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Original Scientific Article

Modeling of Ozone and Hydrogen Peroxide in Air

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Abstract. Ozone (O_3) and hydrogen peroxide (H_2O_2) volume fractions were calculated using the Master Mechanism (MM) model, author S. Madronich (NCAR, Boulder, CO, USA). MM is an atmospheric "box" model program for calculating the time evolution of atmospheric composition from initial amounts of atmospheric gases under chosen or varying conditions using reaction rate data and other physicochemical parameters. The photolysis coefficients were calculated using the Tropospheric Ultraviolet Visible (TUV) program of the same author. Data gathered during the field measurements in 2004[19] and modeled with the MM program[20] are used here to determine how gradual increase of one initial value of the following eight quantities: NO_2, CO, VOC (*i.e.* some volatile organic compounds), BTX (*i.e.* benzene, toluene, xylenes), H_2O_2, O_3, temperature and relative humidity, will in the MM modeling affect the volume fractions of either ozone or hydrogen peroxide. According to the model, H_2O_2 volume fractions in air increase with higher relative humidity and higher initial values of CO, VOC, BTX, H_2O_2 and O_3, and only decrease by NO_2. On the other hand, ozone volume fractions do rise with the increase of initial volume fractions of NO_2, as well as of CO, VOC, BTX, H_2O_2 and O_3. Temperature does not have any significant influence on the formation of H_2O_2 and O_3. The results also may explain the considerably higher ozone values measured at the airport than in the city of Zagreb.[22]

Keywords: free radicals, Master Mechanism model, nitrogen dioxide, peroxides, photochemical smog

INTRODUCTION

The oxidizing capacity of the atmosphere is its capability of "self-cleansing" by oxidation of emitted gases. The most important atmospheric oxidants are oxygen (O_2), ozone (O_3) and hydroxy ($OH^\bullet$) radical. Many compounds (*e.g.* methane, hydrocarbons, carbon monoxide) are removed from the atmosphere through reaction with the $OH^\bullet$ radical. However, elevated oxidant levels in the air have harmful effects on living organisms and many materials.[1–4]

Ozone and hydrogen peroxide (H_2O_2) are indicators of photosmog, photochemical pollution and the oxidative capacity of the atmosphere. In the troposphere, ozone is formed through the photolysis of nitrogen dioxide. The first ozone measurements in Croatia were carried out in the summer of 1975,[5] and it is the only oxidant continuously being measured by now.[6–10] H_2O_2 is formed in gaseous phase mostly by the recombination of two hydroperoxy ($HO_2^\bullet$) radicals, and its levels indirectly depend on the levels of $OH^\bullet$ radical. However, the use of H_2O_2 as an indicator of oxidizing capacity is somewhat limited by the expensive and sophisticated methods of measurements.[11] Ozone and hydrogen peroxide engage in many important atmospheric processes, including not only the reactions in gaseous phase, but also processes on particles and in aqueous phase, as well as on heterogenous surfaces, *e.g.* on gas-aqueous interface.[12] Both, O_3 by comparison with historical measurements,[13] and H_2O_2 by analysis of Greenland ice core samples,[14] show substantial growth of their presence in the atmosphere over the past hundred years. Recently, a simple method for photochemical pollution assessment from long term hourly averages of ozone data by means of calculated indicators has been proposed and applied for twelve EMEP-stations,[15] and later for several Italian, Slovenian and Croatian,[16] as well as some subtropical stations in the USA and in China.[17] Some non photochemical, statistical methods were also developed for ozone modeling. Such models can predict ambient ozone levels from environmental parameters (temperature, humidity, NO_2 levels, *etc.*) with an error of less than 5 ppb.[18]

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In 2004 field measurements of atmospheric constituents and meteorological parameters took place at the Ruđer Bošković Institute (RBI) in Zagreb in cooperation with German scientists.[19] The O_3 and H_2O_2 results were later modeled[20] using the MM and TUV programs developed by S. Madronich (NCAR, Boulder, CO, USA).[21] Here we intend to determine how the modeled O_3 and H_2O_2 values from that study are sensitive to an increase of initial values of eight input parameters (air temperature, relative humidity and levels of NO_2, CO, benzene, toluene, xylene - BTX, some volatile organic compounds – VOC, O_3, H_2O_2) by determining their resulting O_3 and H_2O_2 daily average and daily maximum values for each of the parameters increasing separately over a given range. Another reason for this study was also to explain the considerably higher ozone values measured at the airport than in the city of Zagreb[22] by elevated precursor (NO_2, VOC, BTX, CO) levels in air.

EXPERIMENTAL

In this study ozone and hydrogen peroxide levels in the air were modeled using the NCAR Master Mechanism (MM) model, version 2.4., developed by S. Madronich, and updated in April 2006.[21] The model includes about 5000 reactions in gaseous phase between about 2000 species, but was limited here to about 2300 reactions. Photolysis coefficients for these reactions were calculated using the Tropospheric Ultraviolet-Visible model (TUV), version 4.4, released May 2003, developed by the same author.[23,24]

The Master Mechanism is a multi-task interactive atmospheric box model program that gives an insight into the temporal behavior of atmospheric composition under selected, either fixed or variable, conditions[25,26] given the initial concentrations of various pollutants. It does not include transport, and describes best the reactions and transformations that occur within an air package at rest in a horizontal plane under the influence of sunlight and meteorological parameters. However, the model can also include the effects of some other processes like time-dependent dilution by changes in the height of the planetary boundary layer (PBL), temperature and pressure, emission, or deposition. It allows one to predict the time evolution of any reactive air composition as dictated by the corresponding reaction rate constants and physical parameters.

TUV is a one dimensional FORTRAN 77 radiative transfer model program able to quantify the transfer of radiation in a scattering and absorbing atmosphere. It can be used in the wavelength range of 121−750 nm for calculating the spectral irradiance, the spectral actinic flux, photo-dissociation coefficients and biologically effective irradiance. Output parameters are presented as functions of wavelength and altitude.

Table 1. Environmental data and initial conditions for TUV and MM models*

Parameter		Value
Latitude		45.833° N
Longitude		15.983° E
Altitude		180 m a.s.l.
Albedo		0.1
Aerosol vertical optical depth at 550 nm		0.235
Single scattering albedo of aerosols		0.99
Air number density/ molec. cm^{-3}		2.53×10^{19}
Air temperature / °C		20.0
Air pressure / hPa		1003
Relative humidity / %		35.6
Total ozone column / DU**		335
Volume fraction / ppb	H_2O_2	0.26
	O_3	42.6
	NO_2	9.8
	CO	204
	CO_2	330000
	Benzene	1.8
	Toluene	1.3
	Xylene	2.8
	C_2H_4	1.0
	C_3H_6	1.0
	CH_2O	1.0
	CH_3CHO	1.0
	CH_3COCH_3	1.0

*data for Ruđer Bošković Institute, Zagreb, date 26 June 2004.
**value from NASA/TOMS web site
http://toms.gsfc.nasa.gov/ozone/ozone_v8.html

The accuracy of the MM model was tested previously by comparing modeled[20] and measured H_2O_2 and O_3 values at one location in Zagreb (RBI) during the measuring campaign in summer 2004.[19] In this study, average daily values obtained from the same campaign were used for modeling purposes. As input volume fractions for O_3, H_2O_2, NO_2, CO, H_2O, benzene, toluene and xylene we used data on average volume fractions measured in Zagreb at the Ruđer Bošković Institute on 26 June, 2004. This day was characterized with sunny weather and clear-sky conditions, and for that reason, the data were suitable for MM modeling which is, mostly, limited only to gaseous phase reactions. Table 1 shows the environmental conditions and initial volume fractions for MM and TUV model used in our calculations. Daily variations of temperature and humidity were not simulated in the model. Owing to the lack of accurate data on emission sources, emission data were not included in the model. Instead, the daily cycle of NO was included in the model in order to simulate the influence of transport and emission. For NO, we used the daily cycle measured over the summer of 2004, as described in Acker *et al.*[19] Based on literature data[27] and on the first VOC measurements at Rudjer Bošković Institute, 1 ppb was taken as the input volume fraction for C_2H_4, C_3H_6, CH_2O, CH_3CHO, and CH_3COCH_3. Changes in the PBL during the day were also taken into account within the model, based on the values of Jeričević *et al.*[28]

RESULTS AND DISCUSSION

In previous study, when modeled and measured H_2O_2 and O_3 values were compared at one representative location, it was found that such model needs to be corrected for local emissions, especially due to NO_x emission from vehicle exhausts. Master Mechanism is a "box" model and does not include transport processes. However, Acker *et al.*[19] simulated the influence of NO emission by using daily NO cycle in the model. It was found that on cloudless days, maximum hourly H_2O_2 volume fractions were calculated with relative differences of less than 20 %. For O_3, the relative difference was less than 12.5 % for the calculation of daily maximum hourly values and less than 25.3 % for the calculation of average daily values.[19,20] The model overestimates H_2O_2 and O_3 volume fractions systematically.

For that reason, in further calculations the model with the daily NO cycle was used. Here we included daily NO variations with maximum values at 8:00 and 18:00 hrs. NO levels between 0 and 0.05 ppb were assumed overnight. Figures 1 and 2 show the comparison of modeled H_2O_2 and O_3 values (with and without daily cycle) together with measured values over the 5-day period (26 June – 1 July, 2004). It is obvious that, if only the initial value for NO (average daily value of 0.9 ppb) was used, the model overestimates the average concentrations and also fails to show the characteristic daily variations. In the case of H_2O_2, values increase rapidly over the first two days and then stay between 3.0 and 3.5 ppb. Volume fractions of NO and NO_2 rapidly decrease over the first day and then stay below 0.2 ppb. At the same time other nitrogen compounds are formed (*e.g.* NO_3 radical, HNO_2, HNO_3). In a model with included NO cycle the resulting O_3 and H_2O_2 volume fractions resemble the measured values more closely.

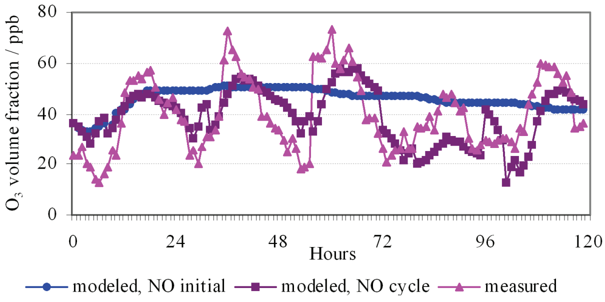

Figure 1. Comparison of modeled O_3 values (with and without daily cycle of nitrogen monoxide) together with measured values over the 5-day period (26 June – 1 July, 2004).

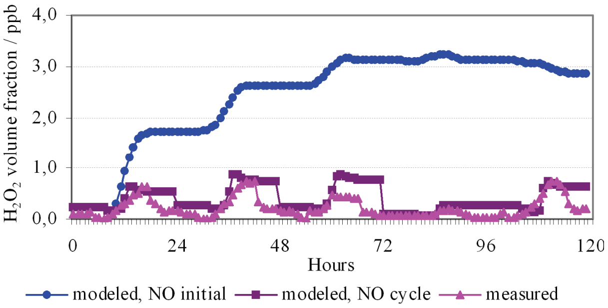

Figure 2. Comparison of modeled H_2O_2 values (with and without daily cycle of nitrogen monoxide) together with measured values over the 5-day period (26 June - 1 July 2004).

Tables 2 and 3 show how changes in some initial conditions do influence the levels of ozone and hydrogen peroxide in the air. The influence of eight parameters in such MM model was analyzed separately. During BTX and VOC calculations, volume fractions of all hydrocarbons were increased consecutively (*e.g.* VOC or BTX volume fraction of 5 ppb means that volume fractions of each hydrocarbon – benzene, toluene and xylene, or C_2H_4, C_3H_6, CH_2O, CH_3CHO and CH_3COCH_3, was 5 ppb). When analyzing the effect of relative humidity on H_2O_2 and O_3 formation, the input values were mass concentrations of H_2O, *i.e.* the absolute humidity of air, but in amounts that correspond to a relative humidity between 30 and 100 % at 25 °C. However, during separate modeling of temperature and humidity some unreal combinations on these two variables have occurred. The sensitivity of H_2O_2 and O_3 formation to changes in initial environmental data was evaluated on the basis of two values: the average daily volume fraction for the selected day and the maximum hourly volume fraction during that day. The rough settings of initial O_3 and H_2O_2 values did not significantly influence the results. Previous studies[19] and data from Figures 1 and 2 show that the first 24 hours of modeling may be taken in account.

The results show that hydrogen peroxide volume fractions in air rise linearly with increasing initial values of CO, VOC, BTX, H_2O_2, O_3 and relative humidity (Table 2). Short-chain (VOC) and aromatic (BTX) hydrocarbons contribute approximately to the same degree to the H_2O_2 formation, and their effect is more pronounced in obtaining a daily maximum. The smallest is the influence of ozone, while the model showed negative correlation between H_2O_2 levels and rise of initial levels of NO_2 (*e.g.* 10 ppb higher initial levels of NO_2

Table 2. The influence of eight different parameters on the levels of H_2O_2 in the air (estimated using the Master mechanism model with included daily NO cycle)

Parameter x	Range	Increment	Average daily H_2O_2 value / ppb					Maximum hourly H_2O_2 value / ppb				
			Equation parameters					Equation parameters				
			a	b	c	d	r^2	a	b	c	d	r^2
$\varphi(NO_2)$ / ppb	0-90	10	−0.0004	0.480			0.994[(a)]	−0.001	0.771			0.986[(a)]
$\varphi(CO)$ / ppm	0-0.9	0.1	0.718	0.297			0.995[(a)]	1.489	0.388			0.996[(a)]
$\varphi(VOC)$ / ppb	0-18	2	0.076	0.341			0.995[(a)]	0.152	0.474			0.997[(a)]
$\varphi(BTX)$ / ppb	0-18	2	0.084	0.336			1.0[(a)]	0.194	0.419			1.0[(a)]
$\varphi(H_2O_2)$ /ppb	0-5	0.5	0.535	0.255			1.0[(a)]	0.927	0.255			0.990[(a)]
$\varphi(O_3)$ / ppb	0-180	20	0.0005	0.419			0.924[(a)]	0.0012	0.615			0.933[(a)]
t / °C	−10-(+35)	5	-4×10^{-6}	0.0002	−0.0013	0.382	0.911[(b)]	-1×10^{-5}	0.0004	−0.0024	0.529	0.865[(b)]
$\gamma(H_2O)$ / g m^{-3}	6.6-33.0	2.2	0.007	0.275			0.999[(a)]	0.017	0.258			0.999[(a)]

[(a)] $y = ax + b$

[(b)] $y = ax^3 + bx^2 + cx + d$

Table 3. The influence of eight different parameters on the levels of O_3 in the air (estimated using the Master mechanism model with included daily NO cycle)

Parameter x	Range	Increment	Average daily O_3 value / ppb					Maximum hourly O_3 value / ppb				
			Equation parameters					Equation parameters				
			a	b	c	d	r^2	a	b	c	d	r^2
$\varphi(NO_2)$ / ppb	0-90	10	0.298	39.47			0.999[(a)]	0.701	41.13			0.990[(a)]
$\varphi(CO)$ / ppm	0-0.9	0.1	13.46	39.82			0.990[(a)]	24.76	45.01			0.989[(a)]
$\varphi(VOC)$ / ppb	0-18	2	2.39	41.93			0.996[(a)]	4.39	47.77			0.998[(a)]
$\varphi(BTX)$ / ppb	0-18	2	1.925 12.7	43.72 35.8			0.902[(a)] 0.995[(b)]	2.336 16.7	55.83 45.7			0.855[(a)] 0.980[(b)]
$\varphi(H_2O_2)$ /ppb	0-5	0.5	0.137	43.37			0.999[(a)]	0.243	50.00			0.990[(a)]
$\varphi(O_3)$ / ppb	0-180	20	0.524	21.99			1.0[(a)]	0.834	22.09			0.976[(a)]
t / °C	−10-(+35)	5	−0.0002	0.0060	−0.0068	42.41	0.836[(d)]	−0.0001	0.0086	−0.0363	48.473	0.812[(d)]
$\gamma(H_2O)$ / g m^{-3}	6.6-33.0	2.2	−0.0013	0.0669	42.51		0.989[(c)]	−0.0015	0.0691	49.30		0.945[(c)]

[(a)] $y = ax + b$

[(b)] $y = a\ln(x) + b$

[(c)] $y = ax^2 + bx + c$

[(d)] $y = ax^3 + bx^2 + cx + d$

cause a decrease of maximum hourly H_2O_2 value by 0.01 ppb). An increase by 1 ppb in initial levels of VOC; BTX; CO, H_2O_2 or O_3 will cause an increase of maximum hourly H_2O_2 value by 0.15, 0.19, 0.0015, 0.93 or 0.001 ppb, respectively.

Data in Table 3 show that ozone volume fractions rise with increasing initial values of NO_2, CO, VOC, BTX, H_2O_2 and O_3. All compounds except BTX show linear relationships. The curve that describes the dependence between ozone levels and initial BTX values may be better described by a logarithmic relationship ($y = 12.7 \times \ln(x) + 35.8$, r^2=0.994 for daily average; $y = 16.7 \times \ln(x) + 45.7$, r^2=0.986, for maximum hourly average, where y stands for the ozone volume fractions in ppb and x stands for the BTX values in ppb). However, within the investigated range, the relationship might still be linear. While the initial values of hydrogen peroxide have only a small influence on O_3 levels, those of NO_2, VOC and BTX influence them strongly, especially the occurrence of high hourly values. An increase by 1 ppb in initial levels of VOC, BTX, CO, NO_2, H_2O_2 or O_3 will cause an increase of maximum hourly O_3 value by 4.4, 2.3, 0.0248, 0.7, 0.2 or 0.8 ppb, respectively. The curve representing the relationship between ozone and humidity is not linear (polynomial) but the contribution of humidity may be safely neglected. According to the model, temperature does not have significant influence on H_2O_2 and O_3 volume fractions. The possible reason is the fact that MM model includes only gas-phase reactions, and as a photochemical box model it is focused primary on the radiation-generated processes with only limited inputs of meteorological variables. The modeling clearly predicts that increase of initial precursor (NO_2, VOC, BTX and CO) concentrations will result in considerably elevated ozone concentrations in Zagreb[22] what particularly is true for the airport neighborhood where air traffic starts very early and at the same time thousands of vehicles from nearby Velika Gorica (by population fourth city in Croatia) stream into Zagreb for work.

CONCLUSION

According to the Master Mechanism model applied to measured and modeled data for 26 June, 2004 in Zagreb, the H_2O_2 volume fractions in air increase with higher relative humidity and higher initial values of CO, VOC, BTX, H_2O_2 and O_3. Higher initial NO_2 values cause a decrease in H_2O_2 volume fractions. Ozone volume fractions in air rise with the increase of initial volume fractions of NO_2, CO, VOC, BTX, H_2O_2 and O_3. Temperature does not have any significant influence on the formation of H_2O_2 and O_3.

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SAŽETAK

Modeliranje ozona i vodikovog peroksida u zraku

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Volumni udjeli ozona i vodikovog peroksida izračunati su pomoću *Master Mechanism* (MM) modela, autora S. Madronicha (NCAR, Boulder, CO, USA). *Master Mechanism* je računalni program za atmosferski model jednodimenzionalne kutije ("box" model) koji iz inicijalnih količina atmosferskih plinova u zadanim, fiksnim ili promjenjivim fizikalnim uvjetima, omogućava promatranje daljnjeg tijeka reakcija na temelju izračunavanja odgovarajućih konstanata brzina reakcija. Konstante fotolize kemijskih reakcija izračunavaju se pomoću Tropospheric Ultraviolet Visible (TUV) programa istog autora. Podaci prikupljeni tijekom mjerenja 2004. godine[19] te modelirani pomoću MM programa[20] korišteni su u ovom radu kako bi se utvrdilo kako porast početnih vrijednosti pojedine od sljedećih osam veličina: udjeli NO_2, CO, VOC (neki hlapljivi organski spojevi), BTX (benzen, toluene, ksileni), H_2O_2, O_3, zatim temperatura i relativna vlažnost, utječu prilikom modeliranja na volumni udio ozona odnosno vodikova peroksida u zraku. Prema modelu, volumni udio H_2O_2 u zraku raste s porastom relativne vlažnosti i porastom početnih vrijednosti CO, VOC, BTX, H_2O_2 i O_3. Više inicijalne vrijednosti NO_2 uzrokuju smanjenje razina H_2O_2. Volumni udjeli ozona u zraku rastu s porastom inicijalnih volumnih udjela NO_2, CO, VOC, BTX, H_2O_2 i O_3. Temperatura nema značajni utjecaj na nastanak H_2O_2 i O_3. Rezultati daju i objašnjenje za znatno povećane koncentracije ozona oko zračne luke u usporedbi s lokacijama u gradu Zagrebu.[22]