

WRF-Chem modeling of sulfur dioxide emissions from the 2008 Kasatochi Volcano

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Abstract

We simulate the dispersion and chemical evolution of the sulfur dioxide (SO₂) plume following the eruption of Kasatochi Volcano in Alaska, USA, on August 7th, 2008 with the Weather Research Forecasting with Chemistry (WRF-Chem) model. The model was initialized with the observed three distinct plumes, which were characterized by a total estimated SO₂ mass of 0.5 to 2.7 Tg. WRF-Chem modeled output was compared to remote sensing retrievals from the Ozone Monitoring Instrument (OMI), and the modeled plumes agreed well in shape and location with the OMI retrievals. The calculated SO₂ column densities showed comparable Dobson Unit values with higher densities especially in the center of the distal plume over northern Canada. We concluded from our analysis that WRF-Chem derived a 9.1-day lifetime of the SO₂ when initialized with a 12km eruption height. Sensitivity tests with varying eruption plume heights revealed significantly increased lifetimes of SO₂ up to 17.1 days for higher plumes.

I. INTRODUCTION

Kasatochi volcano [52.169°N, 175.511°W] is a small (2.7 × 3.3 km, 314 m above sea level, a.s.l.), uninhabited stratovolcano in the Aleutian Arc of Alaska (Scott, Nye, Waythomas, & Neal, 2010). On August 2nd, 2008 US Fish and Wildlife biologists reported small tremors and a sulfur odor while on assignment (Waythomas et al., 2010). They were evacuated prior to a M5.8 earthquake on August 7th, 2008 at 2:00 pm AKDT (22:00 UTC), detected by instruments from the Great Sitkin seismic Network. Infrared satellite retrievals from the Advanced Very High Resolution Radiometer (AVHRR) confirmed the presence of a volcanic plume situated over the volcano's vent during this time (Waythomas et al., 2010). Two additional eruptions followed at 01:50 UTC and 04:35 UTC (Scott et al., 2010). The ash

and SO₂ emissions dispersed in a complex pattern due in large part to a low-pressure cyclogenesis situated nearly on top of the volcano (Krotkov, Schoeberl, Morris, Carn, & Yang, 2010). Coarse ash and fine lapilli deposited quickly while most of the fine ash and SO₂ initially dispersed to the southeast (Waythomas et al., 2010). The resulting SO₂ plume eventually entered the jet stream and traveled into the continental United States and Canada within a week (Krotkov et al., 2010).

The Kasatochi eruption is unique for various reasons. It resulted in the largest injection of SO₂ into the atmosphere since the Mount Hudson eruption in Chile, August 1991. Initial estimates were between 1.20 to 2.7 Tg (Krotkov et al., 2010; Prata, Gangale, Clarisse, & Karagulian, 2010). By using inverse transport modeling, Kristiansen et al. (2010) established a 1.7 Tg

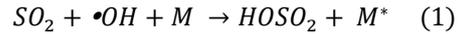
mass loading. In addition, plume altitudes exceeded the tropopause (maxima near 7 to 12 km with smaller emissions up to 20 km) introducing about 1.0 Tg of SO₂ into the stratosphere (Kristiansen et al., 2010).

Modeling SO₂ emissions is useful for various reasons. SO₂ is often collocated with volcanic ash and thus may be used as a proxy for ash where remote sensing is hindered by ice formation, water or cloud cover. Additionally, WRF-Chem studies of historical volcanic eruptions are motivated to test and provide source data and model parameterization schemes capable of predicting volcanic SO₂ and ash eruptions in an operational setting in near real-time. Here, we use the well-defined Kasatochi SO₂ eruption to study WRF-Chem's ability to model volcanic SO₂ transport and conversion.

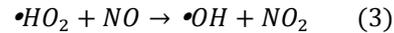
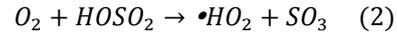
II. BACKGROUND

Sulfur dioxide emissions from Kasatochi have been modeled previously with particle dispersion models (D'Amours et al., 2010; Kristiansen et al., 2010). Wang and others (2010) studied SO₂ dispersion and aerosol formation plume height sensitivity using the Eulerian GEOS-Chem model by initializing the model domain with time-fitted SO₂ column densities from the Ozone Monitoring Instrument (OMI) using the Extended Iterative Spectral Fit (EISF) method. This WRF-Chem study differs from the GEOS-Chem study in that it does not require plume column densities, only specific eruption source data such as location, height, emission rate and duration. These parameters are included in tabulated Eruption Source Parameters (Mastin et al., 2009), which may be used to initialize WRF-Chem for operational volcanic ash and SO₂ forecasts. Sulfur dioxide converts quickly (on the order of days) to sulfate aerosols. In the stratosphere, where the majority of the Kasatochi SO₂ converted to sulfate, the conversion process is

dominated by the interaction of SO₂ with the hydroxyl radical (•OH). Production of •OH begins with the generation of excited states of atomic oxygen from ozone and diatomic oxygen via photolysis. The hydroxyl radical oxidizes SO₂ in the stratosphere according to Equation 1.



M* is a third body quencher required to remove excess energy from the reaction. This process was initially proposed to decrease the ambient amount of •OH, and thus a second order rate equation would be needed to model it. However, as mentioned by McKeen, Liu, & Kiang (1984), there is a cycling of the hydroperoxy radical, HO₂•, and •OH in the presence of nitrogen oxide species, NO_x (McKeen et al., 1984):



This cycling ensures the regeneration of •OH concentration. If we assume [•OH] is constant and [M] varies only with pressure, we may solve the following differential equation to analytically calculate the change in concentration of SO₂ with time:

$$\frac{dSO_2}{dt} = -k_3[SO_2][\bullet OH][M] \quad (4)$$

$$[SO_2]_f = [SO_2]_i e^{-k_3[M][\bullet OH]t} \quad (5)$$

Here, $k_3[M]$ is the pseudo first order rate constant based on Equation 3.

Sulfur dioxide and •OH also interact via aqueous phase reactions. In such reactions, •OH is produced by dissolved hydrogen peroxide in water, which then reacts with dissolved, aqueous SO₂.

III. METHODS

The application of WRF-Chem for simulating the transport and effects of volcanic emissions within the atmosphere has been described in (Stuefer et al., 2013). Importantly, WRF-Chem has been proposed as an operational tool for volcanic emissions modeling. Here, we test the feasibility of using WRF-Chem to capture SO₂ emissions using the well-studied 2008 Kasatochi eruption.

The choice of eruption initialization parameters greatly impacts the ability of the model to predict volcanic ash and SO₂ transport (Mastin et al., 2009; Webley, Stunder, & Dean, 2009). Table 1 lists the domain initialization parameters used in this study and Table 2 provides the initialization parameters for the eruption. We utilized the Global Forecast System (GFS) Final Reanalysis (FNL) datasets as base meteorological fields (NOAA, 2014).

WRF-Chem may use either default values for Eruption Source Parameters (ESP) or if available, source data from plume observations. Karagulian and others (2010) discovered a minimum of 1.7 Tg SO₂ from the Kasatochi eruption using remote sensing data from the Infrared Atmospheric Sounding Interferometer (IASI). Kristiansen and others (2010) utilized inverse transport modeling to establish a similar mass of 1.7 Tg based on measurements from UV, IR and Lidar data. In a recent GEOS-Chem study by Wang et al. (2013) a value of 2.0 Tg SO₂ was used. Herein, we initialized WRF-Chem with a total of 1.7 Tg of SO₂. This mass was gradually added to the model using a constant eruption rate of 23,600 kgs⁻¹ over the course of the three eruptions, using eruption durations and times based on Waythomas et al. (2010) (compare Table .

WRF-Chem initializes, by default, volcanic ash and SO₂ plumes as an umbrella shape with 75% of erupted mass in the plume surrounding the

specified plume height and 25% of the mass linearly detrained underneath (Stuefer et al., 2013). For the eruption plume height, the ESP implemented within the WRF-Chem preprocessor as a default includes a height of 11km for Kasatochi. However, in accordance with Kristiansen et al. (2010), we chose 12 km a.s.l \pm 4 km for this study in order to test the sensitivity of the model to its plume height source. For the example of our mean plume height of 12 km a.s.l, the umbrella will include 75% of the mass between 9 - 13 km a.s.l (peaking at 12 km a.s.l) and 25% below 9 km, linearly decreasing with height (Stuefer et al, 2013).

Table 1: Domain parameters for WRF-Chem

Domain Size	600 x 400
dx, dy	15 km x 15 km
Vertical levels	40, terrain following
Model Height	2,000 Pa
Projection	Lambert-Conformal
Center Lat/Lon	50°N, -120°W

Kasatochi erupted over half of the SO₂ into the stratosphere. Therefore, it is important to capture the gas-phase chemistry behind stratospheric SO₂ oxidation shown in Equation 1. The model simulations utilized the Second Generation Regional Acid Deposition Model Mechanism (RADM2) for gas and aqueous phase reactions. The RADM2 model includes the oxidation of SO₂ by •OH as depicted in Equation 1 using the first order kinetics in Equations 4 and 5 (Stockwell et al., 1990) as well as the treatment of the NO_x species in Equations 2 and 3. Gaseous precursors, such as NO and •OH, were loaded into the model using the Prep-Chem-Source 1.4 preprocessor (Freitas et al., 2011). As mentioned, SO₂ also converts via aqueous phase chemistry with •OH. This scheme is also parameterized within WRF-Chem RADM2.

Table 2: Eruption times and durations

Eruption Date, Time	Eruption Duration	Eruption Rate
8/7 22:00 UTC	60 minutes	23600 kg/s
8/8 01:50 UTC	30 minutes	23600 kg/s
8/8 04:35 UTC	30 minutes	23600 kg/s

Global ozone and other trace gases, such as SO_2 , are detected by the Ozone Monitoring Instrument (OMI), a nadir viewing, ultraviolet (UV)/visible spectrometer aboard the National Aeronautical & Space Administration's (NASA) Earth Observing System's (EOS) Aura satellite. OMI covers a spectral range of 264-504 nm, allowing measurements of ultraviolet and visible SO_2 signals. It provides global coverage once per day with a nadir pixel size of $13 \times 24 \text{ km}^2$ and swath width of 2,600 km and has been used in previous research studies for volcanic emissions analysis (Kristiansen et al., 2010; Krotkov et al., 2010; Lopez et al., 2013; Wang et al., 2013).

For spatial analysis, we utilized NASA's Level 2 SO_2 product, ColumnAmount SO_2 _STL (from here on STL). Column densities of SO_2 in Dobson Units (DU) for this product are shown in Figure 1. Since the STL derived data may underestimate the total amount of SO_2 in plume areas of high concentration, we used values from Krotkov et al. (2010) based on the Extended Iterative Spectral Fit (EISF) method for mass analysis. Applications of this method to Kasatochi SO_2 suggest that it may capture additional SO_2 that other algorithms might miss (Krotkov et al., 2010; Yang et al., 2010).

IV. RESULTS

Figure 1 shows the dispersion of the plume as modeled by WRF-Chem and derived by the OMI STL product. The model captured the

plume's interaction with the meteorology well, as it dispersed over the North American continent. Figure 2 shows a brief spatial analysis along two transects (105W and 145W) marked in red. Plume SO_2 column densities were generally collocated with OMI here, however the normalized masses peaked in different areas. To compare the change in mass in the domain, a linear correlation plot was constructed and presented in Figure 3. We saw a high degree of correlation ($> 0.9 r^2$) for all plume height test cases between the change in WRF-Chem predicted SO_2 mass and those observed by OMI.

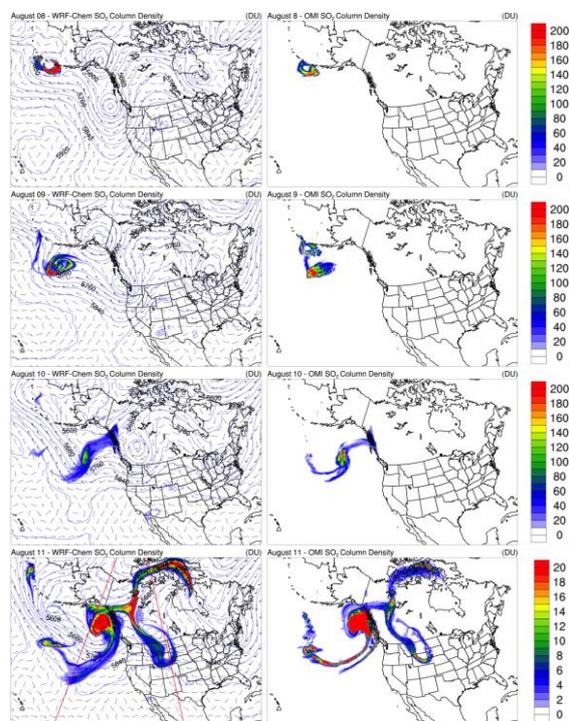


Figure 1: Dispersion of the Kasatochi SO_2 plume as modeled by WRF-Chem (left) and calculated by the OMI STL product (right). The transects used for spatial analysis are shown in red on the August 11th plot. Geopotential height and wind vectors are plotted on WRF-Chem plots.

A lifetime of SO_2 was established using linear regression analysis; the lifetimes significantly

varied with height. The 12km eruption height yielded a 9.1 days lifetime ($r^2=0.74$) while the 8km and 16km plumes resulted in longer lifetimes of 10.6 and 17.1 days ($r_2=0.72, 0.68$), respectively.

V. DISCUSSION

WRF-Chem generally predicted a more disperse plume than was observed by OMI. In addition, there is a higher mass bias in the model results. This is markedly different from the work of Wang et al. (2010) where GOES-Chem produced a low mass bias. In addition, the mass located in the distal plume trended higher than that in the proximal. This is likely a direct result of the chosen ESP used for the modeled case as this varied with the plume height.

The rate of SO₂ conversion agreed well with literature values. We used values from Krotkov et al. (2010) using the EISF method and from Kristiansen et al., (2010) to test WRF-Chem output. In Figure 3 we see that all three initialized eruption heights produced r² values above 0.9. As mentioned, a range of values was produced for the lifetime using linear regression analysis. The 12km eruption produced the shortest lifetime, being about 9 days. This dependence of lifetime on plume height is most likely a direct result of different chemistry at the various levels of the atmosphere. The 12km eruption included SO₂ mass located mostly in the stratosphere where conversion based on Equation 1 dominated, yet also included enough SO₂ in the troposphere where aqueous phase and heterogeneous chemistry can also occur.

WRF-Chem captured the dynamics and mass changes of the Kasatochi plume according to these results. It is, therefore, a robust candidate for volcanic emissions modeling, especially in the operational setting where multiple unknowns such as a specific plume height are present.

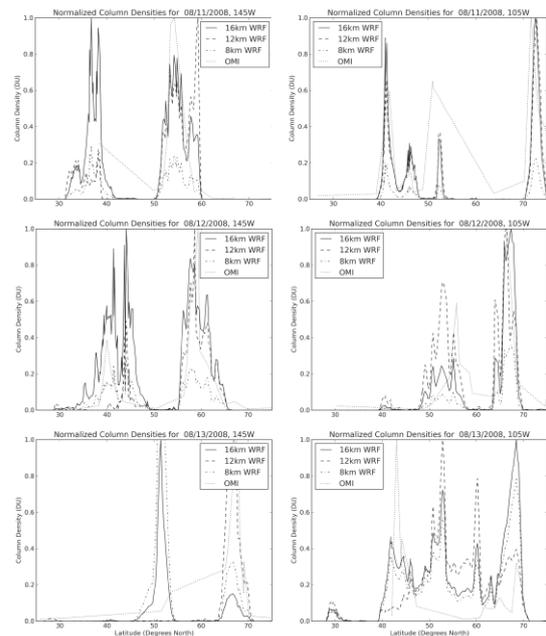


Figure 2: Spatial comparisons of SO₂ column densities from WRF-Chem using 8, 12 and 16 km initialized plume heights and from the OMI STL product.

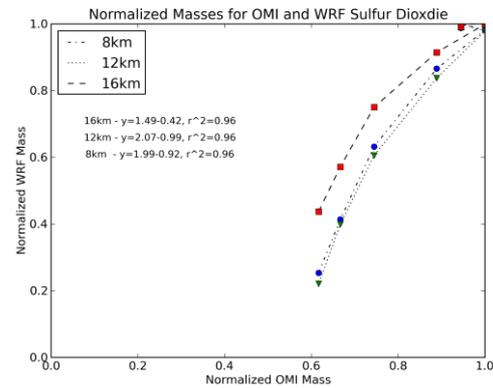


Figure 3: Correlation between WRF-Chem (y-axis) and literature OMI (x axis) SO₂ domain masses for 8, 12 and 16 km plume heights.

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