J.8.2 A NASA MODEL FOR IMPROVING THE LIGHTNING NO_X EMISSION INVENTORY FOR CMAQ

William J. Koshak
Earth Science Office, NASA-MSFC, Huntsville, AL 35805; william.koshak@nasa.gov
Maudood N. Khan
Universities Space Research Association, Huntsville, AL 35805
Arastoo P. Biazar
University of Alabama in Huntsville, Huntsville, AL 35805
Michael Newchurch
University of Alabama in Huntsville, Huntsville, AL 35805
Richard T. McNider
University of Alabama in Huntsville, Huntsville, AL 35805

1. INTRODUCTION

The U.S. Environmental Protection Agency (EPA) Community Multiscale Air Quality (CMAQ) modeling system is used by federal, state, local agencies and other stakeholders to evaluate the impact of air quality management practices for multiple pollutants at a variety of spatio-temporal scales. It enhances the scientific understanding and modeling capability of chemical and physical atmospheric interactions, and guides the development of air quality regulations and standards.

Lightning is a source of nitrogen oxide emissions in the atmosphere. Currently, emissions from lightning are either omitted or are poorly represented in CMAQ. Model predictions suffer as a result, especially in the middle and upper troposphere. A modeling study conducted with funding from the NASA Applied Science Program that compared CMAQ model predictions of ozone against ozonesonde observations, found model bias in excess of 30 percent. In addition to other sources of uncertainty, long-range transport of pollution and emissions from aircraft and lightning might be contributing to these errors. Only a few studies have actually attempted to assess the impact of lightning-induced emissions on air quality model results. Recently, Kaynak et al., (2008) estimated a 2 ppb impact on surface ozone concentration from lightning NO_x emissions. But, the following simplifying assumptions were made regarding lightning modeling:

- The ratio of the number of cloud flashes to ground flashes was held fixed at a value of 3.
- The NO produced by each cloud flash was assumed to be constant.
- The NO produced by each ground flash was assumed to be constant.
- Cloud and ground flashes were assumed to produce the same amount of NO.

In reality, none of these assumptions hold as a general rule. Lightning is highly variable. The physical variables that determine NO production (see section 3) all vary from flash to flash, particularly between ground and cloud flashes.

In this work, we introduce a lightning NO_x production model that combines a detailed theory, routine measurements, and laboratory results to improve the lightning NO_x emission inventory for CMAQ.

2. DATA

Inputs to the model include probability distribution functions (pdfs) of channel length derived from Very High Frequency (VHF) Lightning Mapping Array (LMA) data, ground flash data derived from the National Lightning Detection Network™ (NLDN), and laboratory results derived from Wang et al., (1998). The model also uses the NASA lightning climatology dataset from the combined Tropical Rainfall Measuring Mission (TRMM) Lightning Imaging Sensor (LIS) and the Orbview-1 (formerly called the Microlab-1 spacecraft) Optical Transient Detector (OTD). Specific products include the LIS/OTD High Resolution Full Climatology (HRFC), related monthly/annual climatologies, and the climatological ratio of the number of cloud flashes to the number of ground flashes as deduced using OTD data (Boccippio, 2001).

3. MODEL DETAILS

The model is called the Lightning Nitrogen Oxides Model (LNOM), and is presently under development at the NASA Marshall Space Flight Center. The model implements a realistic description of lightning while at the same time combines useful laboratory findings with state-of-the-art lightning observations to obtain optimum modeling results.

One of the most notable characteristics of lightning is that it is highly variable. This variability in turn produces considerable variability in lightning NO_x production. LNOM is specifically designed to account for the variability in lightning, and thereby provides for a more realistic lightning NO_x emission inventory.

The focus of LNOM is on the production of NO, not its subsequent chemical conversion, transport (convective,

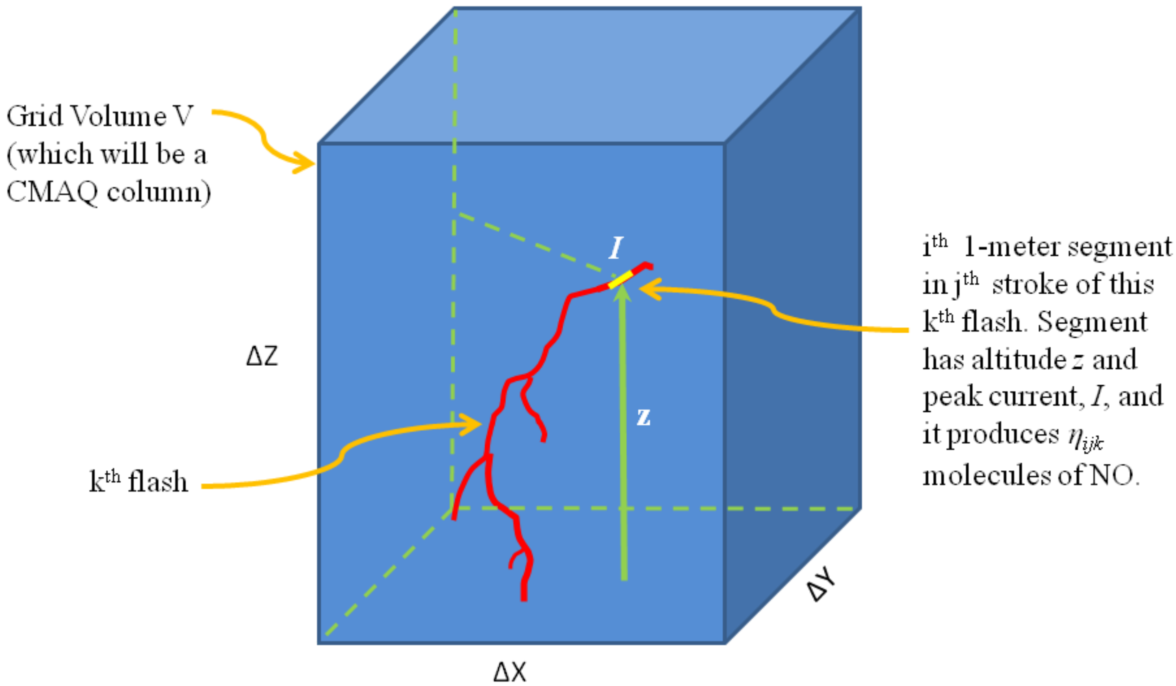

Figure 1. Fundamentals of the NASA lightning NO production model. The k[th] flash occurs in the grid volume, V. This particular flash is one of *N* flashes that occurs within V during time Δt. It is a ground flash having multiplicity = 3 (individual strokes are not shown since they tend to follow the same path forged by the 1[st] return stroke). A 1-meter channel segment is shown in yellow (scale is exaggerated for clarity).

advective), or removal (e.g., wet scavenging). Since only a small percentage of the total NO_x produced in a discharge is NO_2 (Wang et al., 1998), the NO produced from LNOM also serves as the LNOM lightning NO_x production estimate. This estimate is provided as a 1-hr averaged rate in moles/sec for a CMAQ grid volume, V (see Figure 1). The intent is to run CMAQ using 39 vertical layers; each grid volume will have a horizontal dimension of 36 km x 36 km. The Pickering et al. (1998) profiles will be used to appropriately distribute the NO into each vertical layer of CMAQ.

If N is the *number of lightning flashes* that occur in time Δt within a model grid volume V, the NO production, P (in # NO molecules), in that grid volume can be written as

$$P = \sum_{k=1}^{N} \sum_{j=1}^{m_k} \sum_{i=1}^{L_{jk}} \eta_{i\,jk}(I, z) \quad . \qquad (1)$$

Here, $\eta_{ijk}(I, z)$ is the *segment production*; i.e. the # NO molecules produced by the i^{th} 1-meter segment of the j^{th} stroke in the k^{th} lightning flash. It depends on the channel segment *peak current*, I (in kiloamps), and the atmospheric air density or channel segment *altitude*, z (in meters). The larger the channel segment peak current and the lower its altitude, the more NO it produces. The *ijk* indices on I and z are omitted throughout for brevity. Note that the current $i(t)$ in a segment rises to the peak value, I, and then falls to zero; this is repeated for the next (adjacent) segment, and so on. So in the LNOM, a stroke can be viewed as a fixed current waveform pulse $i(t)$ propagating along the stroke channel.

The *stroke channel length* of the j^{th} stroke within the k^{th} flash is given by L_{jk} and it is taken as an integer value (i.e., stroke channel length is modeled to the nearest meter). The number of strokes in the k^{th} flash is given by the *multiplicity* m_k which is equal to unity for cloud flashes, and is typically 3 or 4 for negative polarity ground flashes; a maximum recorded multiplicity of 26 is provided in Uman (1969). Positive polarity ground flashes tend to have smaller values of multiplicity than negative polarity ground flashes.

In summary, equation (1) identifies five variables (N, m_k, L_{jk}, I, z) important to NO production. These variables are chosen not just because of their physical importance, but because they are quantities that are measureable with state-of-the-art lightning detection systems (see section 2).

The importance of each variable is briefly summarized as follows:

- *Number of Flashes,* N: More flashes in the grid volume imply more production.
- *Multiplicity,* m_k: More strokes in a (ground) flash imply more production.
- *Stroke Channel Length,* L_{jk}: Longer channel length implies more production.
- *Segment Production,* $\eta_{ijk}(I, z)$: If a channel segment is more energetic [i.e., the fixed current waveform shape $i(t)$ has a larger peak current value I] it will produce more NO. If the channel segment is lower in altitude z where the air density is high, it will also produce more NO.

Furthermore, note that the effect of *flash-type* (ground flash or cloud flash) on NO production is implicitly accounted for in equation (1). For example, if we are speaking of cloud flashes, then the multiplicity is unity, and the stroke channel length chosen would be representative of cloud flashes rather than ground flashes. Similarly, the segment production would be based on cloud flash properties (higher altitudes and smaller peak currents) rather than ground flash properties (lower altitudes and larger peak currents).

4. IMPLEMENTATION

This section provides specific details on how each variable in the LNOM model is obtained in practice, and what specific lightning measurement datasets and laboratory results are required. By completing the steps below, one obtains the spatio-temporal emission of lightning NO for each CMAQ grid volume. As we have already mentioned above, the Pickering et al. (1998) profiles will be used to appropriately distribute the NO into each vertical layer of CMAQ, thereby completing the implementation/integration process.

4.1 Number of Flashes

The total number of flashes is $N = N_g + N_c$, where N_g is the number of ground flashes and N_c is the number of cloud flashes. Again, these flash tallies are for the grid volume V during time Δt. The value of N_g for any grid volume over the continental US is determined directly from the National Lightning Detection Network™ (NLDN). This network has recently been upgraded and has a high ground flash detection efficiency (90-95%) and a ground flash location accuracy of better than 500 meters (Cummins et al., 2006). The NLDN data is routinely procured and archived by the NASA/MSFC lightning group. The number of cloud flashes is obtained as $N_c = Z_s N_g$ where Z_s is the climatological ratio of the number of cloud flashes to ground flashes derived using NASA OTD lightning satellite data (see Boccippio et al., 2001). The NASA LIS/OTD 0.5 Degree High Resolution Full Climatology (HRFC) total flash data product is also used to adjust the value of Z_s as appropriate. [Further adjustments to Z_s are made using the empirical relationship provided in Price and Rind (1993) given by $Z(D) \equiv N_c/N_g = aD^4+bD^3+cD^2+dD+e-1$, where D is the *cold cloud thickness* (cloud top height minus the height of the 0^oC isotherm), and (a, b, c, d, e) are known empirical constants. GOES cloud satellite data is used to obtain cloud top height and the MM5 model is used to obtain the height of the 0^oC isotherm.]

4.2 Multiplicity

As stated previously, the multiplicity for cloud flashes is unity. For ground flashes, the NLDN directly provides the multiplicity.

4.3 Stroke Channel Length

Vertical-line channel approximations are inadequate because the altitudes of charge centers in the cloud vary and channel tortuosity substantially amplifies total channel length. In addition, since so-called “spider lightning” can propagate hundreds of kilometers in the horizontal, the vertical-line approximation applied to lightning of appreciable horizontal extent is meaningless. Even though channel length is highly variable, LNOM takes advantage of the fact that ground-based VHF lightning mapping systems can map the channel in 3-D space and time with exceptional accuracy (Koshak, 2004). There are several VHF mapping systems presently in operation in the US as shown in Figure 2. An example of a flash detected by the North Alabama Lightning Mapping Array (LMA) is given in Figure 3.

The LNOM assigns a channel length to a flash by randomly picking it from one of two probability distribution functions (pdfs). One pdf is for ground flash channel lengths, and one pdf is for cloud flash channel lengths. The pdfs are produced from VHF lightning mapping data analyses of several thousand flashes. So the approach is statistical and is based on realistic VHF lightning observations.

4.4 Segment Production

The segment production is more formally written as $\eta_{ijk}(w,z)$ where w is the channel segment *energy density* which typically varies between 1-100 kJ/m. However, estimates of *w* vary considerably depending on the method used to make the estimate (Hill, 1979). Even in a simple model where ground flash energy is expressed as the product of the total charge deposited times the cloud electric potential (voltage relative to ground) the total charge transfer typically varies by 2 orders of magnitude (Koshak, 1991), and the specific cloud potential is not usually known or measured.

To overcome these difficulties, note that the LNOM uses readily available observations of peak lightning current, I (in kiloamps), and the laboratory results of Wang et al. (1998) to determine the segment production. That is, Wang et al. (1998) have already

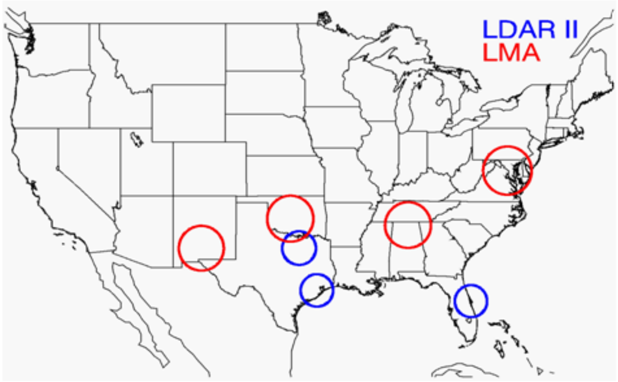

Figure 2. The seven ground-based VHF time-of-arrival lightning mapping networks. Circles are centered on the network location, and circle radius indicates approximate usable detection range. The two network types are Lightning Detection And Ranging II (LDAR II), and Lightning Mapping Array (LMA). [Adapted from D. Buechler, Univ. of Alabama in Huntsville].

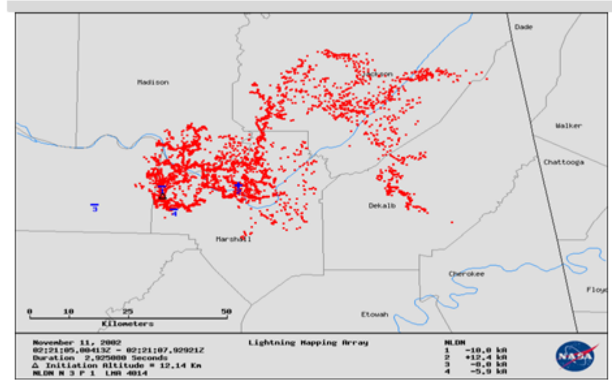

Figure 3. Plan view of a lightning flash detected by the North Alabama Lightning Mapping Array (LMA). Note the extensive horizontal development of the channel.

related NO production to the peak current in laboratory sparks. The laboratory peak current values were as large as 30 kA; i.e., comparable to lightning peak currents. The laboratory results can be reasonably extrapolated to even larger lightning peak current values. In addition, the laboratory results are also used to appropriately adjust segment production as a function of segment altitude.

By combining equations (6) and (9) in Wang et al. (1998), the NO production from a 1-meter channel segment becomes

$$\eta_{ijk}(I,z) = a + bI + cI^2 - \frac{d\eta}{dp}\Delta p \qquad (2)$$
$$= a + bI + cI^2 - B(p_o - p_o e^{-z/h}) \ .$$

Here, the increase in NO production with increasing atmospheric pressure p is constant; i.e., $d\eta/dp = B$. The constant p_o is surface pressure, h is the scale height of the atmosphere (about 8.4 km), and (a, b, c, B) are positive empirical laboratory constants provided in Wang et al. (1998). Substituting equation (2) into equation (1) gives the required final expression for the production P. As expected, equation (2) shows that the NO production increases for a channel segment that has a larger peak current and a lower altitude. Note that the VHF channel mapping data provides the (statistical) values of z.

For ground flashes, values of I are directly inferred from the NLDN data. For cloud flashes, values of I are more difficult to obtain but are typically an order of magnitude smaller than for ground flashes; i.e., the cloud flash peak current is typically about 4 kA (Uman, 1969). So LNOM uses NLDN-observed values of I for ground flashes, and a value of I = 4 kA for all cloud flashes. However, the user can adjust the cloud flash peak current value to assess sensitivity in overall NO production.

5. VALIDATION

In 2007, the University of Alabama in Huntsville (UAH) and the Universities Space Research Association (USRA) conducted baseline air quality model simulations for August 2006 using CMAQ. The results were compared against routine surface observations as well as against ozonesonde measurements launched as part of the IONS-06 field campaign. The baseline simulation and measurements will be used to assess the impact of LNOM on CMAQ results.

To determine the feasibility of our approach, we will use three quantitative metrics. The first is a metric that quantifies how CMAQ model predicted trace gas concentrations change between a model run with and without LNOM lightning modeling. For a given CMAQ model output location, **r**, and time, *t*, the metric is

$$\delta_1(\mathbf{r},t) = T(\mathbf{r},t) - T_b(\mathbf{r},t) \ . \qquad (3)$$

Here, T_b is the baseline (no lightning) trace gas concentration, and T is the trace gas concentration using the LNOM-improved CMAQ model. The baseline run is for the CONUS for calendar year 2006. We will obtain the distribution $\delta_1(\mathbf{r},t)$ for several trace gases, including ozone, and NO_x. This will provide a clear understanding of the basic impact of LNOM.

The second metric will quantify the error between the LNOM-improved CMAQ model predicted ozone concentration *C* and the surface ozone (or ozonesonde) measurement, *M*. The third metric is similar to the second metric, but with the baseline

CMAQ ozone concentration C_b replacing C. The metrics can be written:

$$\delta_2(\mathbf{r}_a, t_a) = C(\mathbf{r}_a, t_a) - M(\mathbf{r}_a, t_a)\,,$$
$$\delta_3(\mathbf{r}_a, t_a) = C_b(\mathbf{r}_a, t_a) - M(\mathbf{r}_a, t_a)\ . \quad (4)$$

These are evaluated at all available ozone measurement locations and times given by ($\mathbf{r}_a$, t_a) that are within the CMAQ domain. Also note that by inter-comparing these two metrics, we will be able to show which of the two CMAQ ozone concentrations (baseline or LNOM-improved) is closer to the measured ozone value.

6. SUMMARY

We anticipate that the application of LNOM will result in a significant improvement in the lightning NO_x emission inventory used by CMAQ, and therefore will improve the accuracy of CMAQ air chemistry and air quality simulations. LNOM carefully identifies and uses those variables that govern lightning NO production; crucial variables that are directly linked to the natural variability of lightning are no longer ignored. Moreover, LNOM picks those variables that can be obtained or estimated using state-of-the-art lightning datasets, empirical models, and laboratory results. Specifically, VHF lightning mapping data will provide realistic channel lengths, and multiplicity data from the NLDN will account for the NO contribution from each stroke in the ground flashes. The VHF data also provide realistic channel segment altitudes which when combined with (NLDN-derived or estimated) channel peak current values and the laboratory spark experimental results discussed, one obtains realistic NO production from the channel segments. Finally, the number of ground flashes is provided by the NLDN data, and the number of cloud flashes is inferred from satellite lightning climatology (adjusted as needed using an empirical model for cold cloud thickness).

7. REFERENCES

Boccippio, D. J., K. L. Cummins, H. J. Christian, and S. J. Goodman, Combined satellite and surface-based estimation of the intracloud:cloud--to-ground lightning ratio over the continental United States, *Mon. Weather Rev.*, 129, 108-122, 2001.

Cummins, K. L., J. A. Cramer, C. J. Biagi, E. P. Krider, J. Jerauld, M. A. Uman, V. A. Rakov, The US National Lightning Detection Network: post-upgrade status, *Second Conference on Meteorological Applications of Lightning Data*, Am. Meteorol. Soc., Atlanta, Ga., January 29 - February 2, 2006.

Hill, R. D., A survey of lightning energy estimates, *Rev. of Geophys. and Space Phys.*, **17**, 155-164, 1979.

Kaynak, B., Y. Hu, R. V. Martin, A. G. Russell, Y. Choi, and Y. Wang, The effect of lightning NO_x production on surface ozone in the continental United States, *Atmos. Chem. Phys. Discuss.*, **8**, 5061-5089, 2008.

Koshak, W. J., R. J. Solakiewicz, R. J. Blakeslee, S. J. Goodman, , H. J. Christian, J. M. Hall, J. C. Bailey, E. P. Krider, M. G. Bateman, D. J. Boccippio, D. M. Mach, E. W. McCaul, M. F. Stewart, D. E. Buechler, W. A. Petersen, D. J. Cecil, North Alabama Lightning Mapping Array (LMA): VHF source retrieval algorithm and error analyses, J. Atmos. Oceanic Technol., **21**, 543-558, 2004.

Pickering, K.E., Y.S. Wang, W.K. Tao, C. Price, and J.F. Muller, Vertical distributions of lightning NO_x for use in regional and global chemical transport models, *J. Geophys. Res.*, **103** (D23), 31203-31216, 1998.

Price, C. and D. Rind, What determines the cloud-to-ground lightning fraction in thunderstorms?, *Geophys. Res. Lett.*, **20**, 463-466, 1993.

Uman, Lightning, New York: McGraw-Hill, 1969.

Wang, Y., A. W. DeSilva, and G. C. Goldenbaum, Nitric oxide production by simulated lightning: dependence on current, energy, and pressure, *J. Geophys. Res.*, **103**, 19149-19159, 1998b.