5.0 ppb/h for the measured and simulated ozone production rates, respectively.**

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