Atmospheric Environment 143 (2016) 237–248

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

Evaluating stomatal ozone fluxes in WRF-Chem: Comparing ozone uptake in Mediterranean ecosystems

J.H. Rydsaa [a,*], F. Stordal [a], G. Gerosa [b], A. Finco [b], Ø. Hodnebrog [c]

[a] Department of Geosciences, University of Oslo, Oslo, Norway
[b] Dipartimento di Matematica e Fisica, Università Cattolica del S.C., Brescia, Italy
[c] CICERO- Center for International Climate and Environmental Research, Oslo, Norway

HIGHLIGHTS

- Validation of WRF-Chem estimates for stomatal uptake of ozone.
- Overestimated daytime ozone stomatal fluxes in particularly dry periods.
- Improved stomatal fluxes with VPD parameterization.
- Revision of both stomatal conductance parameterization and parameter values required.

ARTICLE INFO

Article history:
Received 4 December 2015
Received in revised form
18 August 2016
Accepted 19 August 2016
Available online 21 August 2016

Keywords:
Ozone
WRF-Chem
Wesely
Dry deposition
Ozone flux
Vegetation
Ozone uptake

ABSTRACT

The development of modelling tools for estimating stomatal uptake of surface ozone in vegetation is important for the assessment of potential damage induced due to both current and future near surface ozone concentrations. In this study, we investigate the skill in estimating ozone uptake in plants by the Weather Research and Forecasting model coupled with chemistry (WRF-Chem) V3.6.1, with the Wesely dry deposition scheme. To validate the stomatal uptake of ozone, the model simulations were compared with field measurements of three types of Mediterranean vegetation, over seven different periods representing various meteorological conditions. Some systematic biases in modelled ozone fluxes are revealed; the lack of an explicit and time varying dependency on plants' water availability results in overestimated daytime ozone stomatal fluxes particularly in dry periods. The optimal temperature in the temperature response function is likely too low for the woody species tested here. Also, too low nighttime stomatal conductance leads to underestimation of ozone uptake during night. We demonstrate that modelled stomatal ozone flux is improved by accounting for vapor pressure deficit in the ambient air. Based on the results of the overall comparison to measured fluxes, we propose that additional improvements to the stomatal conductance parameterization should be implemented before applying the modelling system for estimating ozone doses and potential damage to vegetation.

1. Introduction

Near surface ozone is a toxic oxidant, which in cases of high uptake can cause substantial damage to both human health and vegetation. The near surface background concentration of ozone in the Northern Hemisphere has more than doubled since pre-industrial times, and increased concentrations have in many areas reached values at which adverse effects to vegetation can be expected (Hollaway et al., 2012; IPCC, 2013; The Royal Society, 2008). The production efficiency of tropospheric ozone is determined by the availability of precursor gases as well as climatic and meteorological conditions, and the potential for future ozone induced damage is as such dependent on both emission controls and future climatic conditions (Emberson et al., 2013; Fowler et al., 2009; Klingberg et al., 2011, 2014).

There are various metrics in use in order to estimate the risk of ozone-induced damage to vegetation. Concentration-based indexes are the most traditional ones (CLRTAP, 2015; Mills et al., 2007), however; as high ambient air concentrations do not necessarily imply high uptake, adverse effects to vegetation are more

* Corresponding author. Department of Geosciences, Pb 1022 Blindern, 0316 Oslo, Norway.
E-mail address: j.h.rydsaa@geo.uio.no (J.H. Rydsaa).

http://dx.doi.org/10.1016/j.atmosenv.2016.08.057
1352-2310/

appropriately represented by a flux based approach, which relates risk to the actual absorbed stomatal ozone dose (e.g. CLRTAP, 2015; Gerosa et al., 2009c; Mills et al., 2011a; Pleijel et al., 2000; Simpson et al., 2007). The flux-based approach accounts for the various meteorological and environmental factors determining the stomatal flux, estimated by utilizing stomatal conductance parameterizations. Within the United Nations Economic Commission for Europe (UNECE) Convention for Long Range Transboundary Air Pollution (CLRTAP), the flux based approach is used to assess potential damage to present and future ecosystems (CLRTAP, 2015). Application of this approach also requires flux-response relationships, determining the actual damage done per absorbed dose. Such flux-based critical levels for different types of vegetation have been developed (e.g. Mills et al., 2011b). There are several modelling tools available and under constant development for estimating ozone fluxes into vegetation, e.g. the DO_3SE model (Emberson et al., 2000) which is also implemented into the The European Monitoring and Evaluation Programme (EMEP) model (D. Simpson et al., 2003; H. Fagerli et al., 2004).

The Weather Research and Forecasting model (WRF) coupled with chemistry (hereafter referred to as WRF-Chem) (Grell et al., 2005), is employed for e.g. forecasting for field campaigns, testing in relation to air pollution abatement strategies, and assimilation of satellite and in-situ chemical measurements, and could possibly prove a versatile and powerful tool for estimating stomatal flux into vegetation and help indicate both present and future high risk areas for ozone damage to vegetation.

The WRF-Chem model is equipped with a dry deposition scheme based on Wesely (1989) (hereafter referred to as the Wesely scheme), in which stomatal conductance for gaseous species is calculated. This is a widely used dry deposition scheme applied in a range of global and regional chemical transport models and climate models for the purpose of estimating dry deposition velocities for a range of chemical species. As the Wesely scheme is a versatile and widely used parameterization, several studies have been focused on validating the dry deposition velocities produced by it (Fowler et al., 2009; Hardacre et al., 2015; Park et al., 2014; Wu et al., 2011). Some limitations to particularly the surface resistance have been highlighted, related to not accounting for water stress through parameterization of vapor pressure deficit or soil moisture deficit (Fowler et al., 2009; Hardacre et al., 2015). The importance of such effects on dry deposition and particularly stomatal conductance has been demonstrated (e.g. Büker et al., 2007; Fowler et al., 2009). Although identified as a potential source of uncertainty in the Wesely dry deposition scheme, the stomatal conductance and hence the stomatal flux estimates, have to our knowledge not been as thoroughly tested.

In this study, we aim to assess whether or not the WRF-Chem modelling system, with the Wesely deposition scheme, has the potential to provide accurate dose estimates based on ozone stomatal fluxes. Although the traditional purpose of the Wesely scheme has not been to estimate stomatal conductance on a species-specific level, a special investigation into this aspect of the parameterization is required as part of the process of assessing the skill of the modelling system in estimating stomatal ozone fluxes into vegetation. As some known sources of uncertainty in the current parameterization of surface fluxes are related to the parameterization of water deficiency, we place special focus on the ability of the current model system to handle meteorological conditions characterized by limited water availability.

Building on the findings of previous studies evaluating the Wesely scheme, we compare modelled fluxes to measurements in three different Mediterranean ecosystems, during spring and summer periods representing different environmental conditions and particularly levels of water deficiency. This will give an indication of the suitability of the modelling system in estimating potentially harmful ozone doses, and more particularly, how the known weaknesses in the current parameterization potentially influence the results. Also, Mediterranean ecosystems are anticipated to be some of the highest risk areas in Europe for ozone induced damage to vegetation because of high emissions of ozone precursors close to the ecosystems combined with favorable climatic conditions for ozone production both at the present and in the future (Cieslik, 2009; Emberson et al., 2013; Gerosa et al., 2009a). The estimation of stomatal flux in high water use efficient (WUE) Mediterranean ecosystems is especially sensitive to water availability in soil and air (Büker et al., 2007; Cieslik, 2009). We also discuss to what degree the current system may be improved, based on these results and on literature.

2. Model and methodology

To validate the WRF-Chem estimates of environmental conditions, ozone concentration and ozone fluxes into various types of vegetation, we compare modelled estimates with measurements gathered during field campaigns executed at three different sites in Italy, representing different vegetation types. The selected measurement periods represent varying water stress regimes as experienced by the measured vegetation.

2.1. Model setup

WRF (Skamarock and Klemp, 2008) is a weather prediction system with a wide variety of applications, across scales ranging from large-eddy to global simulations. In WRF-Chem, a chemistry module is completely embedded in WRF, allowing it to simulate the coupling between chemistry and meteorology. Here, we use the RADM2 chemical mechanism (Middleton et al., 1990; Stockwell et al., 1990), and for the land use data we have applied the standard USGS data provided within the WRF package. A summary of the setup and choices of key physical parameterization schemes and forcing data used in this study is given in Table 1.

The model is run with 40 s time step and output is written every hour for each of the selected measurement periods. In addition, five spin-up days are added ahead of each period. The vertical resolution is 42 layers from the ground to the model top at 50 hPa. The simulations were conducted for two nested domains. The outer domain is run at a resolution of 9 km $\times$ 9 km and provides boundary conditions for the inner domains, placed to zoom in on the measurement sites in Italy at a resolution of 3 km $\times$ 3 km. The simulation domains are shown in Fig. 1, along with the locations of measurement sites.

The outer domain solutions for the temperature, air moisture and wind are nudged towards the meteorological forcing data with a nudging coefficient of 0.003 s^{-1}. For the meteorological initial and boundary conditions, we use the ECMWF ERA Interim 6 hourly reanalysis. The chemical initial and boundary conditions are gathered from the OsloCTM3 chemical transport model (Søvde et al., 2012), also at a frequency of 6 h. The NMVOC species in the OsloCTM3 model were mapped to the corresponding RADM2 components. For the anthropogenic emissions we use the TNO MACC II (Kuenen et al., 2014) gridded anthropogenic emission database. As demonstrated by Hodnebrog et al. (2011) the resolution of the emission inventory is important in accurate modelling of ozone distribution. Therefore, for the purpose of this study we have been given access to the TNO MACC II high resolution dataset (Denier van der Gon, pers. comm.), covering Europe with a resolution of 1/8° latitude by 1/16° latitude (~7 km $\times$ 7 km) (Denier van der Gon et al., 2010a; Denier van der Gon et al., 2010b). The emissions are re-gridded to fit the WRF-Chem grid and distributed in