PAPER • OPEN ACCESS

Feedbacks between lightning activity, temperature and composition of the atmosphere

View the article online for updates and enhancements.

Feedbacks between lightning activity, temperature and composition of the atmosphere

L Kolomeets[*], S P Smyshlyaev

Russian State Hydrometeorological University, Voronezhskaya 79, St.Petersburg 192007, Russia

E-mail: akvarel@rshu.ru

Abstract. The prediction of lightning-generated nitrogen oxides in the troposphere and low stratosphere is evaluated using the Weather and Research Forecasting model coupled with Chemistry (WRF-Chem) with nested grid spacing of 15 and 5 km where convection is parameterized. The responses of nitrogen oxides, ozone, temperature and peroxyacetyl-nitrate (PAN) are investigated using matching of WRF-Chem sensitivity tests. A high-resolution simulation was performed for the Black sea region to examine feedbacks between atmospheric electricity and local weather. The result obtained shows that storms, occurring near the seaside, cause stronger effect on the land. Temperature fields show that continental difference is bigger than the coast one. The maximum temperature field difference is registered above 10 km altitude.

Introduction

Lightning plays an important role in atmospheric chemistry through generation of nitrogen oxides, especially in the middle and upper troposphere/lower stratosphere (UTLS zone). Nitrogen oxides ($NO_x = NO + NO_2$) are catalytic precursors of ozone (O_3) and also have a strong influence on the hydroxyl radical (OH) concentration [1]. Climate and weather variability can alternate thunderstorm cloud formation resulting in lightning frequency and distribution changes followed by changes in the nitrogen oxides and ozone formation. Thus, positive and negative feedbacks may occur due to interrelation between lightning frequency, atmospheric chemistry and weather, and climate changes [15]. Both regional and global effects of these feedbacks may be important for atmospheric composition and structure variability.

Prediction of lightning flashes in numerical weather and climate models has garnered increasing interest. One of the most important things is the advance in online chemistry models, where chemistry is simulated alongside of physics. To adequately represent the lightning flashes and lightning-generated NO_x (LNO_x) source in regional models, the geographic distribution of flashes, average production of NO per flash, and vertical distribution of LNO_x following convection should be considered. In order to predict UTLS ozone and its climate impact, it is important to be able to simulate the transport, LNO_x and ozone production in chemistry transport models. In this study, we focus on the concentration of LNO_x, and downwind UT production of ozone. Similar studies have been performed for global models, but previous regional-scale modeling studies utilizing PR92 (Price and Rind, 1992) at comparable horizontal grid spacing has not provided evaluations of the lightning

parameterization thus there has been insufficient information to understand the behavior of PR92 in this regime [2].

A variety of schemes have been used to study the horizontal distribution of flashes (cloud top height, upward cloud mass flux, convective precipitation, CAPE etc) [3]. The production of NO per flash has been examined using laboratory experiments, theoretical assumptions regarding the physics of lightning flashes, and observations obtained during field campaigns [3]. The laboratory experiments showed that NO production per unit flash length is also strongly dependent on peak current (Wang et al, 1988). Despite these efforts, a great deal of uncertainty remains regarding NO production on a per flash basis, as well as the relative production by intra-cloud (IC) and cloud-to-ground (CG) flashes. Also uncertainty surrounds a number of other aspects of LNO_x production in addition to the relative production of NOx by IC and CG flashes. It was demonstrated [4], that the amount of NO produced in a lightning channel depended strongly on the temperature in the channel and pressure. [5]presented vertical profiles of LNO_x for use in 3-D CTMs based on the results of 2-D cloud-resolving model simulations of seven convective events. Average profiles of LNO_x mass computed for the midlatitude continental, tropical continental, and tropical marine regimes showed peaks in mass near the surface and in the upper troposphere, leading many CTMs to adopt a C-shaped vertical distribution of LNO_x mass.

Prediction of the lightning flash rate is often based on one or a combination of storm parameters, such as maximum updraft volume, precipitation and non-precipitation ice mass flux product, mid-level graupel mass flux and cloud top height. However, many of these parameters are not represented in model configurations that parameterize convection. When convection is parameterized, the flash rate can be predicted by storm parameters like cloud top height, the upward cloud mass flux, the convective precipitation rate and combination of updraft velocity and cloud thickness. (Romps et al., 2014) have shown, that the lightning flash rate per area is proportional to the precipitation rate times convective available potential energy (CAPE). In mathematical form:

$$F = (\eta/E) \times P \times CAPE \tag{1}$$

Where F is the lightning flash rate per area ($m^{-2}s^{-1}$), P is the precipitation rate (kg $m^{-2}s^{-1}$), and *CAPE* is in J kg^{-1}, η is the dimensionless conversion efficiency, E is the energy discharge per flash. Using an adiabatic definition of *CAPE*, the product of *CAPE* and P is the theoretical maximum rate at which kinetic energy is imparted to ascending water condensates, in units of W m^{-2}. The constant of proportionality, η/E, contains the dimensionless conversion efficiency η and the energy discharge per flash E. The efficiency η is the ratio of power per area dissipated by lightning to the *CAPE* per area time available to condensates. The authors do not propose a specific charging mechanism, but (Romps et al., 2014) note that most charging mechanism is consistent with the notion that higher updraft speeds and water contents should yield higher flash rates. It was shown, that the product of *CAPE* and precipitation explains 77% of the variance in the time series of total cloud-to-ground lightning flashes over the contiguous United States. Storms convert *CAPE* times precipitated water mass to discharged lightning energy with an efficiency of 1%. When this proxy is applied to 11 climate models, *CONUS* lightning strikes are predicted to increase 12±5% per degree Celsius of global warming and about 50% over this century [6].

The following sections are organized as follows. Section 2 describes the experimental set-up and the method used to realize the effects of lightning-produced NO_x on atmospheric chemistry and temperature fields. Section 3 discusses the model results. Section 4 concludes with a summary of the results.

Methodology and argumentation
   WRF-Chem description and Configuration. To study the details of the feedback mechanisms between lightning activity, atmospheric gases and temperature The Weather Research and Forecasting model (WRF-Chem) version 3.6 is exploited: (provides the capability to simulate meteorology, chemistry and aerosols from cloud scales to regional scales).

Scalar transport is integrated with the Runge-Kutta scheme using horizontal and vertical upwind-biased advection operators. Transported scalars include water vapor, the different hydrometeor categories and the chemical species. Mass mixing ratios of cloud water, rain, ice, snow and groupel/hail are predicted. Cloud water and ice are monodispersed and rain, snow, and hail have prescribed inverse exponential distributions. The model predicts the mixing ratios of methane (CH_4), carbon monoxide (CO), ozone (O_3), hydroxyl radical (OH), hydroperoxy radical (HO_2), nitric oxide (NO), nitric acid, hydrogen peroxide (H_2O_2), methyl hydrogen peroxide, formaldehyde (CH_2O), formic acid, sulfur dioxide, ammonia, aerosol sulfate etc. In addition to the chemically active species, a tracer of NOx from lightning (LNO_x) is included in WRF-Chem. LNOx is transported and doesn't undergo any chemical reactions [7]. Adaptation has been performed to cover Black Sea Coast [7] (Figure 1).
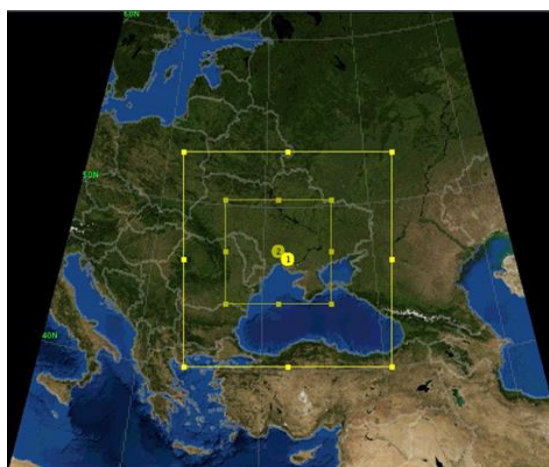
Figure 1. Nested domain of Black Sea Coast.

Meteorology is initialized and continuously nudged with the National Center for Environmental Protection (NCEP) Global Forecasting System (GFS) final (FNL) gridded analysis, which has a 6 hourly time resolution and $0.5^0 \times 0.5^0$ spatial resolution. Winds, potential temperature, pressure, water vapor, and condensed water (i.e., cloud particles), tracer variables, and chemistry species are integrated forward in time using a Runge-Kutta integration method. The LNO_x parameterization is based on the PR92 scheme with some modifications. PR92 is based on maximum convective updraft w (flashes are distributed within reflectivity is up then 20 dBZ) PR92 is used for convection-resolved resolutions with microphysics turned on for reflectivity calculations. To determine LNO_x, the lightning flash rate, the location (both horizontally and vertically), and the amount of NO produced per flash must be estimated. This parameterization of lightning-generated NO_x is valid for both parameterized convection and resolved convection.

The number of lightning flashes is computed based on the maximum updraft speed within each parallel-processing tile of the domain. For both intra-cloud and cloud-to-ground flashes, 330 moles of NO are produced per flash. Included in the simulation are two passive lightning NO_x tracers, one tracing NO_x produced from cloud-to ground flashes and the second tracing NO_x from intracloud flashes. Both tracers have the same source strength determined from the lightning-NO_x parameterization, but then are only transported in the model domain, there are no sinks for these two tracers.

In our simulation there is the concern that changes in the chemistry could lead to a different meteorological scenario because the simulation allows feedbacks between the chemistry and meteorology through radiation and cloud physics.

To track boundary layer air, stratospheric air, and air from the horizontal boundaries, six tracers are included. The boundary layer tracers are defined as having a value of one from the surface to the

planetary boundary layer (PBL) height. The stratosphere tracers are defined as having a value of one from the height of the tropopause to the top of the domain (10 hPa). The horizontal boundary tracers are initially set to zero within the model domain. Their value at the horizontal boundaries is set to one throughout the simulation. Thus, the horizontal boundary tracer allows us to track air that has originated outside the model domain.

The gas-phase chemical mechanism description. The gas-phase chemical mechanism is one of the most important components of any atmospheric chemistry model. WRF-Chem requires high-quality gas-phase chemical mechanisms to calculate the concentrations of atmospheric chemical species. The concentrations of ozone and other air pollutants are determined by the emissions of nitrogen oxides and reactive organic species, gas- and aqueous-phase chemical reaction rates, deposition, and meteorological conditions. In our research we use « Regional Acid Deposition Model, version 2 » (RADM2) mechanisms. Inorganic species include 14 stable species, four reactive intermediates, and three abundant stable species (oxygen, nitrogen and water). Atmospheric organic chemistry is represented by 26 stable species and 16 peroxy radicals. CO_2 and H_2 are not included in the RADM2 transport/transformation model. The reaction of HO with HO_2, which is an important termination channel for HO_x radicals, has been added to the mechanism [8]. Most of the inorganic reactions and rate constants in RADM2 are taken from JPL [9]. The rate constant for the important chain-terminating reactions of HO_2 with HO_2 are from [10,11]. NO_3 chemistry is relatively extensive because of its importance for nighttime chemistry.

The inorganic chemistry of ozone, nitrogen, and sulfur containing species under troposphere conditions is relatively well known. Ozone transported to the troposphere from the stratosphere or generated locally in the troposphere photolysis to produce excited oxygen atoms in the O^1D state. A fraction of the O^1D atoms is quenched by collision with oxygen or nitrogen to produce O^3P atoms, and the remaining fraction reacts with H_2O to produce the hydroxyl radical (HO). HO reacts with both inorganic and organic species. Reactions of HO with CO produce HO_2 radicals, which either react with NO to convert it to NO_2, self react to produce hydrogen peroxide, or react with other organic peroxy radicals to produce organic peroxides. The chain is completed through the photolysis of NO_2, which produces ozone [8].

Results and discussions

It have performed a WRF-Chem model simulation from 1 June to 30 August 2013-2016, for which the 5 July to 30 August periods have been analyzed to avoid the impact of the model spin up during the first few days. To study lightning effect for multi-week integration have been performed model simulations for two types of experiments: 1) experiments without LNO_x parameterization, 2) experiments with LNO_x parameterization. An analysis of these simulated days is performed to understand the role of deep convection on composition and chemistry of the upper troposphere/lower stratosphere. While desirable, event-by-event analysis would be technically challenging because the simulation may not produce the same strength, timing, and location of each convective event. Furthermore, an event-by-event analysis is unnecessary in the context of a mesoscale upper troposphere chemistry study, of which the meaningful timescales often averages biases from many individual events (in this research we use 3-days timescale).

Recent research [7] prove storm activity direct and indirect impact on the atmosphere. This influence is non-linear, non-surface and point-spatial. That's why it's very important to appreciate non-direct effects, which are presented on the picture 1. All atmosphere perturbations, caused by the storm activity are responsible for a new redistribution of thunderstorms. To forecast a new lightning activity there are many different methods [7,12,13] (CAPE, Vaiting method, Fateev method, LIS, CAPE×Precip etc).

Total totals index (TOTL, figure 2), ºC describes atmospheric stability and humidity on the level 850 hPa (important convective cloud lightning development factor) (equation 2)

$$TOTL = (T_{850}\text{-}T_{500})+(Td_{850} - T_{500}) \tag{2}$$

Where T_i – it' s a temperature on a special level (ºC), T_d – dew point temperature (ºC). According to (Kunz, 2007; Schulz,1989), if *TOTL* is equal 45-50 ºC, atmosphere is moderately unstable; if *TOTL* is equal $50 - 55$ ºC, atmosphere is moist unstable (thunderstorm probability is very hight). When *TOTL* values are $55 - 60$ ºC, atmosphere is very unstable, severe thunderstorms have potential to appear.
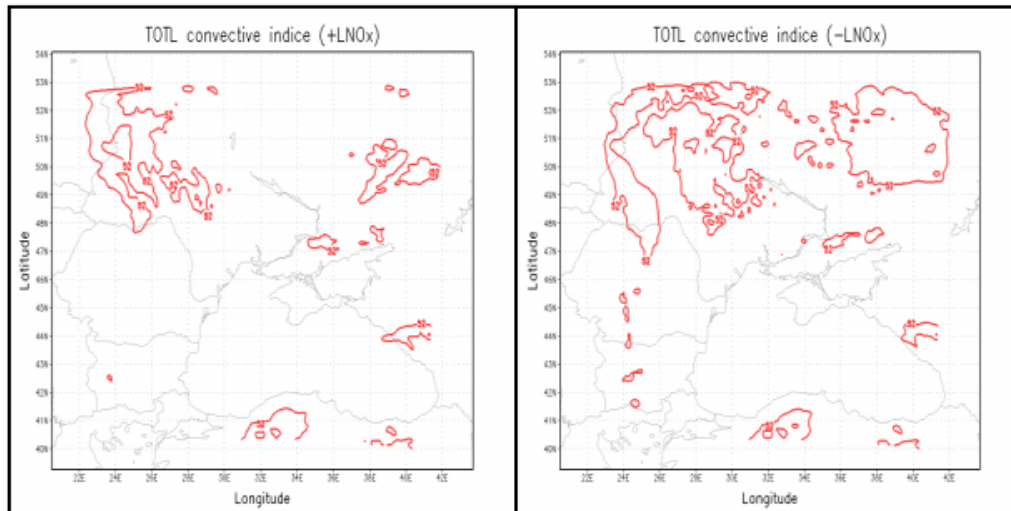
Figure 2. TOTL criterion isolines for 9.06.13 18.00 UT (in case of presence/absence LNO$_x$ atmosphere perturbations).

As is shown at fig. 13-14, WRF-Chem criterion system is capable to forecast lightings in detailed. From the other hand, the results obtained show an essential difference between WRF-Chem simulations with and without LNO$_x$ parameterizations.
 Plane observation of the lightning regions prove, that WRF-Chem usually doesn't describe small convective processes (figure 3).
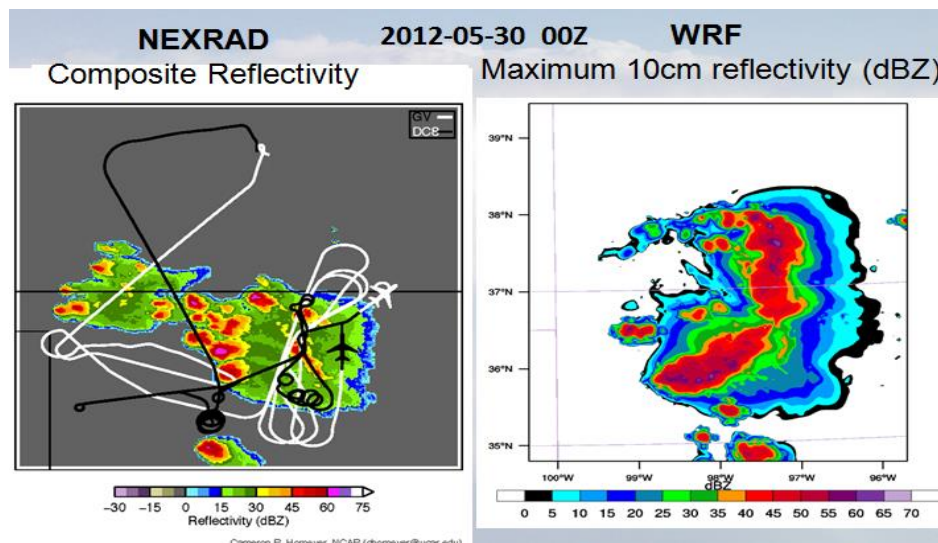

Figure 3. WRF-Chem simulation of maximum 10 cm reflectivity without lightningNOx parametrization – intercomparison between observation and simulation (Megan Bela (U. Colorado), Mary Barth (NCAR), John Wong, O. Brian Toon (U. Colorado)

But using LNOx parametrization, adopted for region of simulation this problem can be minimize (figure 4).
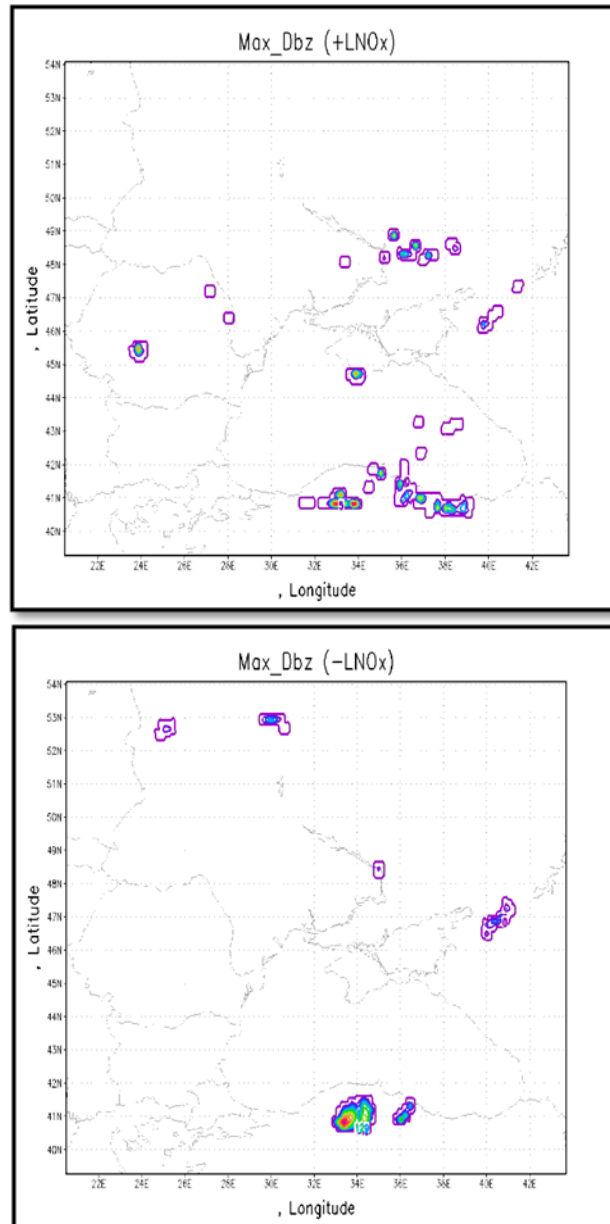
Figure 4. WRF-Chem predicted maximum reflectivity for Black Sea region for 9.06.13 18.00 UT (in case with/without LNOx effects).

It has been calculated CAPE (figure 5a) − convective available potential energy (amount of energy a parcel of air would have if lifted a certain distance vertically through the atmosphere).
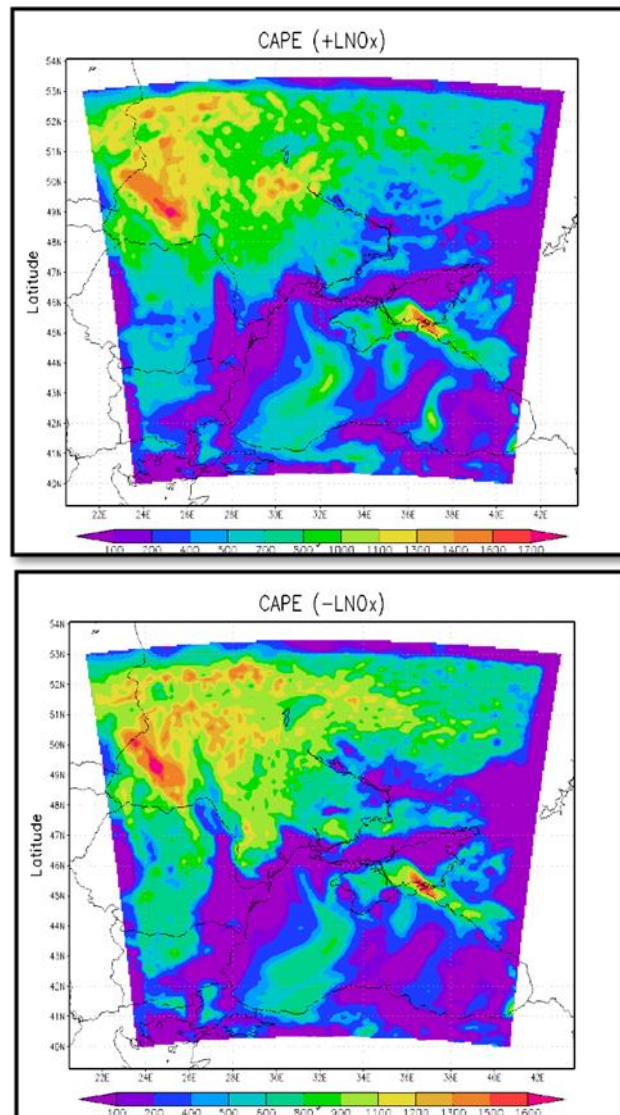
Figure 5 (a). WRF-Chem predicted CAPE for Black Sea region for 9.06.13 18.00 UT (in case with/without LNOx effects).

CAPE is measured in joules per kilogram of air (J/kg). Any value greater than 0 J/kg indicates instability and an increasing potential of thunderstorms and hail. CAPE is calculated by integrating vertically the local buoyancy of a parcel from the level of free convection to the equilibrium level(where positive CAPE is equal a negative one):

$$CAPE = \int_{z_f}^{z_n} \left[g \left(\frac{T_{v, parcel} - T_{v, env}}{T_{v,env}} \right] \right) dz$$

(3)

Where z_f is the height of the level of free convection, z_n is the height of the equilibrium level (neutral buoyancy). $T_{v, parcel}$ is the vertical temperature of the specific parcel, $T_{v, env}$ is the virtual temperature of the environment, g is the acceleration due to gravity.

Using WRF-Chem data simulation for 9.06.2013 we appreciate atmosphere stability criterion, which are responsible for lightning forecast for 10.06.2013.It's shown, that simulation with using

lightning parameterization are better to describe convective processes in atmosphere. Simulations without LNOx parametrization are overestimated near the Black sea region.

Also it has been calculated CIN (convective inhibition) difference between the results with and without additional source of NOx of lightning orogin (figure 5b), that also demonstrates atmosphere sensitivity to electrical and convective processes.
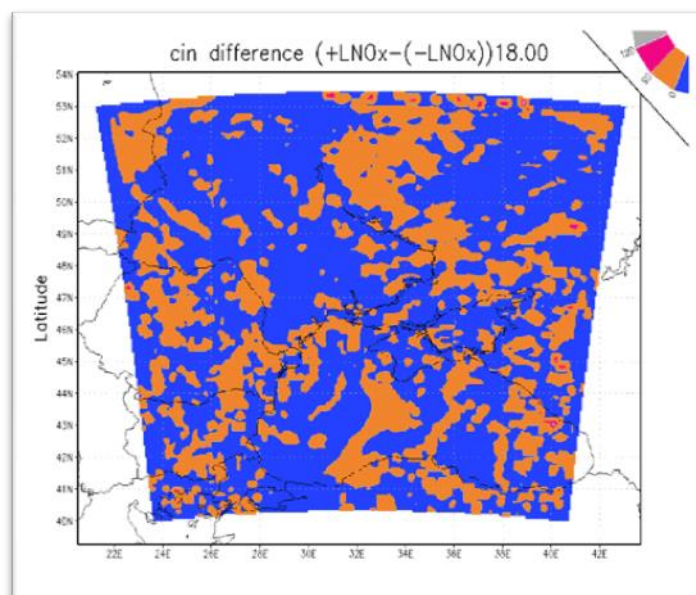
Figure 5b. WRF-Chem predicted Cin difference for Black Sea region for 9.06.13 18.00 UT (in case with/without LNOx effects).

These facts prove the presence in atmosphere feedbacks between local climate, weather, and atmospheric chemistry.

Summary and conclusions
A high-resolution simulation of meteorology and chemistry was been performed for the Black sea region to examine feedbacks between atmospheric electricity and regional climate. An analysis of summer days is performed to understand the role of deep convection on the composition and chemistry of the upper troposphere/lower stratosphere. We have run lightning NO_x as a conserved tracer in these calculations over a period of 72 hours. In reality, some part of LNO_x is oxidized to other reactive nitrogen compounds. Application of mean production per flash and the vertical distributions of LNO_x must be carefully evaluated in all Black Sea regions through comparison with available satellite, ground- and aircraft-based data. Field experiments with lightning and chemistry observations are needed to further verify and improve this approach.

Data availability.The data used in this study are supported by the Russian State Hydrometeorological University and available by request to Ludmila Kolomeets (akvarel@rshu.ru).

References
[1] Lawrence M G, Chameides W L, Kasibhalta P S, Levy II H, Moxim W 1995 *Lightning and atmospheric chemistry: The rate of atmospheric NO production (*CRC Press, Inc.m) **189** 202.
[2] Barth M C, Lee J, Hodzic A, Pfister G, Skamarock W C, Worden J, Wong J, Noone D 2006 *Thunderstorms and upper troposphere chemistry during the early stages of the 2006 North American Monsoon* (Atmos. Chem. Phys. Discuss.) **12** 16407–16455. DOI:10.5194/acpd-12-16407-2012, 2012.

[3] Allen D J, Pickering K E 2002 *Evaluation of lightning flash rate parameterizations* (D23), 4711, DOI:10.1029/2002JD002066

[4] Chameides W L 1986 *The role of lightning in the chemistry of the atmosphere, in The Earth's Electrical Environment* (Studies in Geophysics, Natl. Acad. Press, Washington, D. C.) 70 -77.

[5] Wang Y W, DeSilva G C, Goldenbaum, Dickerson R R 1988 *Nitric oxide production by simulated lightning: Dependence on current, energy, and pressure* (J. Geophys. Res.) **103 (D15)** 149 – 19, 159. DOI:10.1029/98JD01356

[6] Pickering K E, Wang Y, Tao W-K, Price C, Muller J – F 1988 *Vertical distributions of lightning O_x for use in regional and global chemical transport models* (J. Geophys. Res.) **103** (31) 203 – 216. DOI:10.1029/98JD02651

[7] Kolomeets L I, Smyshlyaev S P 2016 *Direct and indirect effects between thunderstorm activity, temperature and atmosphere composition on a regional scale: sensitive tests with WRF-CHEM* (Proceedings of MGO) **585** 187—211.

[8] Stockwell W R, Middleton P, Chang J S 1990 *The Second Generation Regional Acid Deposition Model Chemical Mechanism for Regional Air Quality Modeling* (Journal of Geophysical Research) **95 (16)** 343-16,367, September 20, 1990

[9] Sander S P, Abbatt J, Barker J R, Burkholder J B, Friedl R R, Golden D M, Huie R E, Kolb C E, Kurylo M J, Moortgat G K, Orkin V L, Wine P H 2011 *Chemical kinetics and photochemical data for use in atmospheric studies* (JPL Publication 10-6, Jet Propulsion Laboratory, Pasadena) **17**.

[10] Sander S P, Peterson R T, Watson, Patrick R 1982 *Kinetic studies of the $HO_2 + HO_2$ and $DO_2+ DO_2$ reactions at 298 K* (J. Phys. Chem.) **86** 1236 – 1240.

[11] Kirtcher C C, Sander S P 1984 *Kinetic and mechanism of HO_2 and DO_2 disproportionations* (J. Phys. Chem.) **84** 2082 – 2091.

[12] Kunz M 2007 *The skill of convective parameters and indices to predict isolated and severe thunderstorms* (Natural Hazards and Earth System Sciences) **7** 327-342.

[13] Schulz P 1989 *Relationships of several stability indices to convective weather events in northeast Colorado* (Weather Forecasting) **4** 73-80.