Effect of the soil wetness state on the stomatal ozone fluxes over Hungary

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Abstract: A coupled Eulerian photochemical reaction-transport model and a detailed ozone dry deposition model have been utilised for the estimation of stomatal ozone fluxes over Hungary. Ozone concentrations were modelled on an unstructured triangular grid using a method of lines approach to the solution of the reaction–diffusion–advection equations describing ozone formation, transport and deposition. The model domain covers Central-Europe including Hungary, which was located at the centre of the domain and covered by a high resolution nested grid. The dry deposition velocity of ozone was calculated based on the aerodynamic, quasi-laminar boundary layer and canopy resistance. The effect of soil water content on the stomatal ozone flux was analysed. The stomatal ozone flux calculations were performed for two cases, with and without taking into account the effect of the soil moisture stress on the ozone deposition. The meteorological data were generated by the ALADIN meso-scale limited area numerical weather prediction model. It was found that soil water deficiency can strongly reduce the stomatal conductance and hence the ozone flux through it.

Keywords: dry deposition model; photochemical air pollution model; root-zone soil water content; ozone; stomatal flux.

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1 Introduction

Due to substantial emissions of ozone precursor species across Europe, elevated ozone concentrations may cover large areas of Europe for either shorter episodic or longer periods under certain meteorological conditions (Hjellbrekke and Solberg, 2002). These elevated concentrations can be harmful to agricultural and natural vegetation. Air quality measures, based on Accumulated exposure Over a Threshold (AOT) such as AOT40 were therefore developed based on experiment in order to try to mitigate the damage (Fuhrer et al., 1997). However, since ozone enters plants through the stomata, the response of vegetation to changes in the atmospheric ozone concentrations is more directly influenced by the stomatal ozone flux than the atmospheric concentration itself. Therefore, it has been suggested that the stomatal ozone flux is a more appropriate measure for ozone damage than the AOT40 value (Emberson et al., 2000a). This flux depends on several factors including the soil wetness state in moderate soil water availability conditions. To this end, the goal of this study was to analyse the sensitivity of stomatal ozone flux to the soil wetness state over Hungary.

Root-zone soil water content plays an important role in stomatal conductance. In the Soil-Vegetation-Atmosphere (SVAT) models, the effect of available soil moisture on stomata in general is described in two different ways. Some of these models use the leaf water potential (Ács and Hantel, 1998, 1999; Brook et al., 1999; Zhang et al., 2002) and others the soil water potential or soil water content (Bassin et al., 2004; Calvet et al., 2004; Emberson et al., 2000b; Grünhage and Haenel, 1997; Meyers et al., 1998). Ács (2005) showed, that these two different estimations should give the same results for a consistent soil parameter set. Since the latter method is simpler than the former one, it is more suitable for routine applications. It must be noted that in some other models (Smith et al., 2000) the effect of soil moisture stress is omitted. This approximation can be suitable in well-watered regions, but under continental climatic conditions, especially during the summer months, soil wetness cannot be neglected.

Based on a previous investigation (Lagzi et al., 2004), it seems that in continental regions, soil water deficiency can strongly reduce the stomatal conductance and so the ozone flux through it. This former study has pointed out that in Hungary the dry deposition velocity of ozone depends on the soil water content during the daytime, when stomatal deposition is dominant. For high soil water contents, deposition is also influenced by atmospheric and surface characteristics and can be highly spatially variable. However, in the earlier studies only prescribed soil water fields were used. In contrast, in this study the soil water field has been calculated using a simple water-budget model developed by Mintz and Walker (1993). Utilising the results of this model, an Eulerian photochemical reaction–transport model coupled with a detailed ozone dry deposition model was applied for estimating the stomatal deposition of ozone over Hungary. The combined model was tested for a sunny, summer day (23 July 1998). The stomatal ozone flux was estimated with and without taking into account the effect of the soil moisture stress. Results show that under continental climatic condition, the soil state can be a crucial factor in determining the extent of stomatal ozone deposition.

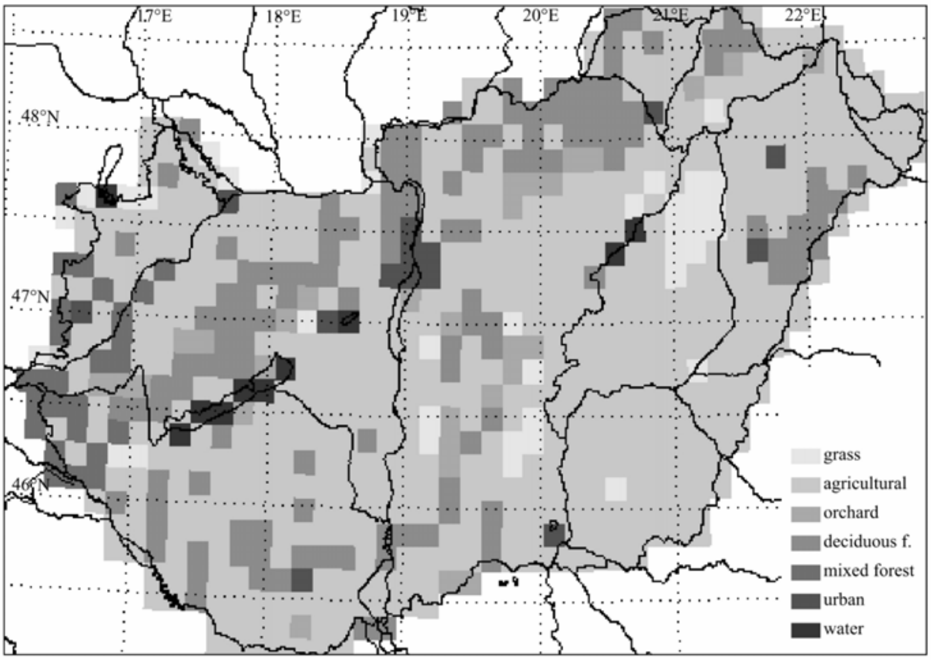
2 Materials and methods

2.1 The coupled dipersion–deposition model

An Eulerian reactive transport and a deposition model have been coupled for estimating the effective ozone load over Hungary. The deposition velocity of ozone was calculated as the inverse of the sum of the atmospheric and canopy resistances, where this latter term was parameterised by stomatal, mesophyll, surface and cuticular resistances. The reaction–diffusion–advection equations relating to ozone formation, transport and deposition were solved on an unstructured triangular grid using the 'method of lines' technique. This approach reduced the partial differential (reaction–diffusion–advection) equation set to a system of ordinary differential equations where the independent variable is the time. The two main steps of 'method of lines' were the spatial discretisation and time integration. Our model uses a flux limited, cell centred finite volume scheme on an unstructured triangular mesh (Berzins and Furzeland, 1992; Berzins and Ware, 1995, 1996; Berzins et al., 1989). The resulting system of ordinary differential equations can then be solved as an initial value problem using the code SPRINT2D (Berzins and Furzeland, 1992; Berzins and Ware, 1995, 1996; Berzins et al., 1989). The model grid structure during the simulations included a fixed fine nested grid over Hungary (980 km × 920 km), which had edge size of 12.5 km and a coarse grid outside of the rectangle covering Hungary. This coarser grid was characterised by edge length of 100 km. The model applies Dirichlet and Neumann type boundary conditions depending on the advective fluxes over boundary edge. The boundary conditions are imposed through the approximate Riemann solver. The vertical stratification is presented using four horizontal layers. These are the surface, the mixing, the reservoir and the free-troposphere layer, respectively. The vertical mixing of pollutants is approximated by a parameterised description of mixing between the layers. This is achieved by parameterisation of the vertical eddy diffusion (set of coupled ordinary differential equations) between the surface and mixing layers and fumigation between the mixing layer and either the reservoir or upper layer above it. The coupled air quality model used the Emission Inventory for Budapest (1 km × 1 km), the National Emission Inventory (20 km × 20 km) for Hungary and EMEP inventory data for outside the country. The model uses the Generic Reaction Set (GRS) gas-phase chemical kinetic scheme to describe the photooxidant formation (Azzi et al., 1992). This mechanism represents seven species interacting in seven reactions. Although, the model also allows the utilisation of larger reaction schemes. Photolysis rate constants are expressed as *m*th order rate constants with units (molecule cm^3) $m^{-1}s^{-1}$.

The dry deposition velocity of ozone was estimated over different types of vegetation. The land-cover map was generated using a Hungarian land-use map (Figure 1) (National Atlas of Hungary, 1989). The model was applied on the grid of the meso-scale limited area numerical weather prediction model ALADIN (Horányi et al., 1996). The time and space resolution of the data was 6 hrs and 0.10° × 0.15°, respectively.

Figure 1 Land use categories in the model



The total ozone flux (F_t) was calculated as a product of the deposition velocity of ozone (v_d) and the ozone concentration (C_r) at a reference height (within the surface layer of the model).

$$F_t = v_d C_r \tag{1}$$

The deposition velocity is defined as the inverse of the sum of the atmospheric and surface resistances, which retard the ozone flux:

$$v_d = \left(R_a + R_b + R_c\right)^{-1} \tag{2}$$

where R_a, R_b and R_c are the aerodynamic resistance, the quasi-laminar boundary layer resistance and the canopy resistance, respectively.

The aerodynamic resistance is calculated using Monin-Obukhov's similarity theory taking into account the atmospheric stability. The procedure is described in detail in the work of Ács and Szász (2002). The boundary layer resistance is calculated by an empirical relationship after Hicks et al. (1987). The canopy resistance R_c is parameterised by equation:

$$R_c = \frac{1}{\left(R_{st} + R_{mes}\right)^{-1} + \left(R_s\right)^{-1} + \left(R_{cut}\right)^{-1}} \tag{3}$$

where R_{st}, R_{mes}, R_s and R_{cut} are the stomatal, mesophyll, surface and cuticular resistances, respectively.

The stomatal resistance can be calculated from the empirical formula of Jarvis (1976) referring to a vegetation canopy. This parameterisation requires knowledge of the soil and plant physiological characteristics:

$$R_{\mathrm{st}} = \frac{1}{G_{\mathrm{st}}(\mathrm{PAR}) f_t(t) f_e(e) f_\theta(\theta) f_{D,i}} \tag{4}$$

where G_{st}(PAR) is the unstressed canopy stomatal conductance, a function of PAR, the photosynthetically active radiation. This term is estimated after Zhang et al. (2001). The factors in the denominator range between 0 and 1 and modify the stomatal resistance: $f_t(t)$, $f_e(e)$ and $f_\theta(\theta)$ describe the effect of temperature, the vapour pressure deficit and plant water stress on stomata (Lagzi et al., 2004), while $f_{D,i}$ modifies the stomatal resistance for the pollutant gas of interest (for ozone, $f_{D,i}$ = 0.625 after Wesely (1989)).

The mesophyll resistance for ozone in the model is taken to be zero. Cuticular resistance, R_{cut} and surface resistance, R_{s} for ozone deposition were obtained as in Lagzi et al. (2004).

Ozone basically reacts by vegetation through the stomata. Therefore it is important to know the part of the total flux, which represents the stomatal uptake. Since we assumed that the flux is constant between the reference height and the top of the canopy, the total flux can be written as follows:

$$F_{\mathrm{t}} = C_{\mathrm{r}} \left(R_{\mathrm{a}} + R_{\mathrm{b}} + R_{\mathrm{c}} \right)^{-1} = C_{\mathrm{c}} R_{\mathrm{c}}^{-1} \tag{5}$$

where C_{c} is the concentration at the top of canopy. For estimating stomatal ozone flux, the total flux at the canopy top level is divided into stomatal (F_{st}) and non-stomatal (F_{nst}) deposition pathways:

$$F_{\mathrm{t}} = F_{\mathrm{st}} + F_{\mathrm{nst}} \tag{6}$$

and

$$F_{\mathrm{t}} = C_{\mathrm{c}} R_{\mathrm{st}}^{-1} + C_{\mathrm{c}} R_{\mathrm{nst}}^{-1} \tag{7}$$

Accordingly from Equation (5), the stomatal flux is calculated separately:

$$F_{\mathrm{st}} = C_{\mathrm{r}} R_{\mathrm{c}} \left(R_{\mathrm{a}} + R_{\mathrm{b}} + R_{\mathrm{c}} \right)^{-1} R_{\mathrm{st}}^{-1} \tag{8}$$

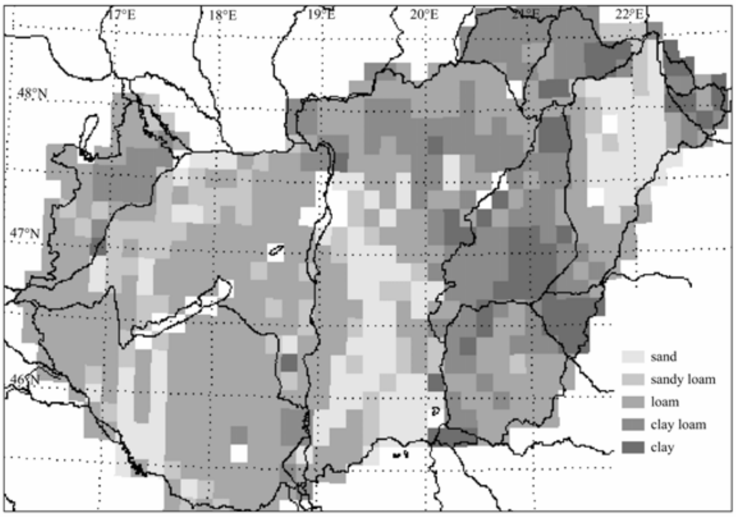
2.2 *The water-budget model*

Previous investigations (Lagzi et al., 2004) have shown that soil water content can strongly affect the stomatal flux. This influence is described by Equation (4) with the soil water stress function term $f_\theta(\theta)$. This can be parameterised using soil water content (θ):

$$f_\theta = \begin{cases} 1 & \text{if } \theta > \theta_f \\ \max\left\{ \dfrac{\theta - \theta_w}{\theta_f - \theta_w},\ 0.05 \right\} & \text{if } \theta_w < \theta \le \theta_f \\ 0.05 & \text{if } \theta \le \theta_w \end{cases} \tag{9}$$

where θ_w and θ_f are the wilting point and the field capacity soil moisture contents, respectively. These terms depend on the soil texture of the grid cell. The soil texture was determined from the work of Várallyay et al. (1980). The grid cell soil texture was represented by the dominant soil texture (Figure 2). The following soil texture categories were used in the model: sand, sandy loam, loam, clay loam and clay. The θ_w and θ_f values for different soil textures were taken from Ács (2003).

Figure 2 Soil types in the model



In Hungary, under continental climatic conditions, deposition is frequently obstructed by soil water deficiency. Soil water content, θ can be modelled by a simple bucket model (Mintz and Walker, 1993). The model estimates the soil water content in the root-zone using a daily time step. Vegetation can take up water from the root-zone. Horizontal water transport in the root-zone and interaction with deeper soil layers are neglected. Water surplus overflows at the surface.

The soil water content on the ith day (θ_i) is calculated as the sum of the soil water content and the water budget component on the (i – 1)th day:

$$\theta_i = \theta_{i-1} + \left(P_{i-1} - I_{i-1}\right) - \left(T_{i-1} + E_{i-1}\right) \tag{10}$$

where P_{i-1}, I_{i-1}, T_{i-1} and E_{i-1} are the precipitation, the interception, transpiration and vaporation on the (i – 1)th day, respectively (all terms expressed in mm). Interception is parameterised as:

$$I_{i-1} = \min\left(P_{i-1}, \mathrm{PE}_{i-1}\right) \tag{11}$$

where PE_{i-1} is the potential evapotranspiration. There are a number of possible parameterisations for potential evapotranspiration, but a common one used for Hungary has been constructed by Antal (1966):

$$\mathrm{PE}_{i-1} = \frac{1-(f/100)}{2-(f/100)} t_n \tag{12}$$

where f [%] and t_n [°C] are the average daily values of relative humidity and temperature on the (i – 1)th day, respectively. For temperatures below 0°C, the potential evapotranspiration is equal to zero in the model. In this case water cannot diminish in the bucket and can only increase by precipitation.

The term T_{i-1} + E_{i-1} (transpiration + evaporation) is expressed by a $\beta_{T,E}$ stress coefficient:

$$\left(T_{i-1} + E_{i-1}\right) = \beta_{T,E}\left(\mathrm{PE}_{i-1} - I_{i-1}\right) \tag{13}$$

where

$$\beta_{T,E} = \frac{\theta_{i-1} - \theta_{\omega}}{\theta_{f} - \theta_{\omega}} z_r \tag{14}$$

Here θ_{i-1} is the soil water content on the previous day and z_r is the root-zone in mm.

3 Results and discussions

The coupled transport-deposition model was applied for a simulation period from noon 22 July to midnight 23 July 1998. This case study was chosen since during the selected days, the high temperature, low cloud cover and low wind speed resulted in high photooxidant levels in Hungary. The initial concentrations of the major species were 0.4 ppb for NO_2, 2.0 ppb for NO, 80 ppb for O_3 and 4.1 ppb for VOC, which corresponded to typical daytime species concentrations. The initial concentrations were equal in each layer across the whole simulated domain.

To analyse the influence of soil moisture on the ozone flux, the soil water content has been calculated by a simplified water-budget model. This model was started from 1 July 1998 to obtain a realistic value of soil moisture content for the simulation day (23 July 1998). The initial θ values were chosen for each grid cell as the average of the wilting point and the field capacity soil moisture contents with respect to the given soil types. Distribution of soil water content is shown in Figure 3. The results indicate a good correlation with Figure 2, because the meteorological conditions before the simulation day had been optimal for soil water content (precipitation and evaporation were roughly in balance) and therefore the soil water content was mainly determined by soil type. The lowest soil moisture content values occur in the region where the soil type is sand, whereas the highest ones occur in the case of clay soil.

Figure 3 Calculated soil moisture content on 23 July 1998

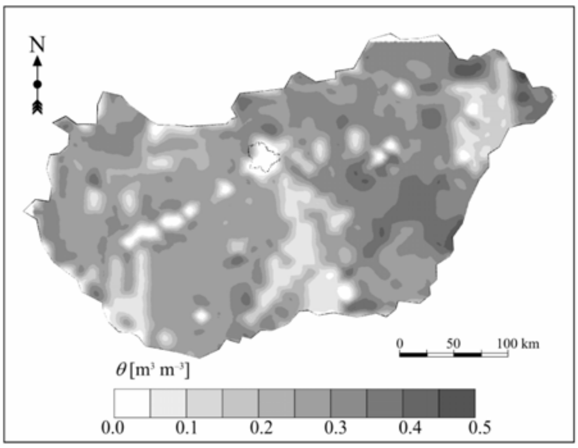
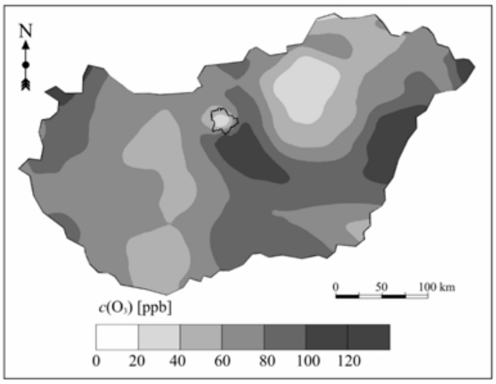


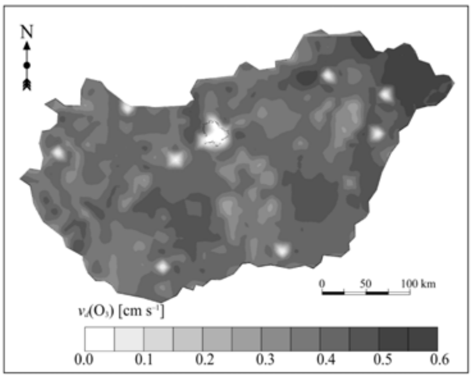
Figure 4 shows the simulated spatial distribution of ozone concentration at 12 UTC on 23 July 1998. The chosen period was the same as described in our previous paper (Lagzi et al., 2004), where model results were compared with measurement data. We have pointed out that the soil moisture practically does not affect the calculated ozone concentration. High ozone concentrations are obtained in the north-western and eastern parts of Hungary and also in southeast of the city of Budapest. In this region, elevated ozone concentrations appear due to the formation of a plume from the city's emissions. At the same time, low concentrations are observed in the city of Budapest, because of high concentrations of nitrogen oxide in the urban atmosphere, which titrates a large proportion of the ozone transported into the city.

Figure 4 Calculated ozone concentration on 23 July 1998 at 12 UTC



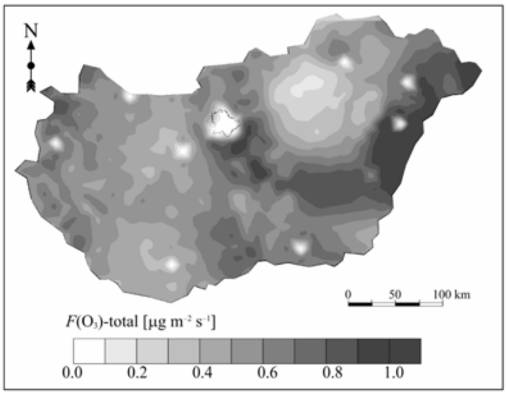
The distribution of the deposition velocities at 12 UTC on 23 July 1998 is presented in Figure 5. The calculated deposition velocities of ozone over different vegetation types are shown to vary between 0.1 and 0.6 cm s^{-1}, showing good agreement with the published observed data (see Lagzi et al. (2004)). The spatial variability within this range is quite high due to varying land use and soil types through soil wetness state.

Figure 5 Calculated dry-deposition velocity of ozone on 23 July 1998 at 12 UTC



The total ozone flux is the product of the deposition velocity and ozone concentration. Figure 6 shows the distribution of total ozone flux, where the effects of both concentration and deposition fields are apparent. For example, the highest values of the total ozone flux (around 1 μg $m^{-2}s^{-1}$) can be seen in the Eastern and North-Eastern parts of the country. In these regions both the concentration of ozone and its deposition velocity are higher. In the South Eastern region, the ozone concentrations were predicted to be high (>80 ppb). However, the predicted total ozone flux is relatively low due to low deposition velocities in this region, demonstrating possible flaws in the assumption that damage can be directly related to ozone concentrations.

Figure 6 Calculated total ozone flux on 23 July 1998 at 12 UTC



To utilise the soil moisture field, the stomatal part of ozone flux was calculated for two cases. The first represents a situation where the effect of soil moisture was neglected. This means that during the model run, the soil water stress function, $f_\theta(\theta) = 1$ was applied across the whole region. In line with this assumption, Figure 7 shows the distribution of stomatal ozone flux without considering spatial variability in soil moisture. This figure characterises a theoretical well-watered situation, where the soil moisture content is considered to be equal to the field capacity soil water content for the whole country. It also represents a high flux case since the stomatal conductance is not limited by soil water deficiency. A more realistic distribution of predicted stomatal ozone flux can be seen in Figure 8, where in the model calculations, an estimated soil water content field (see Figure 3) has been used.

Figure 7 Calculated stomatal ozone flux on 23 July 1998 at 12 UTC. Result corresponds to a supposed condition with sufficient soil wetness

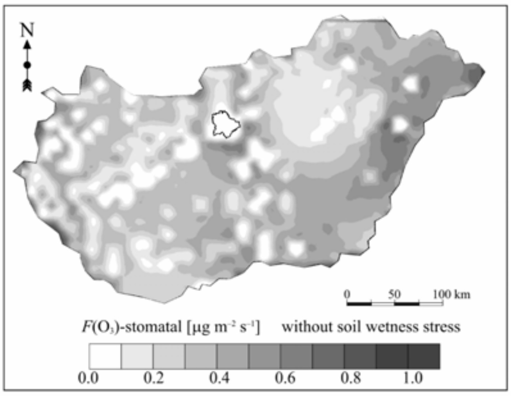
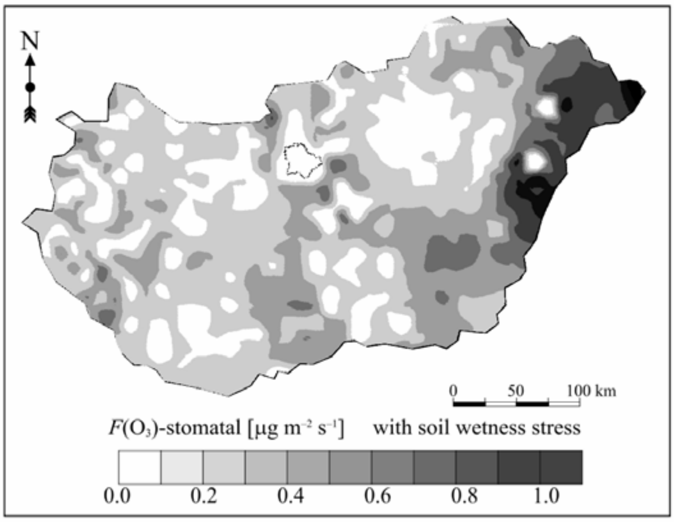


Figure 8 Calculated stomatal ozone flux on 23 July 1998 at 12 UTC. Result corresponds to the effective soil wetness condition



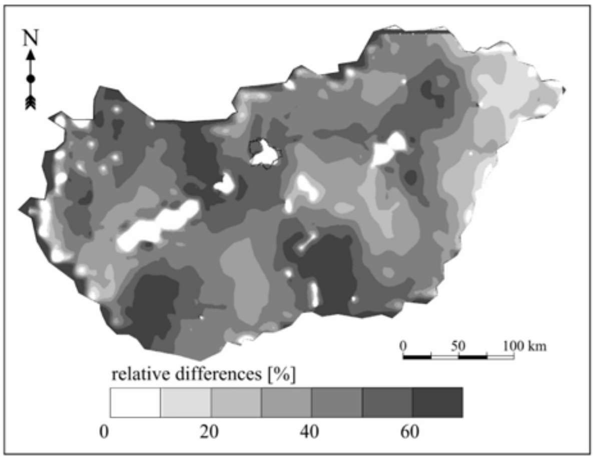
In both the cases the highest predicted stomatal fluxes are directly to the South East of Budapest and to the East of Hungary where the predicted ozone concentrations are over 100 ppb. Where soil wetness state is taken into account however, the predicted stomatal fluxes are substantially lower in most areas, reflecting the influence of soil water deficiency. The percentage differences between estimated stomatal fluxes for the two cases vary between 0% and 70% (Figure 9(a)). This term was calculated using $100(F_{st1}–F_{st2})/F_{st1}$, where F_{st2} and F_{st1} are the stomatal fluxes with and without taking into account the effect of the soil moisture stress, respectively. Figure 9(b) shows the equivalent absolute differences in stomatal fluxes between the two cases.

Evidently, there are no differences over urban and water covered areas where the stomatal flux for the base case was effectively zero. The effect of the soil wetness state however, influences the percentage differences between the two cases, as does the predicted ozone concentration.

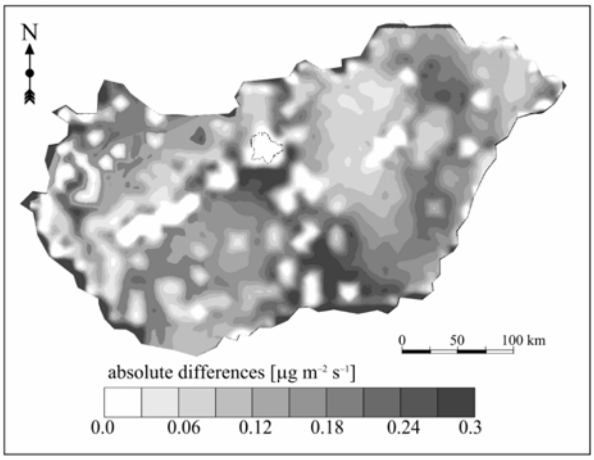
The greatest relative and absolute differences are seen in the South Eastern part of the country where sand and loam soil types with low soil moisture content are present and the predicted ozone concentrations are over 80 ppb. High absolute differences are also seen directly to the South East of Budapest where the predicted ozone concentrations are high and again the soils are mainly sandy. Both of these regions are predominantly agricultural. High relative differences are seen in the South West of the country, although the absolute differences here are lower due to the lower predicted ozone concentrations (around 60 ppb) in this region. Much lower relative differences between the two cases are seen in regions of clay soils such as the North Eastern tip of Hungary, where θ is effectively higher.

Although the results refer to a single day case study, they serve to illustrate the importance of representing the spatial variability of soil moisture content in calculating stomatal ozone fluxes. Further conclusions about the importance of such effects over a longer period, such as a growing season, will be the subject of future investigations.

Figure 9 Effect of soil wetness state: (a) relative and (b) absolute differences of stomatal resistances with and without soil wetness stress



(a)



(b)

4 Conclusions

A chemical transport model and a dry deposition model were coupled for the purpose of simulating ozone fluxes over Hungary. Accurate estimation of both the ozone concentration and deposition velocity fields facilitates the calculation of stomatal ozone flux. This flux is an accurate measure of the effective ozone load and has been shown to differ from the ozone concentration field due to spatial variability in land use and soil type. The stomatal ozone flux depends on the atmospheric conditions and the vegetation physiology. Previous investigations (Lagzi et al., 2004), have also shown that soil water content is another important factor which governs the deposition of ozone. The soil water deficiency can strongly reduce the stomatal conductance and so the ozone flux through it. In earlier studies, prescribed soil water fields had been used. In contrast, in this study the soil water field has been calculated using a simplified water-budget model. Stomatal ozone flux calculations were performed with and without taking into account the effect of the soil moisture stress on the ozone deposition.

The main conclusions that can be drawn from the study can be summarised as follows. For the hot, summer day tested, a significant difference in the spatial distribution of the stomatal flux between the two case studies was predicted. The obstructive effect of the soil wetness stress on the stomatal ozone deposition varies between 0% and 70%. These relative differences were shown to depend on both the atmospheric state, the vegetation type and also strongly on soil types and soil characteristics. This suggests, that the effect of soil water content cannot be neglected in the continental climate region, especially in the hot summer period. However, a particular analysis of the influence of soil on overall ozone deposition requires additional model calculations. In the future, it is planned to couple the transport-deposition model with the ALADIN meso-scale limited area numerical weather prediction model to estimate ozone deposition over Hungary for a routine application. Such longer term predictions, coupled with sensitivity analyses, will allow more detailed investigations about the relationships between soil, vegetation and the resulting ozone fluxes over the growing season.

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