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Extreme ozone events: Tail behavior of the surface ozone distribution over the U.S.

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HIGHLIGHTS

- Analyze the concentration of ozone using extreme value theory.
- Transform the data to get rid of inter- and intra-annual effects.
- Generate synthetic data to compare and verify the methods used.
- Calculate upper limits (if applicable) and 20-year return levels of ozone.
- NOx SIP call decreases the mean but increases shape parameter of the distribution.

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ABSTRACT

The ground level ozone concentration over the continental United States is analyzed from the point of view of modern Extreme Value Theory using ozone data from the Clean Air Status and Trends Network (CASTNET) at 25 measurement sites. At each site the data is analyzed separately for two time periods (1992–2002 and 2003–2013) approximately separated by the NO_X SIP call. The Generalized Pareto Distribution is fit to extremes of the ozone concentration by using a combination of maximum likelihood estimates (MLEs) and Hill estimates. The data is appropriately transformed prior to extreme value analysis and data in the right tail is separated from that in the middle part of the distribution. This analysis is compared to current approaches by using synthetic data. Under a variety of conditions the procedure using the MLE approach is likely to underestimate the tail of the distribution. The analysis of the CASTNET ozone data shows that at some locations the ozone probability distribution is not exponentially bounded, and thus can be characterized as heavy tailed, and that at other locations this distribution is not heavy and is bounded to the right so that the ozone concentration is bounded for any return period. The tails of the distribution of ozone concentration become heavier following the NO_X SIP call at most of the sites with heavy tails prior to this call.

1. Introduction

Chronic and acute exposure to surface ozone has been associated with increased risk of death from cardiovascular and respiratory causes (Bell et al., 2004; Jerrett et al., 2009) and damage to agriculture estimated in 2000 at $14-$26 billion per year (van Dingenen et al., 2009). Ozone, a secondary pollutant, is generated through the oxidation of volatile organic carbons, carbon monoxide and methane in the presence of NO_X and sunlight. The analysis of Duncan et al. Duncan et al., 2010 shows that across most of the continental U.S. ozone production is NO_X limited. Ozone shows significant temporal variability within the continental boundary layer across a wide range of timescales with pronounced inter-annual, seasonal, daily and hourly variability. The ozone

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distribution in the Eastern U.S. has a summertime temporal distribution with heavier than Gaussian tails (Rieder et al., 2013). It is the more extreme events that exceed the Environmental Protection Agency (EPA) ozone regulated limits. The purpose of this paper is to use extreme value theory to analyze high ozone concentrations over the continental U.S.

Ozone has been regulated in the U.S. under the Clean Air Act since 1971. In 1997 the NAAQS (National Ambient Air Quality Standard) for ozone was set to a maximum daily 8-h average ozone (MDA8 O_3) of 84 ppb. To meet this standard, the NO_X State Implementation Plan (SIP) was implemented for controlling NO_X emissions in 22 states in the Eastern U.S. The result was an approximate 50% decrease in eastern U.S. NO_X emissions from point sources between 1999 and 2003 (Frost et al., 2006). Rieder et al., 2013 shows that both the mean ozone concentrations and the 1 and 5 year return level concentrations decreased between 1989 and 1998 (prior to the NO_X SIP implementation) and 1999–2009 (subsequent to the NO_X SIP implementation) over the Eastern U.S..

Summertime ozone concentrations over the U.S. can be thought to be comprised of two portions: a portion amendable by U.S. emissions controls and a background value not sensitive to these controls (e.g., Fiore et al., 2014). Summertime background values range from 25 to 40 ppb over high-altitude western sites to 20–30 ppb over the Eastern U.S. (Fiore et al., 2014). Extreme ozone pollution concentrations above background levels can sometimes be associated with tropopause folds (Lin et al., 2012) or with wildfires (e.g., Jaffe and Wigder, 2012), but more frequently with an intensification of pollution events in association with particular meteorological conditions. Intense pollution events are often associated with warm stagnant conditions over the East Coast of the U.S. (Hegarty et al., 2007; Vukovich, 1995) and often occur with weak, slow-moving and persistent high-pressure systems (Logan, 1989). The 2003 European heat wave and the associated strong stagnation is an example of a severe meteorological event accompanied by dangerous ozone concentrations (Vautard et al., 2005; Vautard et al., 2007; Guerova and Jones, 2007; Solberg et al., 2008). Summertime ozone concentrations are highly correlated with temperature (Brown-Steiner et al., 2015 and references therein). This is at least partly explained by the correlation between temperature, air stagnation, and solar radiation (e.g., Jacob and Winner, 2009). There is a number of feedbacks between the severity and duration of heat waves and surface pollution concentrations including changes in natural emissions particularly those from fire and vegetation (Fang et al., 1996; Guenther et al., 2006; Guenther et al., 2012) and changes in stomata ozone uptake with its impact on dry deposition (Vautard et al., 2005; Solberg et al., 2008). On the other hand, the tropospheric chemical system appears to be highly buffered (Shindell et al., 2003; Stevenson et al., 2006) so that the response of ozone to changes in chemical or meteorological forcing may be weaker than expected.

Temperatures (IPCC, 2013), the frequency and severity of heat waves (Russo et al., 2014), and in many parts of the globe air stagnation days (Horton et al., 2014) are expected to increase during this next century. However, NO_X emissions, in many locations the limiting ozone precursor, are expected to decrease. A number of studies have suggested that climate change alone will preferentially increase the frequency of extreme pollution events on the high end of the cumulative probability distribution (Mickley et al., 2004; Hogrefe et al., 2004; Tagaris et al., 2007; Wu et al., 2008) although other studies do not show this (Murazaki and Hess, 2006; Lin et al., 2008; Rieder et al., 2015). The projected future decrease in NO_X emissions, on the other hand, is expected to decrease both the mean and the 90th percentile ozone concentrations (Rieder et al., 2015) over the Eastern U.S. with the 90th percentile more sensitive to NO_X changes than the mean concentration.

Extreme value theory (EVT) provides a useful mathematical framework to examine the tail of the ozone distribution, which we usually refer to as the right end of the distribution Coles, 2001. Most notably Rieder et al. (Rieder et al., 2015; Rieder et al., 2013) used extreme value theory to quantify ozone extreme values over the Eastern U.S. and the extreme response of ozone to emission changes.

The goal of this paper is to further characterize ozone extremes over the continental U.S. The results are used to characterize the geography of the extreme behavior of measured ozone concentrations. We achieve this goal by refining the approach in Rieder et al., 2013 via specialized methods for estimating tail properties of the ozone distribution. These methods are tested on synthetic data and applied subsequently to analyze CASTNET (The Clean Air Status and Trends Network) ozone data over the continental U.S. The analysis of the CASTNET dataset allows us to examine continental scale geographic differences in extreme behavior of ozone and how this behavior changes following the NO_X SIP implementation. CASTNET provides a regional characterization of ozone concentrations representative of rural background conditions, and is thus more suitable for an evaluation of global chemistry climate models than data ozone measurements more specific to local conditions. In contrast to Rieder et al., 2013, we present results over the entire U.S. and focus on the shape of the tail of the ozone distribution. We show that at some locations the ozone probability distribution is not exponentially bounded, and thus can be characterized as heavy tailed; however, in other locations the distribution is not heavy tailed. In these latter locations the distribution is bounded and the ozone concentration has an upper limit for arbitrarily long return periods. In these locations we characterize the distribution as having light tails. We show that following the reduction of NO_X emissions in association with the NO_X SIP call the number of locations where the ozone distribution is heavy tailed increases significantly.

The paper is organized as follows. In section 2 we review the data used and how it is transformed so as to apply extreme value theory to the CASTNET ozone measurements. In section 3, we briefly review extreme value theory and apply it to synthetic distributions so as to recommend a best practice procedure for applying extreme value theory to measured ozone distributions. Our contention is that applying extreme value theory and estimating extreme behavior is trickier than it may appear initially, for several reasons. In section 4 we analyze the geography of extreme values throughout the U.S. using CASTNET data and in section 5 we give our conclusions.

2. Data

Ozone measurements from the CASTNET (www.epa.gov/castnet) observational network are used to analyze the ozone extremities at 25 sites throughout the continental U.S. (see Table 1). The hourly CASTNET data is converted into daily data by calculating the maximum daily 8-h average of ozone concentration (MDA8), which is denoted by $x_{y,d}$ for the day d in year y. We use the summertime (June, July and August—JJA) ozone measurements between 1992 and 2013. We have further divided the CASTNET data into 2 periods: 1992–2002 and 2003–2013 so as to investigate the effect of the NO_X SIP call on the ozone extremes.

It is necessary to further transform the daily observations in order to make them approximately stationary (i.e. to prevent significant distributional changes from day to day). Such potential distributional changes can be thought of as arising from two different phenomena: overall inter-annual changes from year to year and intra-annual seasonal variations within the same year. This leads to a 2-step method of data transformation. In the first