Final Report

Biogenic VOC Emission Estimates for the TexAQS 2000 Emission Inventory: Estimating Emissions During Periods of Drought and Prolonged High Temperatures and Developing GloBEIS3

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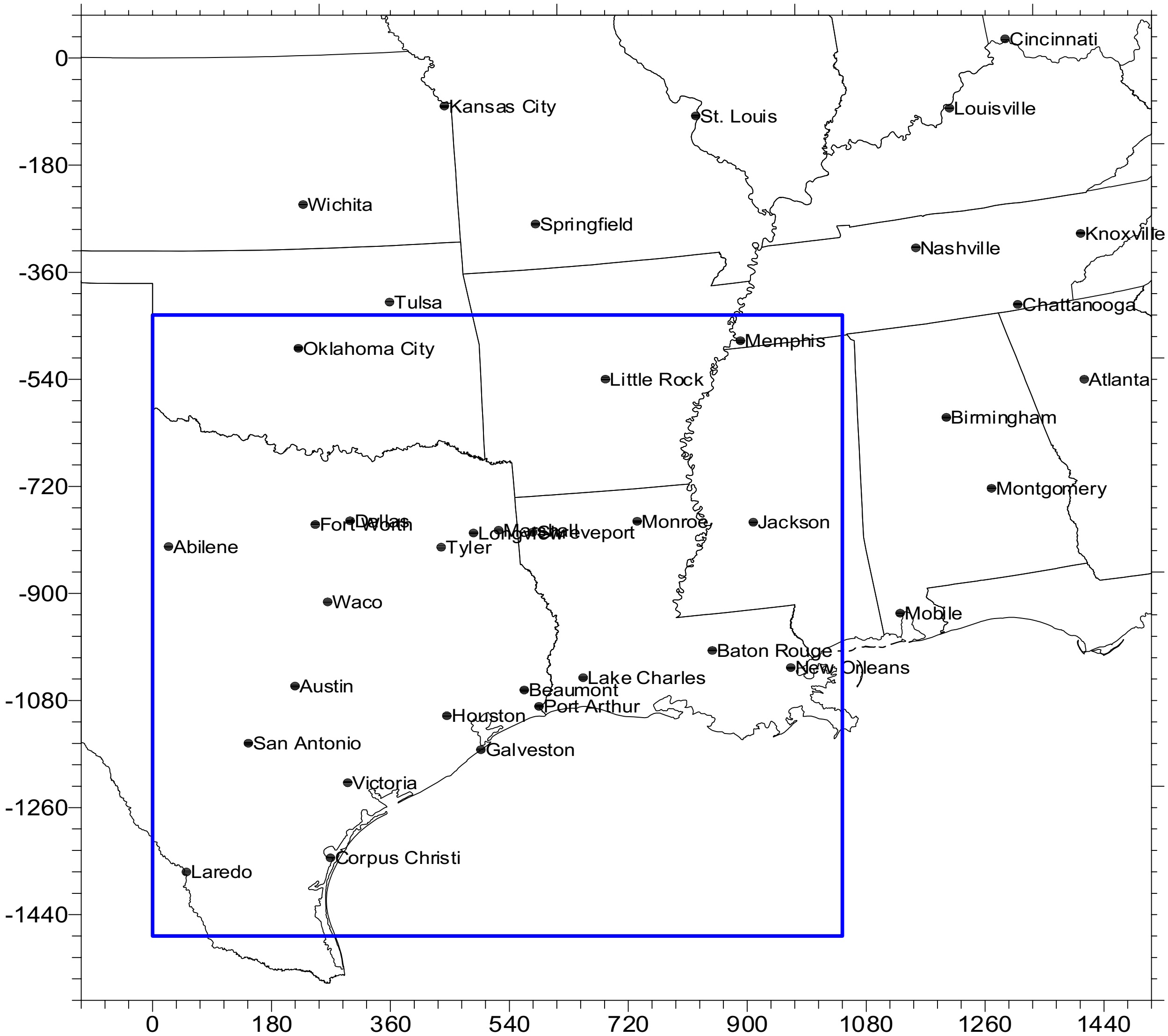
1. INTRODUCTION

Emissions from natural sources are important to the photochemistry of the lower atmosphere. In particular, emissions of volatile organic compounds (VOCs), nitrogen oxides (NOx) and carbon monoxide (CO) from plants and soils (biogenic emissions) are precursors to the formation of tropospheric ozone (Fehsenfeld et al., 1992). The TNRCC is responsible for developing plans to ensure that air quality in the state of Texas meets the National Ambient Air Quality Standards (NAAQS) for ozone. The TNRCC uses the CAMx photochemical grid model (ENVIRON, 2000) to develop air quality plans for ozone, and an accurate biogenic emission inventory is an important input to the CAMx modeling.

The TNRCC uses the GloBEIS emissions model (ENVIRON, 1999) to prepare biogenic emission inventories. The area included in the TNRCC's biogenic emission inventories is shown in Figure 1-1. The modeling grids are defined in a Lambert Conformal Projection (LCP) with central latitude of 40 degrees North and a central longitude of 100 degrees West. The new modeling grids include a 36 km grid covering the south and central U.S. ('regional' domain) and a nested 12 km grid covering eastern Texas and several surrounding states ('arklatx' domain). In addition, one or more nested 4 km grids will be included over ozone Texas nonattainment areas (Houston, Galveston, Beaumont, Port Arthur, Dallas, Fort Worth) and/or near nonattainment areas (Austin, Corpus Christi, San Antonio, Victoria, Tyler, Longview).

Previous biogenic VOC emission models, e.g., GloBEIS 2.2, do not account for the influence of drought on VOC emissions, but it is well known that drought will impact most plant physiological processes. The physiological responses to moderate drought include significant reductions in stomatal conductance and photosynthesis rates. Extreme drought reduces these rates to zero and results in senescence (the plant drops its leaves) in some plants. Investigations of the influence of drought and prolonged high temperatures on isoprene emissions suggest that these factors will be important in determining emission variations. Extreme and extended drought will lower the isoprene emission capacity of a plant and lower the total leaf area. However, moderate drought might actually increase isoprene emission due to the influence of prolonged high leaf temperatures that result for lower water potentials.

This report introduces the GloBEIS 3.0 model, which has an improved capability for predicting isoprene and other biogenic VOC emissions during periods of drought. The GloBEIS 3.0 framework is suitable for modeling emissions during drought, but there currently is a lack of observations for specifying some of the parameters in this model. It should be recognized that the resulting predictions of the impact of drought on biogenic VOC emissions have large uncertainties but can be used to determine the sensitivity of emissions to drought and indicate whether additional observations are required to provide a more accurate prediction.



CAMx GRID DIMENSIONS
LCP Grid with reference origin at (40 N, 100 W)

36 km Grid: 45 x 46 cells from (-108, -1584) to (1512, 72)
12 km Grid: 87 x 87 cells from (0, -1476) to (1044, -432)

(nested grid dimensions do not include buffer cells)

Figure 1-1. Regional 36 km and 12 km resolution modeling grids for which biogenic emissions model inputs will be prepared at 12 km and 4 km resolution, respectively.

2. METHODS

The procedures used to accomplish each task are described in this section. Details on modifications to the GloBEIS code required to implement each of the new features are given in Appendix 1.

Drought

Potential drought index data were investigated to determine the best candidate for including in GloBEIS at this time. There are several indices used to describe the severity of a drought or the availability of water. These are primarily used by governmental and agricultural agencies to estimate relief needs and crop health. Examples of these indices include the Palmer Drought Severity Index (PDI) (Palmer, 1965) (an indicator of meteorological drought), the Crop Moisture Index (CMI) (Palmer, 1968), (a derivative of the PDI that represents short-term moisture in major crop- producing regions), and the Standardized Precipitation Index (SPI) (McKee et al., 1993) (based on the probability of precipitation for any time scale, and an indicator of hydrological drought). Many of these indices are described and provided by the National Drought Mitigation Center at the University of Nebraska-Lincoln (URL: http://drought.unl.edu/ndmc/enigma/indices.htm). Links to current drought data, background information and specific state-run sites are provided by the National Oceanic and Atmospheric Administration (NOAA) (URL: http://www.drought.noaa.gov/).

Another index that was investigated is the Vegetation Health Index (VHI) developed by Felix Kogan of NOAA. The VHI is calculated from processed Normalized Difference Vegetation Index (NDVI) and brightness temperature (BT) data observed by the Advanced Very High Resolution Radiometer (AVHRR) satellite instrument. These indices are directly related to drought stress in vegetation, and could be used to determine the extent of drought and water stress on vegetation, and it's effects on biogenic emissions. Global vegetation health is calculated at 16km resolution on a weekly time scale (Kogan, 1997). Currently, VHI data (mostly in image format) are available at URL: http://orbit-net.nesdis.noaa.gov/crad/sat/surf/vci/index.html. Electronic datasets of VHI for the United States for the years 2001 and 2002 are available via ftp directly from Felix Kogan. Weekly VHI data for the United States at the climatic division resolution for the year 2000 was provided by Felix Kogan upon request. The VHI appears to be a very good indicator of vegetation water stress within the United States and around the world. The best resolution of the data that could have been obtained was at the same spatial resolution (climatic divisions, see Figure 2-1) as other, more easily available drought index data sets.

The Palmer Drought Severity Index (PDI) is used to assess long-term drought, based on meteorology and moisture conditions. The original Palmer Drought Severity Index was developed by W.C. Palmer (1965) and was updated by Heddinghaus and Sabol (1991). The indices and their definitions are given in Table 2-1.

Table 2-1. Modified Palmer Drought Severity Index definitions.

< -4	Extreme drought
-3.99 to –3.0	Severe Drought
-2.99 to –2.0	Moderate drought
-1.99 to –1.0	Mild Drought
-0.99 to –0.5	Incipient drought
-0.49 to 0.49	Near Normal
0.50 to 0.99	Incipient Wet Spell
1.0 to 1.99	Slightly wet
2.0 to 2.99	Moderately wet
3.0 to 3.99	Very wet
> 4.0	Extremely wet

The PDI is assigned to climatic divisions within each state, which are regions defined by factors such as soil type (Guttman and Quayle, 1996). For example, the state of Texas has 10 climatic divisions. Figure 2-1 shows the climatic divisions within the continental United States. Metadata or ArcINFO files containing the climatic division geodata can be downloaded from the U.S.G.S. at URL:
http://water.usgs.gov/GIS/metadata/usgswrd/climate_div.html

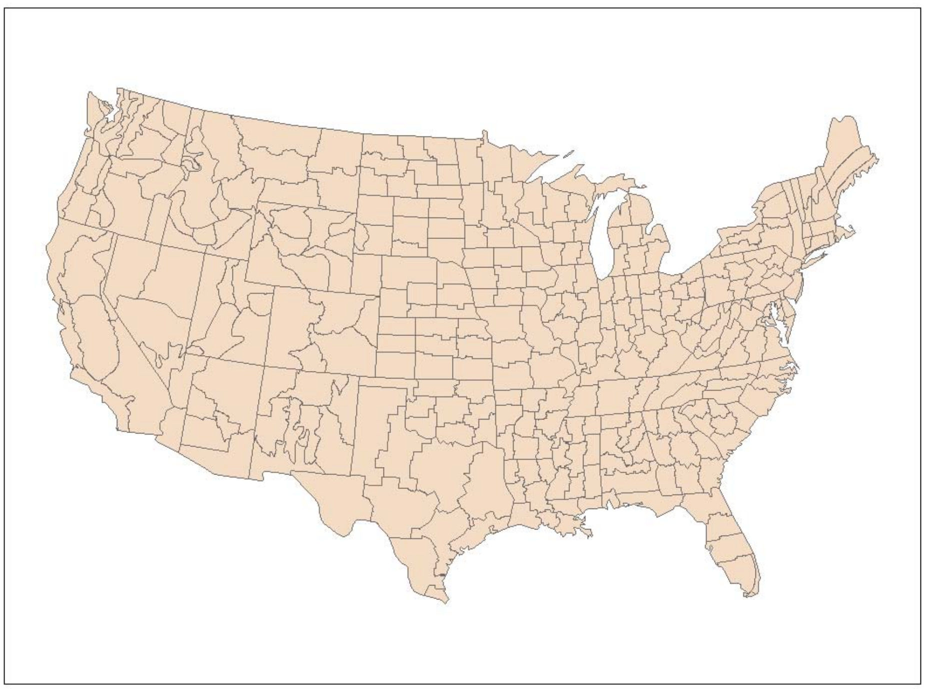


Figure 2-1. Climatic divisions of the United States.

A weekly PDI value is used to assign the severity of drought in each of the climatic divisions for 2 months in August and September, 2000 for all areas within the ‘regional’ and the ‘arklatex’ modeling domains. These PDI data were provided directly by Thomas Heddinghaus of the Climate Operations Branch (CPC, NCEP, NWS) of NOAA. A FORTRAN program was also provided to interpret the datasets.

To create the drought index files necessary for GloBEIS, a polygon shapefile of each modeling domain was produced. This was accomplished by calculating the centroids of each domain from the domain information provided by Mark Estes of TNRCC and Greg Yarwood of ENVIRON (the 'regional' domain with 12km resolution and the 'arklatx' domain with a 4km resolution, see Figure 1-1). These centroids were imported to ArcGIS and converted first to a point shapefile and then to a polygon shapefile using programs provided on the web. The polygon domain coverages were joined with the climatic division data within ArcGIS so that a climatic division was assigned to each grid cell. The weekly PDI value assigned to each Climatic Division was further joined to the geo data, and a final PDI file was output for each week for both domains. For areas covered with water, the PDI value is assigned as -9999. Since no drought data similar to the PDI were available for areas within Mexico, the areas in northern Mexico included in the modeling domains were assigned the PDI of the closest climatic division within Texas.

The qualitative descriptions of the influence of drought reported by several investigators (Tingey et al. 1981; Sharkey and Loreto, 1993; Fang et al., 1996; Guenther et al., 1999a) was used to develop a relationship between Palmer Drought Severity Index (PDI) and emissions of isoprene. The same activity factor is used for other VOC emissions, with the exception of the emission of monoterpenes that are contained in large pools, to reflect their presumed association with biological activity. The emission of monoterpenes from Texas vegetation is likely to be insensitive to drought (Lerdau et al. 1994) and GloBEIS 3.0 assumes that these emissions are not directly influence by drought. A reduction in stomatal conductance with increasing drought was also characterized in a simple linear relationship based on the above studies.

Leaf Area Index

A leaf area index (LAI) database has been prepared for the Texas 2000 study. LAI values are based on a standard 8-day average LAI product (MOD15A2 ISIN Grid V001) from the Moderate Resolution Imaging Spectroradiometer (MODIS). LAI data were acquired from the EROS Data Center (Sioux Falls, SD) at 1 km resolution for the following dates:

19 July 2000 (day 201)
20 August 2000 (day 233)
28 August 2000 (day 241)
05 September 2000 (day 249)
13 September 2000 (day 257)
21 September 2000 (day 265)
29 September 2000 (day 273)

(LAI data products were not available for the period between days 201 and 233).

LAI data were delivered in the Integerized Sinusoidal Projection, with 1 km pixels, in 10 x 10 degree sections. The data were reprojected to the Lambert Conformal Conic projection used in this study with the MODIS Reprojection Tool v.2.1 (EROS Data Center, Sioux Falls, SD). The reprojected 10 degree sections were mosaicked into continuous single-date images using ENVI software (RSI, Boulder, CO). Average LAI values for pixels inside the 4 km and 12 km grid cells were calculated using algorithms written in IDL (RSI, Boulder, CO) and applied using ENVI. The original LAI data use a no-data mask value of 255. These pixels were ignored when calculating the average grid cell values. Grid cells composed entirely of mask pixels were assigned a LAI of 0. Grid cell average LAI values were joined to grid cell polygons using Arc GIS 8.1 software (ESRI, Redlands, CA). Additional details describing the raw data are available for the MODIS sensor (http://modis.gsfc.nasa.gov/about/index.html), the 8-day average LAI product, MOD15A2 ISIN Grid V001, (http://edcdaac.usgs.gov/modis/mod15a2.html), and the MODIS Reprojection Tool (http://edcwww.cr.usgs.gov/programs/sddm/modisdist/info/index.shtml)

Leaf Temperature

The methods used for calculating leaf temperature are based on the work of Goudrian and Van Laar (1994) and Leuning et al. (1995). This includes both new modules for calculating leaf energy balance and improved methods for calculating radiation penetration into the canopy. In addition to the leaf temperature calculation, various components of the energy balance are computed and can be output by GloBEIS (as an option).

Antecedent Leaf Temperatures

We have implemented four numerical algorithms into GloBEIS 3.0 to describe this behavior: one each to describe the results of the three studies and a fourth that combines the results of all three studies. One option is to use the Petron et al. (2001) method which assumes that isoprene emissions are influenced by the average temperature during the past 360 hours. Emissions are calculated as:

$$\gamma_T = E_{opt}\, C_{T2} \exp(C_{T1}\, x)/[C_{T2} - C_{T1}\{1 - \exp(C_{T2}\, x)\}] \qquad (1a)$$

where $x = [(1/T_{opt})-(1/T)]/R$, T is current leaf temperature (K), R is the gas constant (=0.00831), E_{opt} is the maximum normalized emission capacity, T_{opt} is the temperature at which E_{opt} occurs, and the empirical coefficients C_{T1} (=95) and C_{T2} (=230) represent the energy of activation and deactivation, respectively. The maximum normalized emission capacity and the temperature at which it occurs are estimated as

$$E_{opt} = 1.9 \times \text{Exp}(0.125 * (T_{360} - 301)) \qquad (1b)$$

and

$$T_{opt} = 312.5 + 0.5 * (T_{360} - 301) \qquad (1c)$$

where T_{360} is the mean temperature (K) of the past 360 hours (15 days). Equation 3a is nearly equivalent to the algorithm of Guenther et al. (1993) for E_{opt} = 1.9 and T_{opt} = 312.5 K.

The second option is based on Geron et al. (2000) and assumes that emissions are influenced by the average temperature of the past 24 hours using the following algorithm:

$$\gamma_T = \gamma_{T1} [1 + 0.04 (T_{24} - 301)] \quad (2)$$

while the third is based on Sharkey et al. (2000) and calculates the antecedent temperature activity factor as

$$\gamma_T = \gamma_{T1} [1 + 0.06 (T_{48} - 301)] \quad (3)$$

where T_{48} is the average ambient air temperature (K) over the past 48 hours and γ_{T1} is the activity factor accounting for the temperature of the past hour. The fourth option combines all three models as

$$\gamma_T = \gamma_{T1} [1+0.04 (T_{18} - 301)+0.02 (T_{48} - 301))+0.14 (T_{360} - 301)] \quad (4)$$

3. RESULTS

Drought

It is well known that drought will impact plant physiological processes and several investigators have attempted to characterize the influence of drought on isoprene emissions. In addition to any direct influence on isoprene emission, drought can significantly reduce stomatal conductance and thus increase leaf temperatures. Algorithms that simulate these expected trends have been incorporated into GloBEIS and are available as an option.

The Palmer Drought Severity Index (PDI) was chosen as the best option for specifying drought in GloBEIS. The PDI is basically a soil moisture algorithm calibrated for relatively homogeneous regions, and is widely used. These data are applicable for Texas and its surrounding states. Qualitative evaluation of the data during the summer of 2000 (see URL: http://www.cpc.ncep.noaa.gov/products/analysis_monitoring/regional_monitoring/palmer/2000/weekly_PALMER_2000.html) concluded that these indices provided a good identification of the areas affected by drought in the summer and fall, 2000, and the extent of its effects. As shown in Figure 3-1, areas within Texas often had PDI indices of less than –4 during the study period of August through September 2000. The cost and time associated with obtaining and incorporating the higher spatially resolved VHI data were not feasible for this project. It is recommended that these data be further evaluated in the future, as it is likely that VHI could be used to identify the extent of drought.

A separate file is supplied for each week. The file is in GloBEIS input format (described in the GloBEIS Users Manual). The PDI in each file contains 3 significant figures. Nine files for each modeling domain were created, representing July 30 through September 30, 2000. A README file is included with these GloBEIS inputs to further explain the file-naming methods.

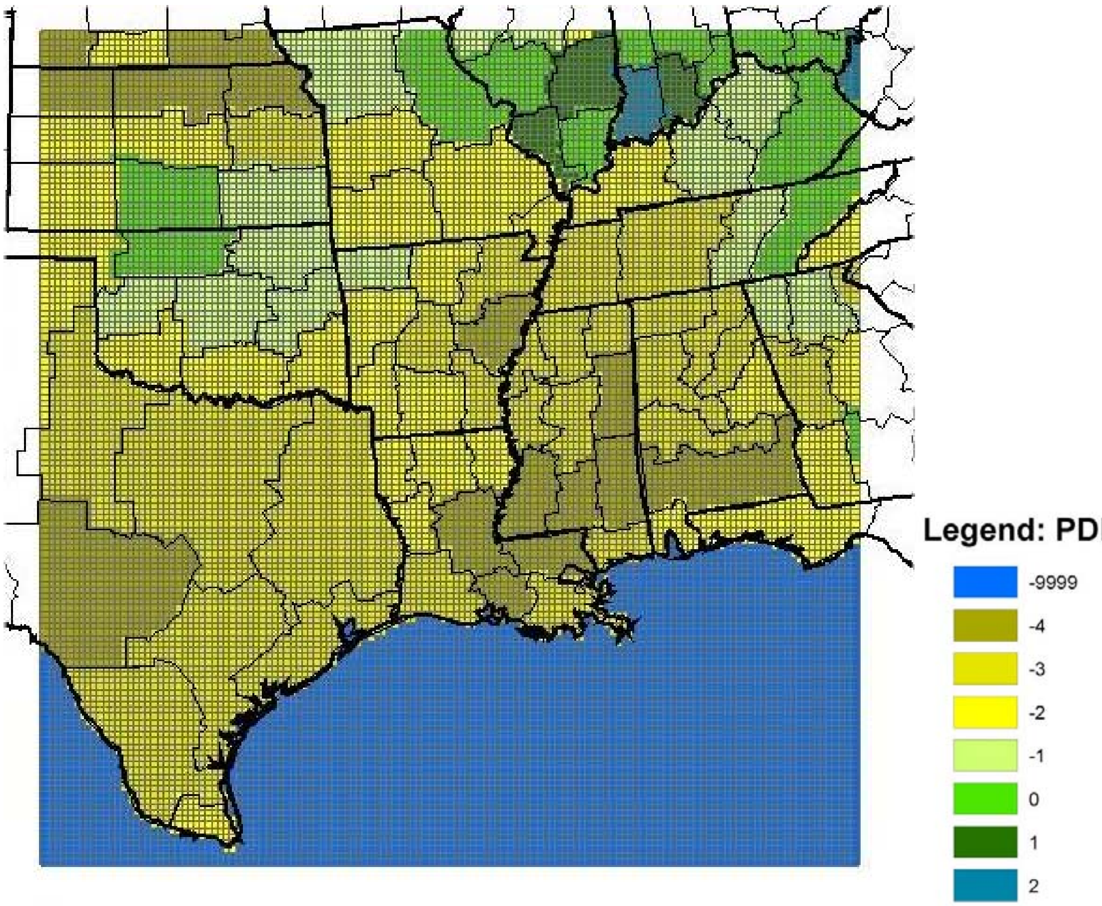


Figure 3-1. Illustration of the distribution of Palmer Drought Indices for the *U.S.* area of the regional domain (at a 12km resolution) compiled for input to GloBEIS 3.0 for the week of September 3 through 9, 2000.

Extreme drought reduces isoprene emission rates to zero and results in senescence (the plant drops its leaves) in some plants. However, several studies (Tingey et al. 1981; Sharkey and Loreto, 1993; Fang et al., 1996; Guenther et al., 1999) have shown that moderate drought conditions decrease photosynthesis rates but not isoprene emission. However, these studies have not produced a general numerical relationship between drought and isoprene emission and it is likely that specific responses vary considerably among different species. For example, some oak species are fairly drought resistant, while others are sensitive to drought conditions. The studies indicate that mild drought levels are accompanied by almost no change in isoprene emission but that severe drought ceases all biological activity, including isoprene emission. GloBEIS 3 assumes that isoprene emission is not directly influenced by drought for a Palmer Drought Severity Index (PDI) above –2 and decreases linearly to 10% of no-drought conditions for a PDI of –5 (Figure 3-2). We apply this activity factor to other VOC emissions, with the exception of the emission of monoterpenes that are contained in large pools, to reflect their presumed association with biological activity. The emission of monoterpenes from Texas vegetation is likely to be insensitive to drought (Lerdau et al. 1994) and GloBEIS 3.0 assumes that these emissions are not directly influence by drought.

GloBEIS 3.0 also simulates the reduction in stomatal conductance that occurs with drought. This means that the leaves can no longer use the release of water (transpiration) for cooling and they can heat up by several degrees. The relationship between PDI and stomatal conductance assumed by GloBEIS 3.0 is shown in Figure 3-2.

The net result of drought predicted by GloBEIS 3.0 on isoprene and “other VOC” is that mild drought (PDI= -0.5 to –2) tends to increase emissions, moderate drought (PDI= -2.5 to –4) tends to decrease emissions significantly, and extreme drought (PDI<-4) greatly decreases emissions. GloBEIS 3.0 does not decrease monoterpene emissions as a result of drought although these emissions probably do decline during an extended severe drought. However, this can be accounted for in GloBEIS 3.0 using the variable LAI option, which would account for the decreased LAI that occurs during an extended severe drought.

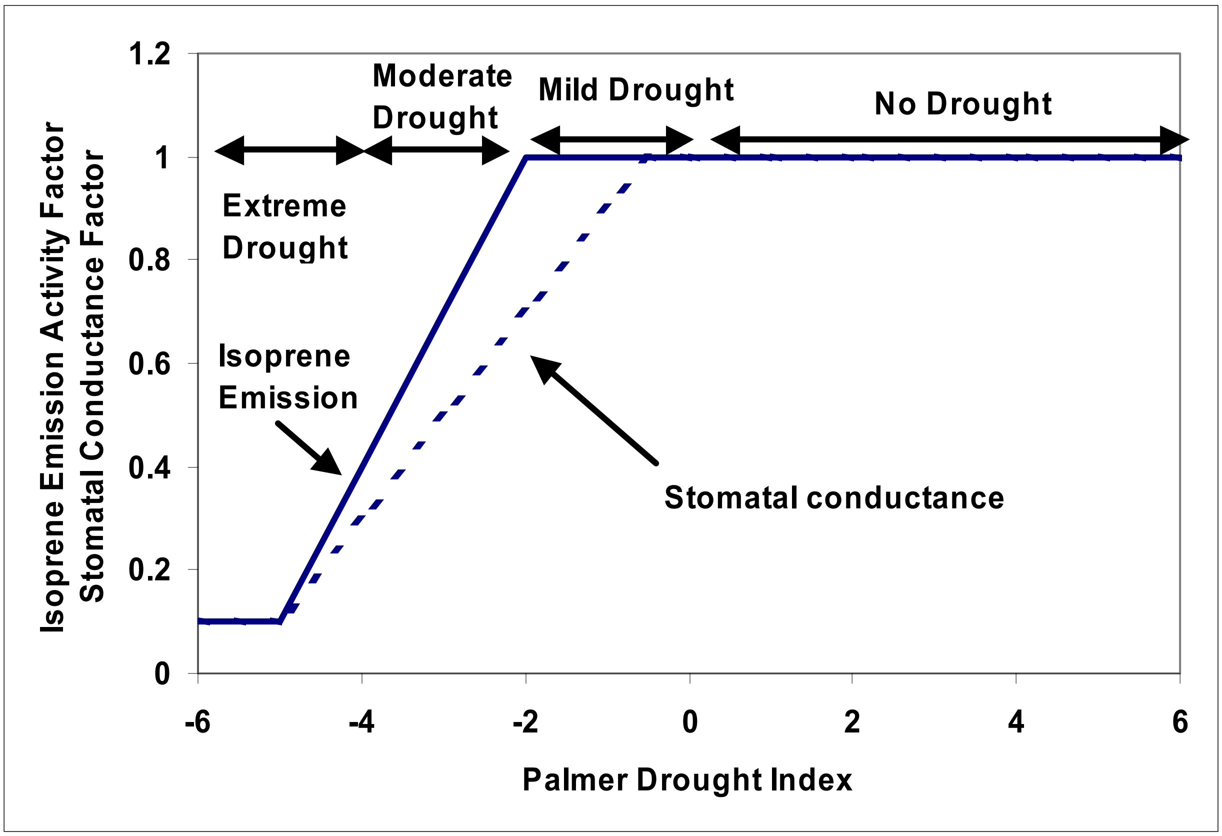


Figure 3-2. Relationship between Palmer Drought Index and isoprene emission (solid line) and stomatal conductance (dashed line) assumed by GloBEIS 3.0.

Leaf Area Index

All biogenic VOC emission models assume that emissions are related to Leaf Area Index (LAI, the area of leaves per unit of ground area) but they often do not use representative LAI data. GloBEIS 2.2 introduced an algorithm that lowered isoprene emissions according to the fraction of leaves that were new or old (both of which tend to have very low emission rates). The amounts of old and young leaves were estimated from the change in LAI from one month to the next. However, GloBEIS 2.2. used a low resolution LAI database that was based on the average of several years (and so likely did not represent the scenario being modeled). GloBEIS3 includes the option of importing LAI at the same spatial resolution used for other input variables and with a temporal resolution that can be as high as daily, but will more typically be about 7-10 days.

Seven LAI files were prepared for use with GloBEIS 3.0. The input data extend over the Texas 2000 study and include dates from July 19, 2000 to September 29, 2000. The LAI distribution for August 28, 2000 is shown as an example in Figure 3-3.

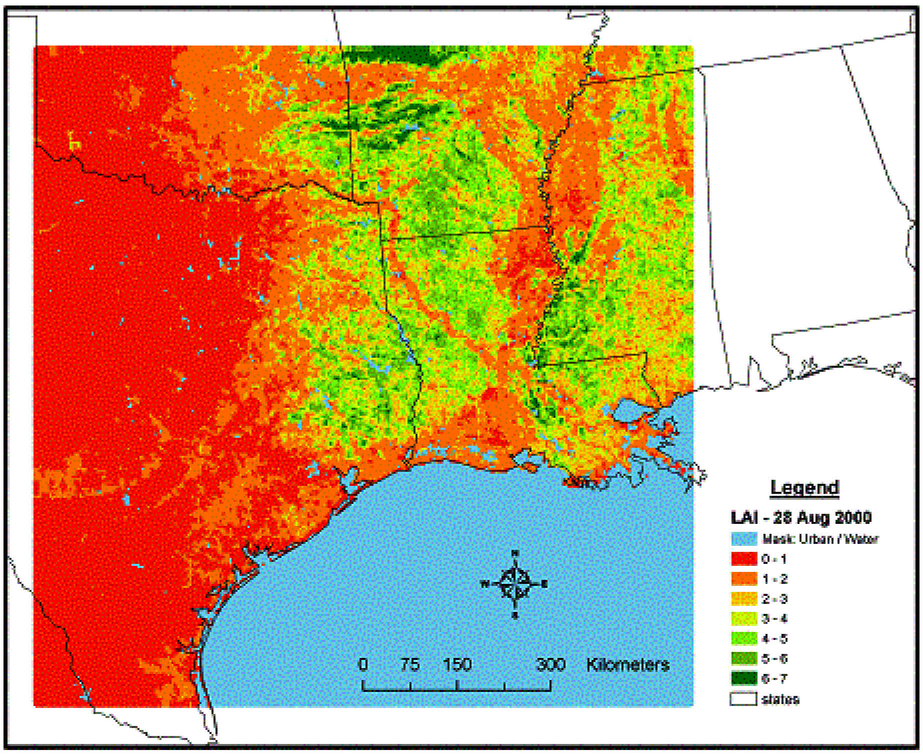
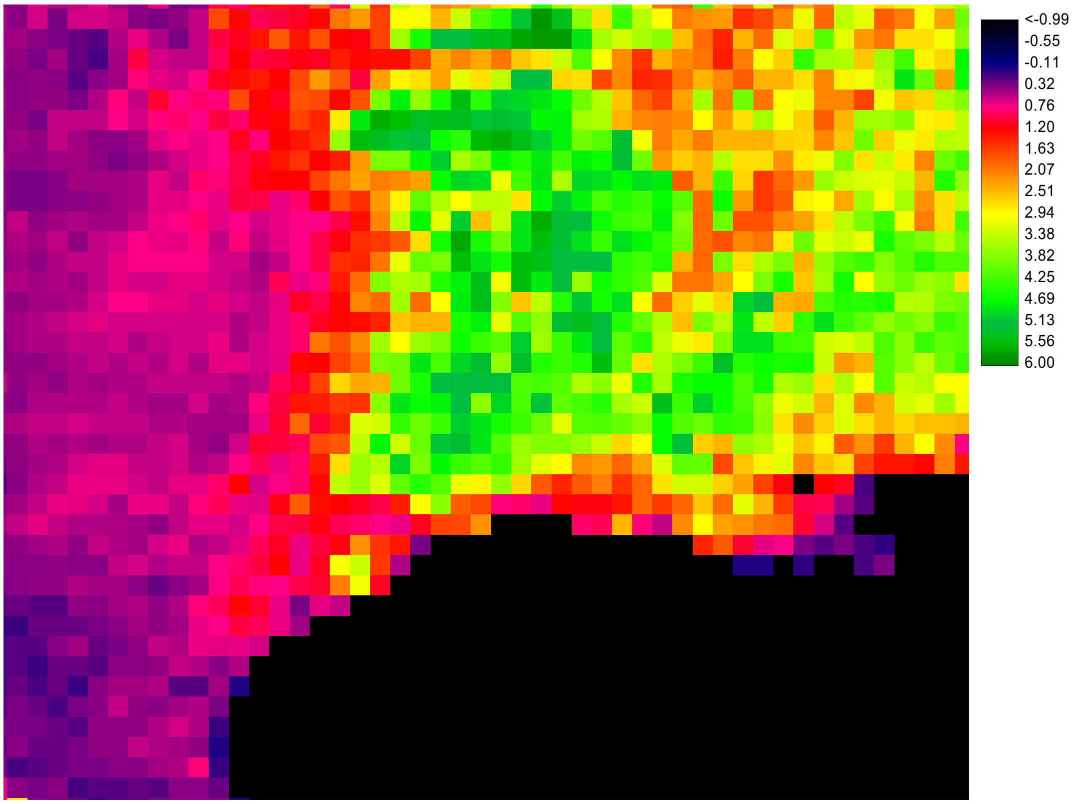


Figure 3-3. Illustration of the distribution of Leaf Area Indices compiled from MODIS for input to GloBEIS 3.0 for August 28, 2000.



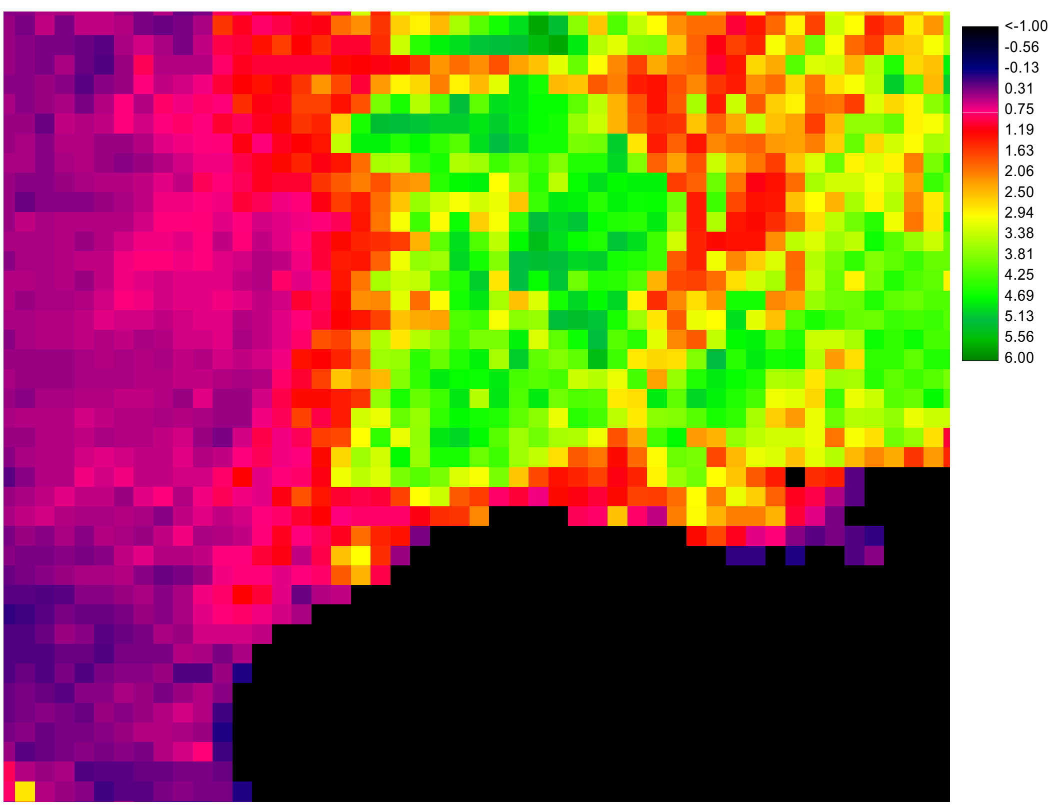


Figure 3-4. 10-year average (1981-1990) LAI estimated from AVHRR by Myneni et al. (1997) for the same region shown in Figure 3-3 for August (top) and September (bottom).

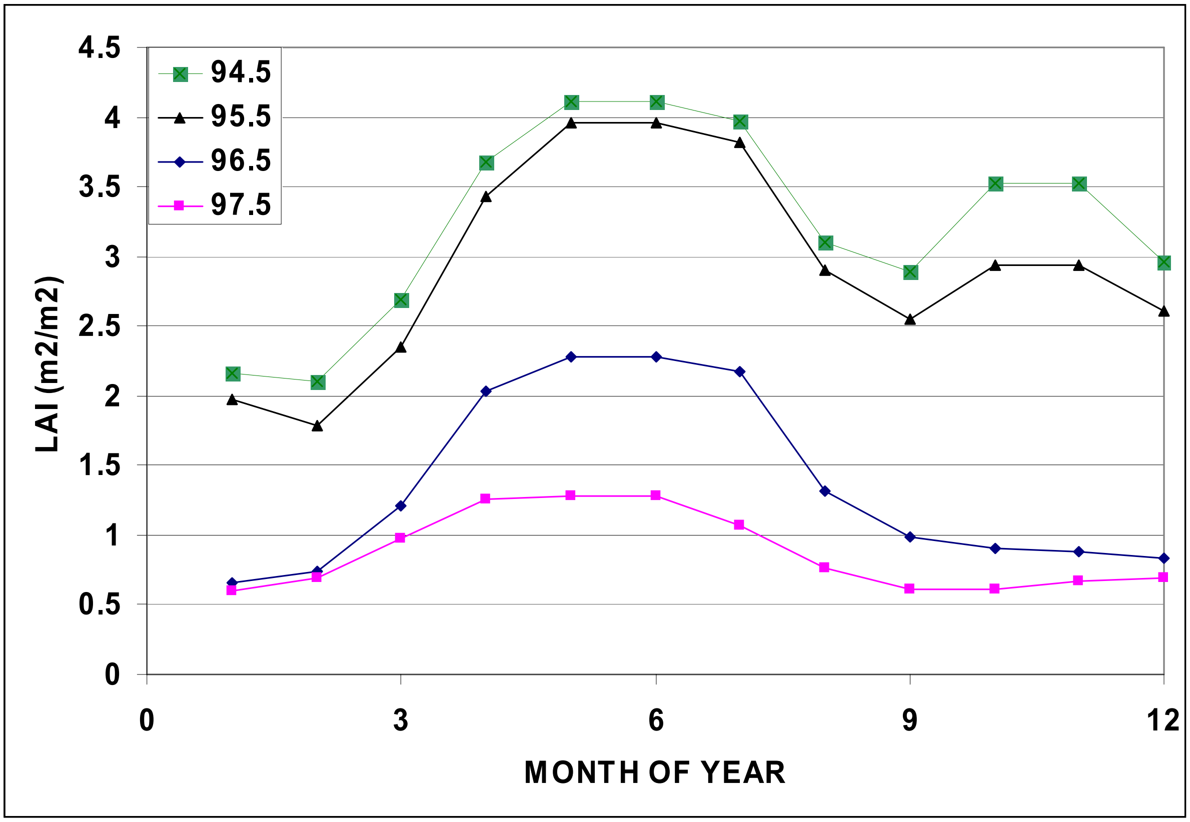


Figure 3-5. Monthly variation in LAI averaged over 1° grids (derived from AVHRR by Sellers et al. 1994) centered at a latitude of 31.5 N and four longitudes (94.5W, 95.5W, 96.5W, and 97.5W). The vegetation covering the grids range from forest (for the longitude94.5 near the Texas/Louisiana border) to shrub and grass in the west. The LAI estimates are an average for 1987 and 1988, which was a period of drought in this region.

The MODIS derived LAI observations shown in Figure 3-3 are compared with estimates calculated from AVHRR in Figures 3-4 and 3-5. Figure 3-4 shows a long term average (10 years: 1981 to 1990) for August and September (from Myneni et al. 1997). The values are generally comparable with the estimates shown in Figure 3-3 indicating that the LAI values for the drought of 2000 do not differ dramatically from the normal values. An idea of the seasonal variation in LAI for east Texas forests and shrublands is shown in Figure 3-5 (from Sellers et al. 1994). The LAI shown is an average for 1987 and 1988 which was a period of drought similar to 2000. Figure 3-5 shows that LAI decreases considerably (about 0.5 to 1.5 m^2 m^{-2}) in both forests (longitude $<$96W) and shrublands (longitude$>$96W). However, the percentage decrease is much less for the forests. The minimum LAI occurs in September in most of this region.

Leaf Temperature

Although it is well known that leaf temperature, rather than ambient temperature, controls foliar VOC emissions, most BVOC modeling approaches have assumed that leaf temperature is equal to ambient temperature. An earlier model (BEIS) attempted to estimate leaf temperatures but the predicted behavior did not appear reasonable in some cases. Because of this, and due to the high computational effort, later models (e.g., BEIS2) reverted to assuming that leaf temperature was equal to ambient temperature.

The leaf temperature calculation implemented in GloBEIS 3.0 has a considerably more efficient routine, compared to BEIS, for solving the leaf energy balance equation and so it's use does not greatly increase the required computational time. More importantly, GloBEIS 3.0 uses numerical routines that result in a more accurate simulation of leaf temperatures. The methods used are based on the work of Goudrian and Van Laar (1994) and Leuning et al. (1995). Another improved feature of the GloBEIS 3.0 code is that several variables that can be measured in-situ or estimated from satellite observations (e.g., whole canopy sensible and latent heat fluxes, fraction of PAR that is absorbed by the canopy, reflected radiation) are calculated and can be output by the model and used as a check of model performance.

Two extreme cases for summertime Texas conditions are shown in Figure 3-6. Daytime differences between leaf and ambient temperature for sun leaves range from 5K higher to 7K lower. Shade leaves in daytime have a lower range of deviations (1.5 K higher to 4K lower). At nighttime, leaves range from being slightly (<0.5K) cooler than ambient to over 6K cooler. The difference between leaf and ambient temperatures is increased at low wind speeds. Conditions that result in daytime leaf temperatures that are higher than ambient include cool ambient temperatures, high humidity, and clear skies. Conversely, overcast skies with hot temperatures and low humidity generally result in leaf temperatures that are lower than ambient. Drought conditions (low soil moisture) tend to increase leaf temperatures (if that option is selected). Under more typical summertime conditions for Texas, GloBEIS 3.0 predicts that the average canopy is about 1K cooler than ambient at nighttime and about 0.5 K warmer during daytime (Figure 3-7).

GloBEIS3 assigns one of seven canopy types to each landcover type. The canopy types include broadleaf forest, mixed forest, needleleaf forest, mixed vegetation, shrub, grass and crop. The canopy types can differ in their leaf and canopy dimensions and in their canopy radiation diffusion properties.

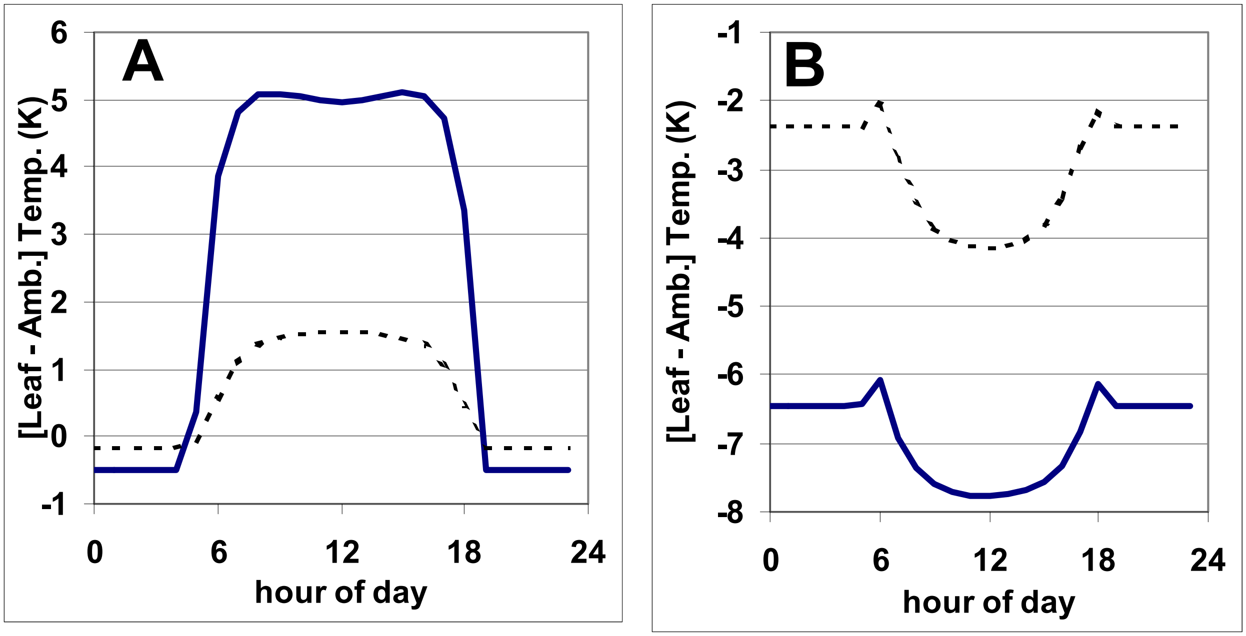


Figure 3-6. Diurnal cycle of deviation between leaf and ambient temperatures (K) predicted by GloBEIS3 for constant meteorological conditions for an oak forest canopy. Case A represents cool ambient temperature (290K), humid (100% humidity), clear skies and low winds (0.1 m s-1). Case B represents hot ambient temperature (310K), dry (1 g kg-1), overcast skies and low winds (0.1 m s-1). Sun leaf predictions are represented by a thick solid line and shade leaves by a narrow dashed line.

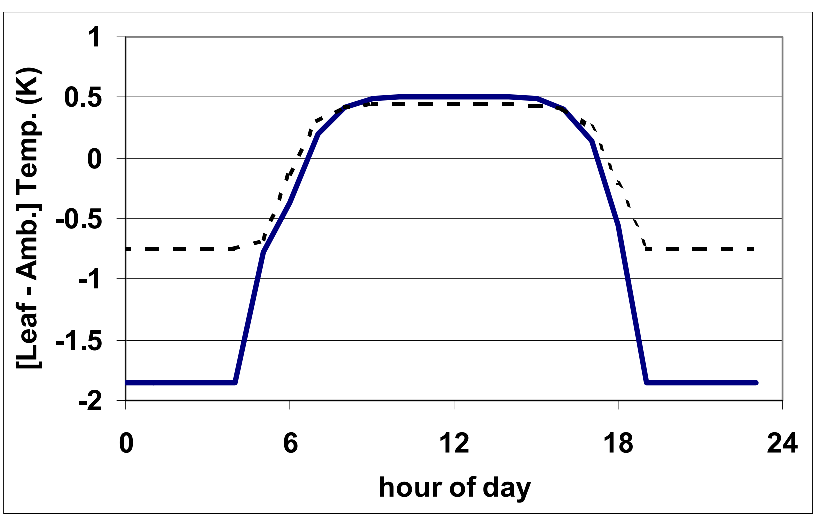


Figure 3-7. Diurnal cycle of deviation between leaf and ambient temperatures (K) predicted by GloBEIS3 for constant meteorological conditions: warm ambient temperature (300K), moderate humidity (10 g kg-1), clear skies and moderate winds (4 m s-1) for an oak forest canopy. Sun leaf predictions are represented by a thick solid line and shade leaves by a narrow dashed line.

Antecedent Leaf Temperatures

Biogenic VOC emissions are very sensitive to changes in temperature and all efforts to model these emissions have included some algorithm describing temperature dependence. In most cases, the temperature dependence algorithm simulates the only response that is observed when temperature changes fairly quickly (over a time scale of an hour or less). Other plant physiological processes (e.g., photosynthesis) are sensitive to changes in the temperature history of the plant so it is not surprising that isoprene emission would also be similarly influenced. There have been three recent studies that demonstrate that the temperature of past days can impact isoprene emissions (Sharkey et al. 2000; Geron et al. 2000; Petron et al. 2001). Each study found that higher temperatures during past days resulted in higher isoprene emissions. However, the specific pattern reported for each study differs considerably. Both the observed magnitude of the effect differed among the three studies and the length of the period influencing current emissions was very different (ranging from about 1 to 15 days).

A 3 month (~2200 hours) record of summertime (June-August) ambient temperature variations was used to demonstrate the difference in the isoprene emissions predicted by the four options (Figure 3-8). This temperature series was observed at a research site (Blodget Forest) in the lower slopes of the Sierra Nevada mountains in California. The maximum daily temperature ranged from about 10ºC to 30ºC during this season. The antecedent temperature correction factor ranged from about 1.4 (i.e. 40% higher emissions than if not used) to about 0.5 (i.e., 50% lower emissions). The differences in the predictions of the four methods ranged from about 8 to 30%.

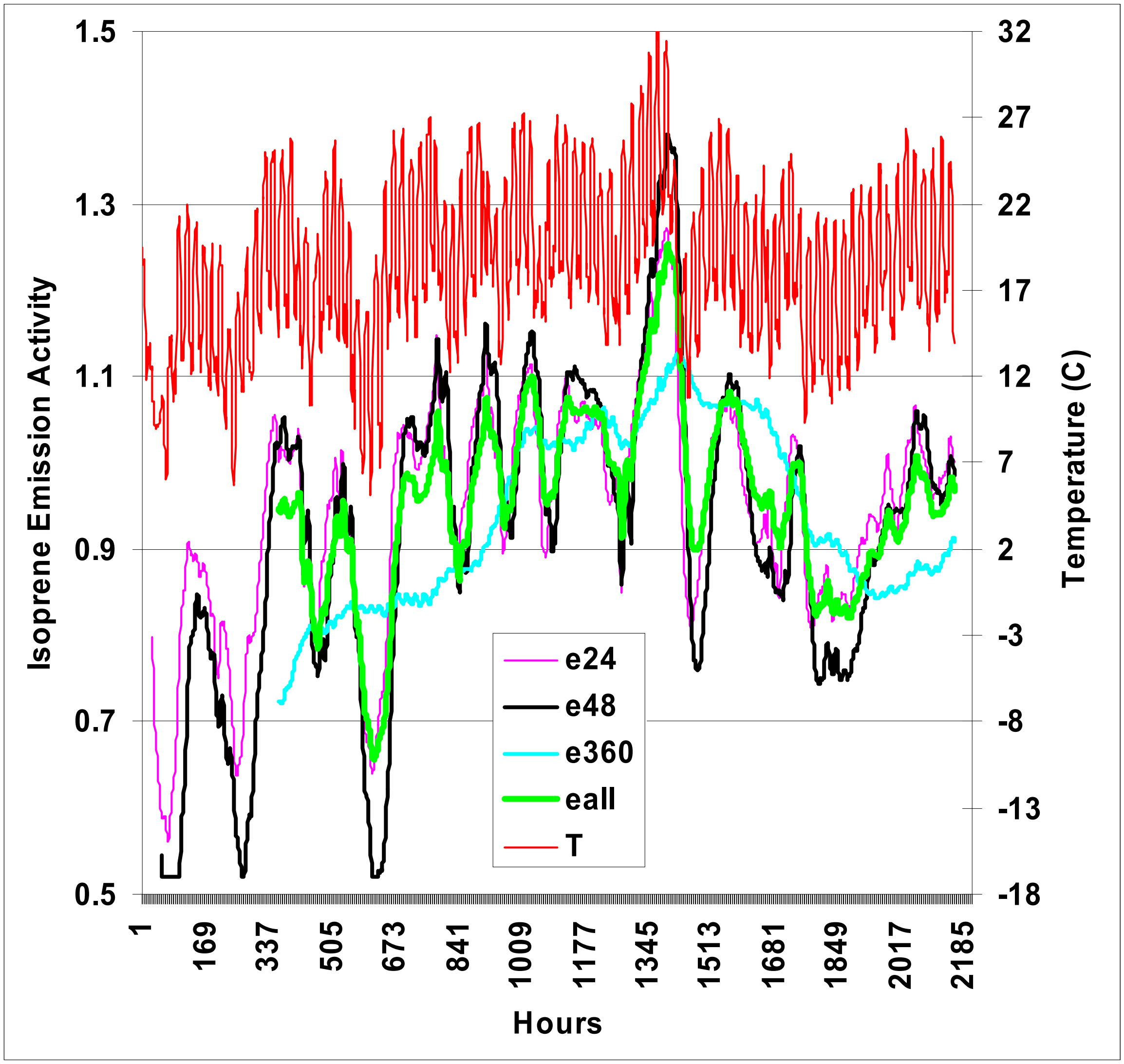


Figure 3-8. Isoprene emission activity predicted by four methods for predicting the influence of antecedent temperature. Ambient temperature (ºC) is shown as solid red line.

4. SENSITIVITY TESTING

A series of sensitivity tests were performed with the new GloBEIS3 code for quality assurance, model evaluation and documentation purposes. Tests were performed for a section of the 12-km regional modeling domain shown in Figure 1-1 covering the Houston area. Specifically, grid cells (43, 31) to (66, 54) were extracted to form a 24 by 24 cell domain suitable for testing. The test case area is shown in Figure 4-1. All emissions calculations were for a 24-hour period (nominally July 18, 2000) assuming constant temperature of 300 K and two tenths cloud cover. Twenty-three scenarios were run as shown in Table 4-1.

GloBEIS versions 2.2 and 3

The first four calculations checked consistency between GloBEIS2.2 and GloBEIS3. The modified BEIS2 emission factor algorithm gave identical results in GloBEIS2.2 and GloBEIS3 (scenarios v2modb2 and v3modb2). The BEIS99 emission factor algorithm in GloBEIS2.2 corresponds to the default GloBEIS3 algorithm, and the only difference in emissions between the v2b99 and v3gb3 scenarios is a 0.2% decrease in isoprene emissions. This small difference is attributed to updates to the canopy radiation model. These first four tests show that there is continuity in results between versions 2 and 3 of GloBEIS. Figures 4-2 through 4-4 which show the isoprene, total VOC and NOx emissions for the GloBEIS3 base case scenario (v3gb3).

Antecedent Temperature

Eight calculations were performed to investigate the effects of the antecedent temperature algorithms in GloBEIS3 (Table 4-1). The scenarios modeled were antecedent temperatures of 300 K and 295 K for periods of 24, 48, 360 and "all" hours. Only isoprene emissions are affected by antecedent temperature, as shown in Figure 4-3. Prolonged periods of 300 K average temperature (81 °F) increased isoprene emissions by up to 60 %. Prolonged periods of 295 K average temperature (72 °F) increased isoprene emissions by up to 14 %.

Leaf Temperature

GloBEIS3 includes an option to model leaf temperatures rather than assuming that all leaves are at ambient temperature. This option depends upon the wind speed and humidity (and also interacts with drought, as discussed later) so three scenarios were modeled with wind speeds 4 and 0 m/s and humidities of 10 and 4 g/kg. These scenarios changed isoprene and other VOC emissions by up to about 10 % (Table 4-1 and Figure 4-4). Isoprene emissions increased when the wind speed was reduced from 4 m/s to zero. Isoprene emissions decreased when the humidity was reduced from 10 g/kg to 4 g/kg.

Drought Index

Three scenarios looked at the effects of drought by changing the palmer Drought Index (PDI) values specified for all grid cells. The leaf temperature algorithm was deactivated, so drought index influenced VOC emissions by closing the stomata. PDI values of +1 and −1 had no effect on emissions (consistent with the algorithm design when leaf temperatures are not calculated) but a PDI value of −3 decreased isoprene emissions by 30% (Table 4-1 and Figure 4-5).

Drought Index and Leaf Temperature

Two scenarios looked at the effects of drought with the leaf temperature algorithm activated. PDI values of −1 and −3 were used with a wind speed of 4 m/s and humidity of 10 g/kg. Figures 4-6 and 4-7 compare the effects of changing the PDI with and without the leaf temperature algorithm. A PDI of −1 (mild drought) had no effect on emissions without leaf temperature effects, and slightly increased isoprene emissions with leaf temperature effects. A PDI of −3 (moderate drought) reduced isoprene emissions by 30% without and by 24% with leaf temperature effects.

Leaf Area Index

GloBEIS3 can use gridded leaf area index (LAI) data to determine the amount of leaf biomass and/or model effects due to leaf age. Three scenarios investigated these effects separately and in combination using LAI data from August 28 and August 21, 2000 (Figure 4-7). The development of the LAI data from satellite observations is described above. Effects on leaf biomass were based on the LAI observed on August 28th, whereas as leaf age effects depended upon the change in LAI between August 20th and 28th. Leaf mass effects decreased both isoprene and other VOC emissions by about 10%. Leaf age effects reduced isoprene emissions by about 30% but did not effect other VOCs. In combination, the leaf mass and leaf age effects were approximately additive.

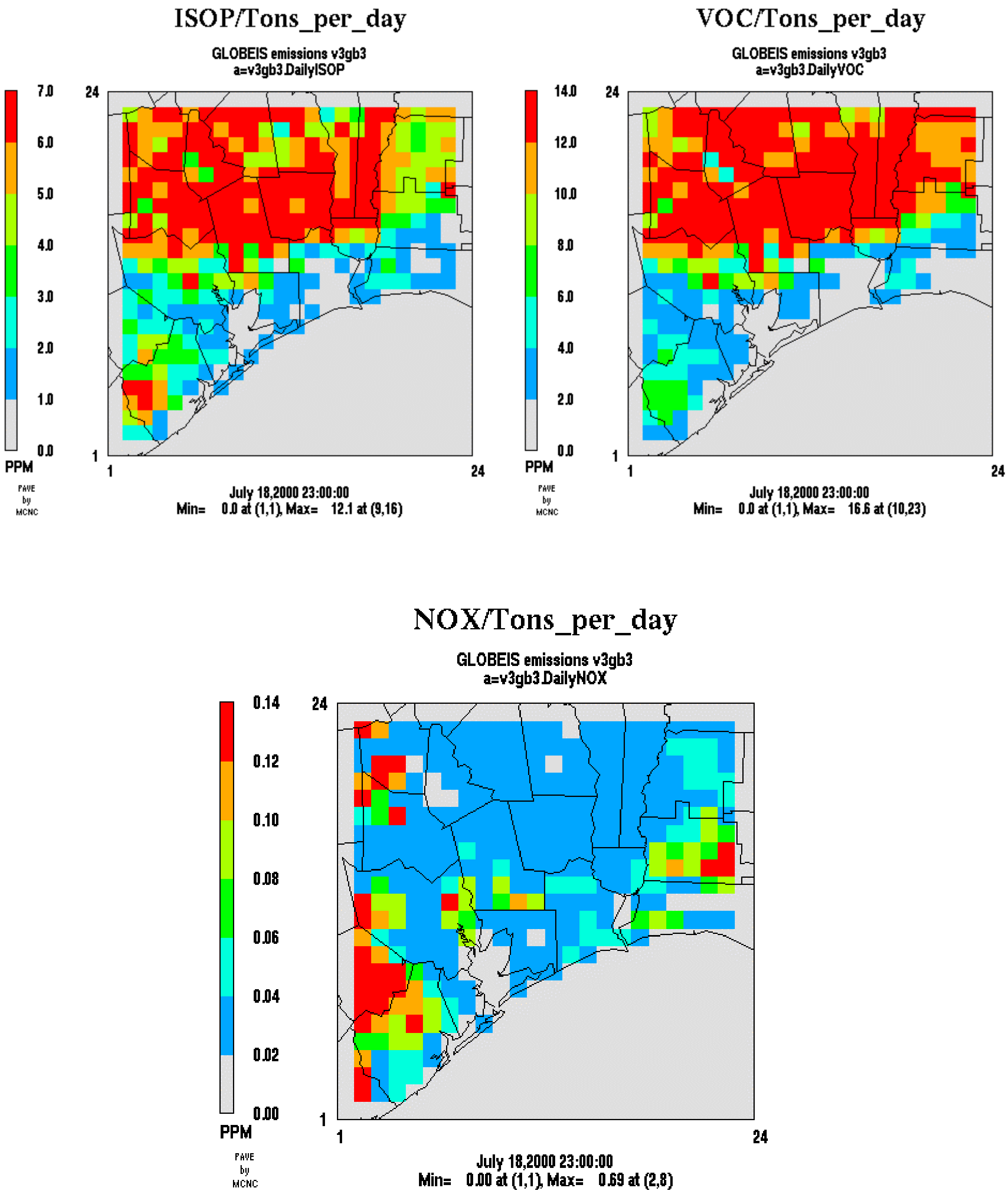


Figure 4-1. Biogenic isoprene, total VOC and NOx emissions (ton/day) for the GloBEIS3 base case in the Houston area 12 km grid testing domain.

Table 4-1. Results of GloBEIS sensitivity runs for idealized scenarios of the Houston area.

Run number	GloBEIS Options						Description of options and input values	CB4 Emissions (tons/day)				
	GloBEIS3	Antecedant T	Leaf Temp	Drought	Leaf Mass	Leaf Age		Isoprene	Other VOCs	Total VOCs	CO	NOx
v2modb2							GloBEIS2, modified BEIS2	1545.0	1790.4	3335.5	379.3	27.0
v3modb2							GloBEIS3, modified BEIS2	2207.3	1790.4	3997.7	379.3	27.0
v2b99							GloBEIS3, BEIS99	1888.0	1790.4	3678.5	379.3	27.0
v3gb3	X						GloBEIS3	1884.5	1790.4	3675.0	379.3	27.0
v3gb324a300	X	X					24 hr antecedant T of 300 K	2412.7	1790.4	4203.2	379.3	27.0
v3gb324a295	X	X					24 hr antecedant T of 295 K	2035.3	1790.4	3825.8	379.3	27.0
v3gb348a300	X	X					48 hr antecedant T of 300 K	2676.4	1790.4	4466.9	379.3	27.0
v3gb348a295	X	X					48 hr antecedant T of 295 K	2111.1	1790.4	3901.6	379.3	27.0
v3gb3360a300	X	X					360 hr antecedant T of 300 K	3047.7	1790.4	4838.1	379.3	27.0
v3gb3360a295	X	X					360 hr antecedant T of 295 K	2162.3	1790.4	3952.7	379.3	27.0
v3gb3alla300	X	X					all hr antecedant T of 300 K	2809.6	1790.4	4600.0	379.3	27.0
v3gb3alla295	X	X					all hr antecedant T of 295 K	2108.5	1790.4	3899.0	379.3	27.0
v3gb3lt4ms10g	X		X				4 m/s wind, 10 g/kg humidity	1873.9	1714.1	3588.0	363.0	27.0
v3gb3lt0ms10g	X		X				0 m/s wind, 10 g/kg humidity	2012.4	1717.9	3730.3	363.9	27.0
v3gb3lt4ms4g	X		X				4 m/s wind, 4 g/kg humidity	1691.4	1623.6	3315.0	344.1	27.0
v3gb3di+1	X			X			Palmer drought index (PDI) +1	1884.5	1790.4	3675.0	379.3	27.0
v3gb3di-1	X			X			PDI -1	1884.5	1790.4	3675.0	379.3	27.0
v3gb3di-3	X			X			PDI -3	1319.2	1573.7	2893.0	265.5	27.0
v3gb3lt4ms10g-1di	X		X	X			4 m/s wind, 10 g/kg humidity, PDI -1	1900.4	1721.3	3621.7	364.5	27.0
v3gb3lt4ms10g-3di	X		X	X			4 m/s wind, 10 g/kg humidity, PDI -3	1424.2	1547.4	2971.6	261.1	27.0
v3gbvlai	X				X		LAI data from 8/20 to 8/28/01	1665.8	1652.3	3318.1	339.2	27.0
v3gbvage	X					X	LAI data from 8/20 to 8/28/01	1346.6	1790.4	3137.0	379.3	27.0
v3gbvlaivage	X				X	X	LAI data from 8/20 to 8/28/01	1197.6	1652.3	2849.9	339.2	27.0

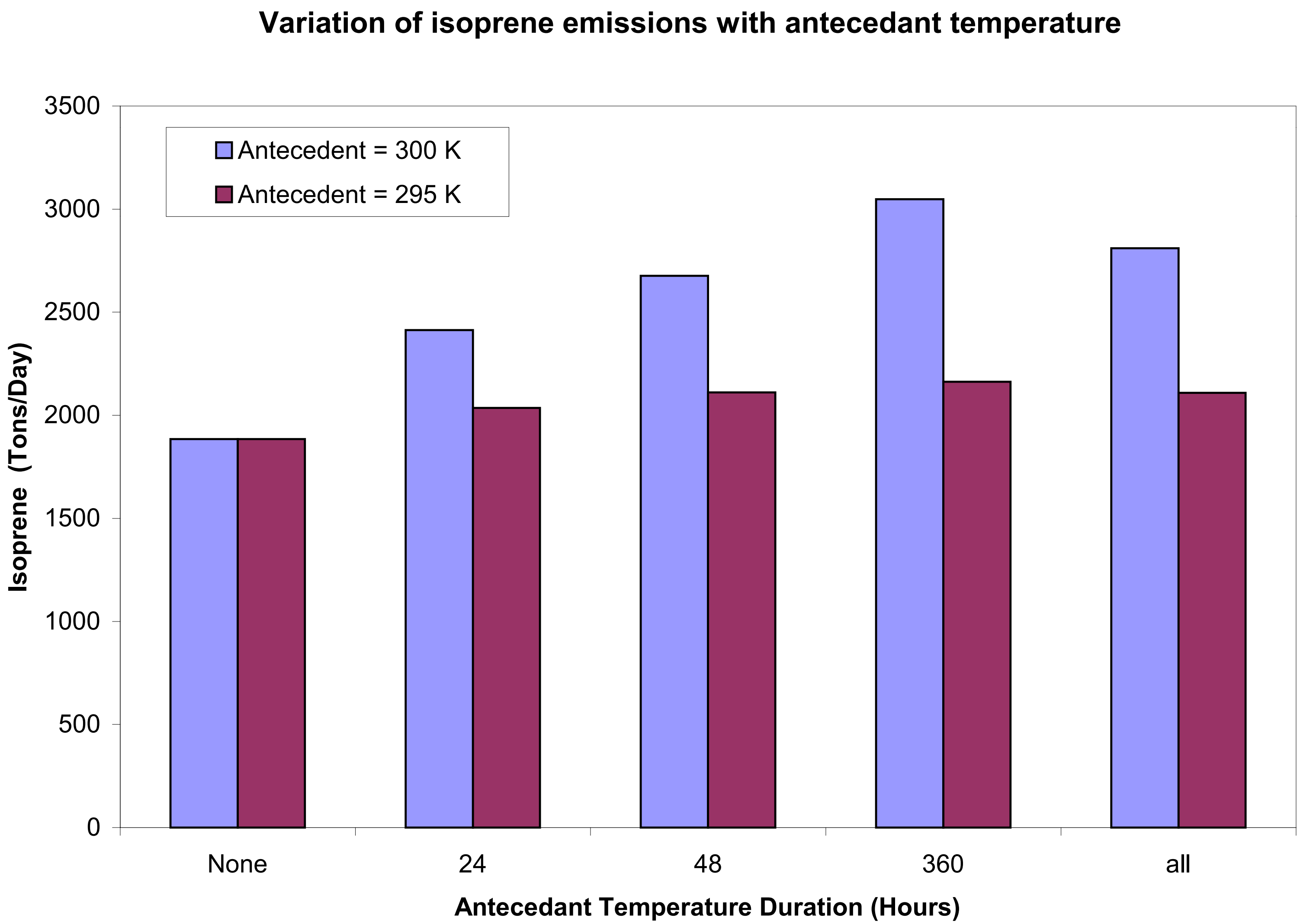


Figure 4-2. Variation of isoprene emissions with antecedant temperature.

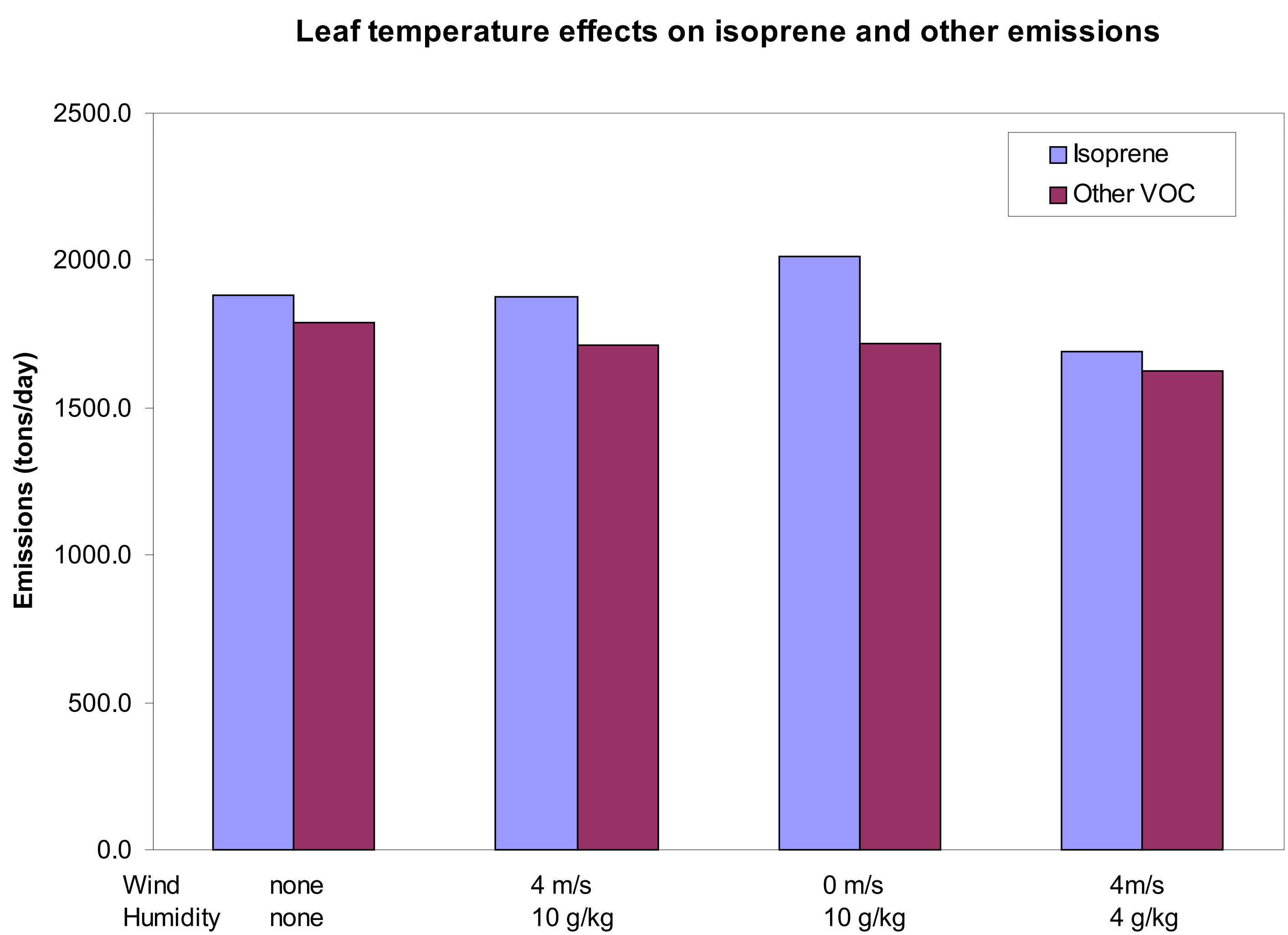


Figure 4-3. Leaf temperature effects on isoprene and other emissions.

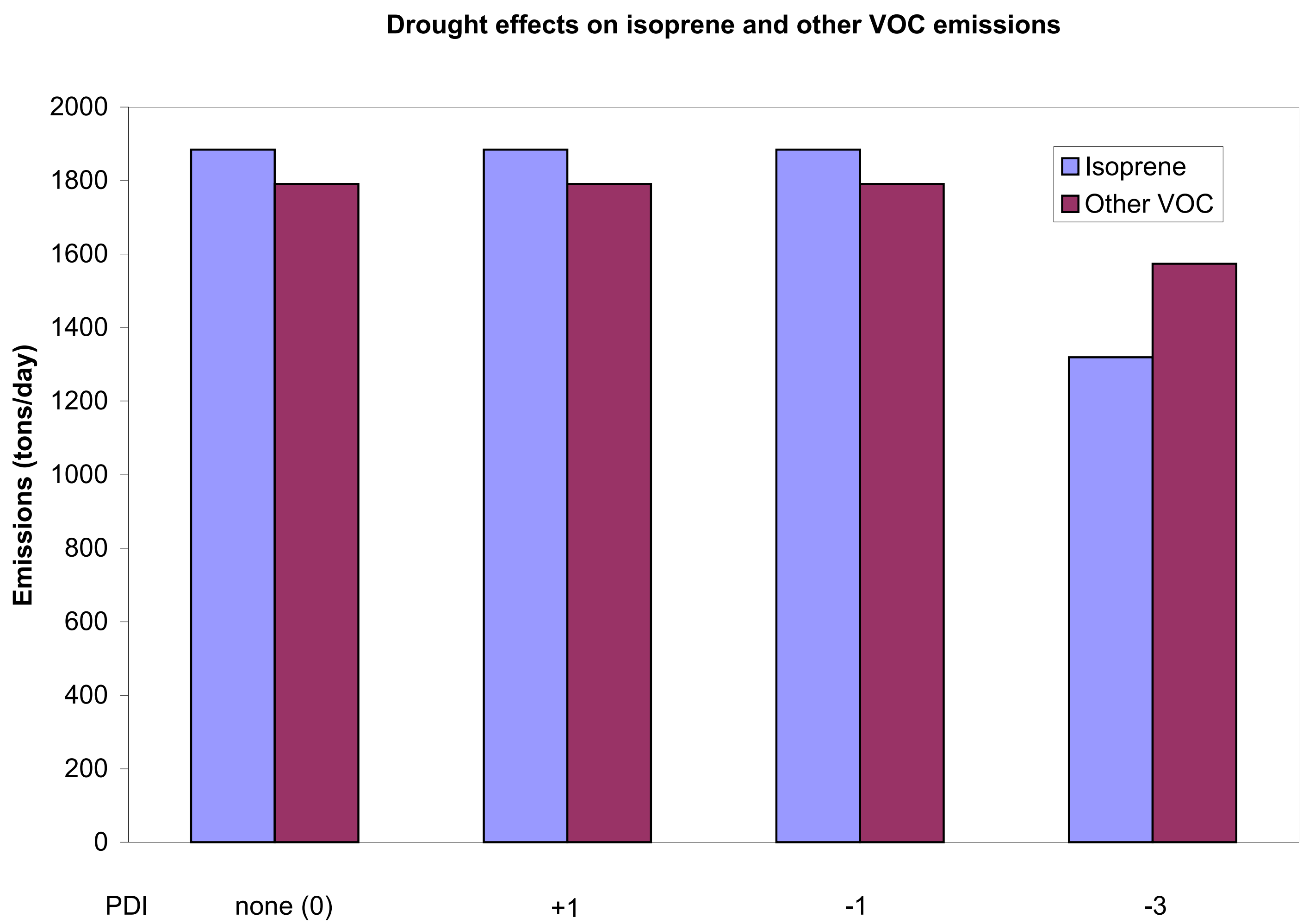


Figure 4-4. Drought effects on isoprene and other VOC emissions.

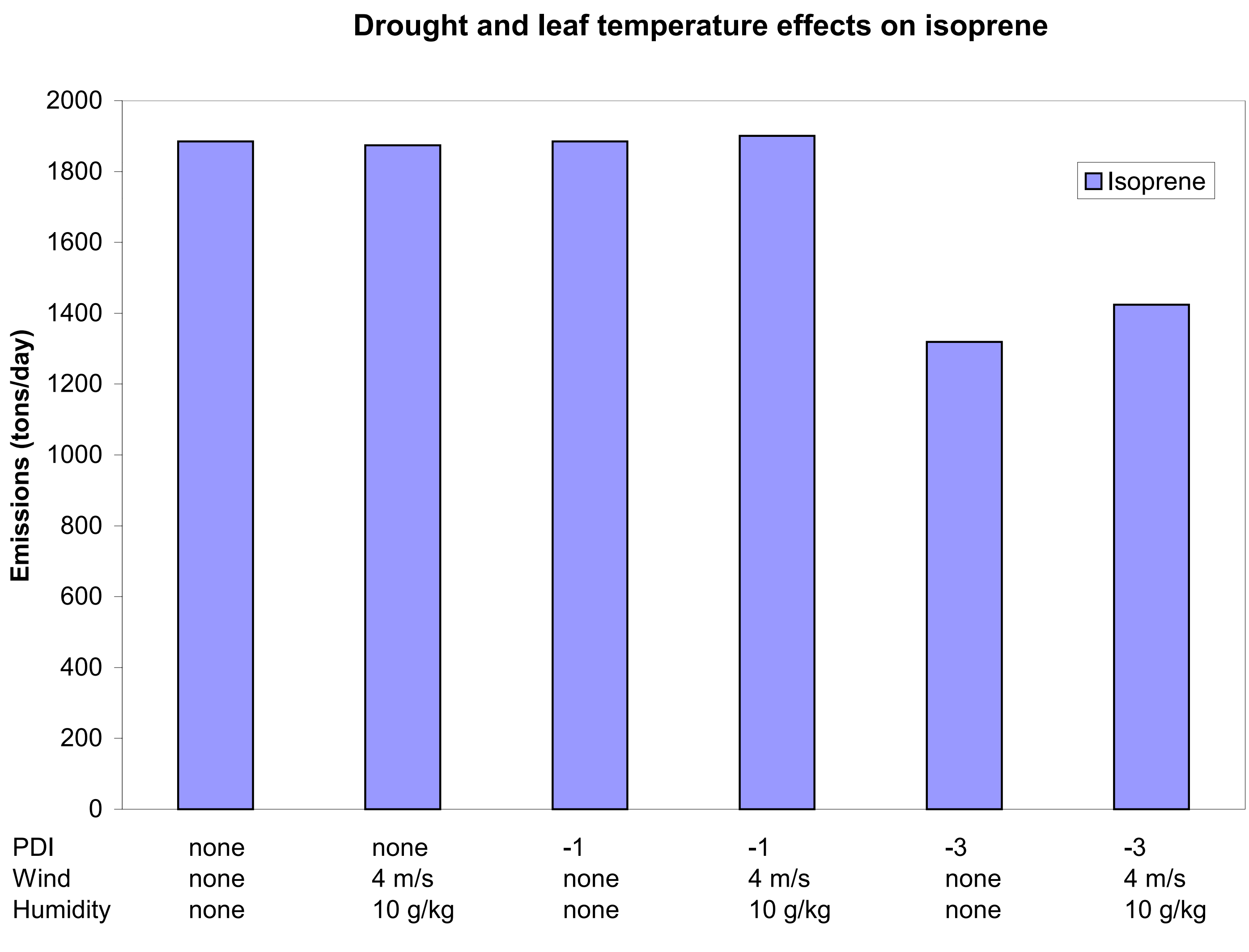


Figure 4-5. Drought and leaf temperature effects on isoprene.

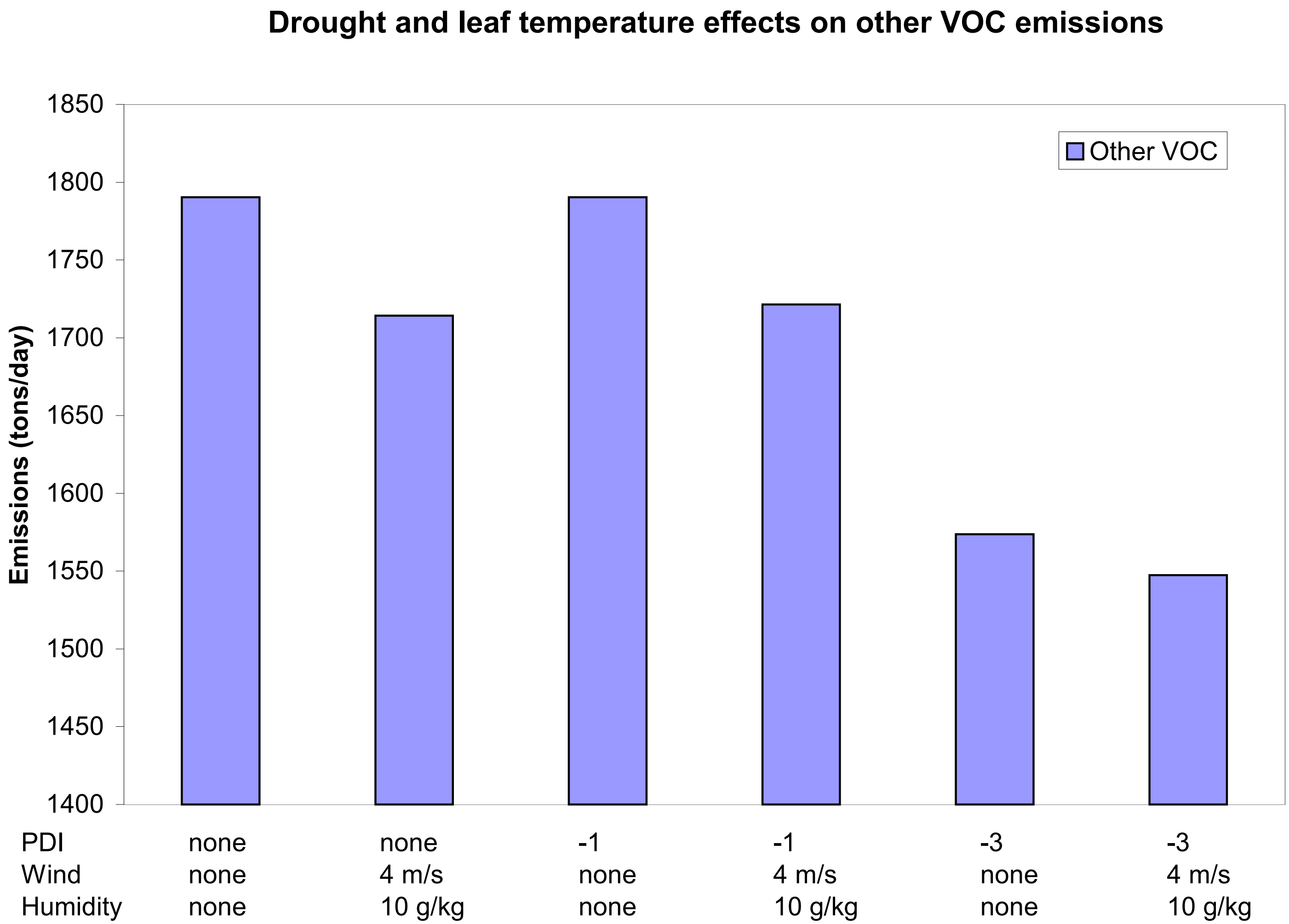


Figure 4-6. Drought and leaf temperature effects on other VOC emissions.

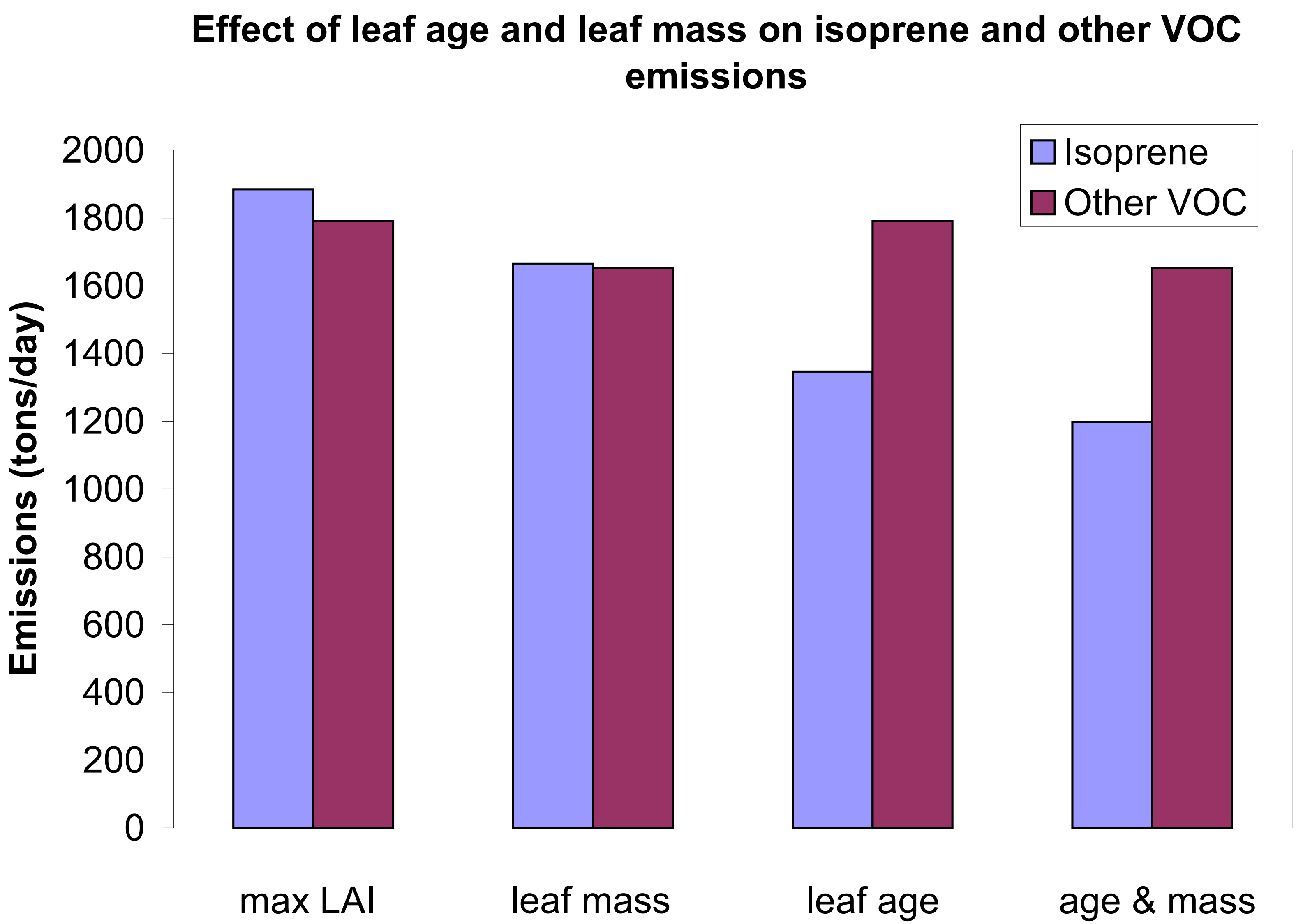


Figure 4-7. Effect of leaf age and leaf mass on isoprene and other VOC emissions.

5. RECOMMENDATIONS

GloBEIS3 provides a number of options and so the following guidance is provided to help you decide how to use the model.

Choosing Between BEIS2, Modified BEIS2, and GloBEIS3

BEIS2 should be used only if you are trying to generate estimates that agree with the BEIS2 model. If you would like to use the BEIS2 procedures but want to adjust the "cosla" variable (which is not set to a realistic value in BEIS2) then the "modified BEIS2" model should be used. GloBEIS3 must be selected if you want to use many of the provided options.

Options Available for All Models

"Number of layers": 5 is recommended for accurate calculations of canopy radiation transfer. If the model run time is a concern then 3 can be used.

"Database Max. Iso. EF" and "revised Max. Iso EF": the values for these two variables should both be exactly the same UNLESS you would like to use this option as a convenient way of uniformly increasing/decreasing the isoprene emission factors specified in the internal landcover characteristics data. This option is useful if the internal landcover characteristics database contains BEIS2 emission factors but you would like to use GloBEIS3 options. If this is the case, you should enter 79.3 (the maximum BEIS2 isoprene emission factor) for "Database Max. Iso EF" and 113.3 (the maximum isoprene emission factor if using the GloBEIS3 model) for revised Max. Iso EF"

Options Available for "Modified BEIS2"

The recommended value for the canopy extinction coefficient, "Extcoeff", is 0.6 unless you want to simulate a specific type of canopy. The recommended value for the cosine of the mean leaf angle, "Cosla", is 0.5 unless you want to simulate a canopy that has a non-uniform leaf angle distribution.

Options Available for "GloBEIS3"

The "Leaf temperature" option is recommended if you have wind speed and humidity data available. The "Output Energy Balance terms" should be selected only if you are interested in using these energy flux terms to evaluate model performance.

The "variable LAI" option should be used if you have leaf area index estimates available that are more representative than the specified peak LAI estimates that are included in the landcover characteristics database. This option is always recommended for months outside of the peak growing season.

The "variable leaf age" option should be used if you have an available time series of leaf area index estimates. It is recommended that the time series used should be at least monthly and no more than 5 day. This option is always recommended for months outside of the peak growing season.

One of the antecedent temperature options ("24 hr", "48 hr", "360 hr" or "24, 48, 360 hr") should be used if you have a temperature time series available and would like to investigate the sensitivity of emissions to antecedent temperature. It should be recognized that although each of the options is based on a published quantitative description of the influence of antecedent temperature, the relationship between antecedent temperature and emissions is not well understood.

The "Drought index" option should be used if you have Palmer Drought Index estimates available and would like to investigate the sensitivity of emissions to drought. It should be recognized that the GloBEIS3 is a crude approximation of limited qualitative observations and that no quantitative descriptions of the impact of drought on biogenic emissions were available for this version.

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6. CONCLUSIONS

We have implemented four new features into the GloBEIS model: 1) leaf temperature calculation, 2) importation of satellite observations of Leaf Area Index, 3) importation of drought indices and prediction of the impact on emissions, and 4) calculation of past temperature history on current emissions. All four of these features can influence BVOC emissions by at least 25% under well-watered conditions. Each of the four new features are expected to produce the greatest differences between GloBEIS 2.2 and GloBEIS 3.0 in the presence of drought conditions.

The leaf temperature calculation has been tested over a range of conditions and appears to be fairly robust and reasonable. The main improvement that could be made to this module would be to incorporate a "state of the art" land surface model that would characterize all of the biophysical variables (e.g., soil moisture, leaf water potential) that control leaf physiology.

The LAI and drought indices data provided for the Texas 2000 study are currently the best available estimates. Future advances in satellite remote sensing technology should improve both the LAI and drought index the datasets that can be used in GloBEIS 3.0.

The direct influence of drought on emissions, and the indirect influence through stomatal conductance, implemented in GloBEIS 3.0 are rough approximations of the qualitative descriptions that have been reported. The GloBEIS 3.0 algorithms for simulating the influence of past temperature on isoprene emissions have a similar high level of uncertainty. Additional observations of all of these behaviors are needed to improve and test these parameterizations. It is important that these investigations be conducted with the goal of developing numerical algorithms suitable for regional modeling.

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APPENDIX 1

Changes to the GloBEIS Code

Task 2. Incorporate drought conditions into GloBEIS model.

1. The banner page was modified to allow the user to import leaf area index, wind speed, humidity, drought index, and antecedent temperature files if GloBEIS3 is selected as the model in the "Model Parameters" screen. Depending on the additional options selected in the "Model Parameters" screen for the GloBEIS3 model (i.e., variable LAI, variable leaf age, drought index, leaf temperature, or antecedent temperature), the corresponding import modules are enabled or disabled on the banner screen appropriately.
2. The "Model Parameters" screen was modified to include all the additional options for running the GloBEIS3 model. The screen was divided into two tabs, where the input file names are on one tab, and all the remaining parameters are on another.
3. A new button called "Create Drought Index File" was added to the "Simple Inputs" utility. This new feature creates a drought index table of constant values for all cells in the domain, so the user does not have to import a drought index file.
4. The new modules "Procedures: 2001" and "Procedures: Canopy MicroClimate" were added to the module "7 Make EMISSIONS." These modules introduce 1) a function "ea1DI2002" that reduces isoprene emission with increasing drought stress and 2) function "Distomata" that increases stomatal conductance (typically resulting in higher leaf temperatures) with increasing drought stress.

Task 3. Incorporate variable green leaf area into GloBEIS model

1. The banner page was modified to allow user to select to input antecedent temperature file (Form "banner" and associated class object were modified, the Queries "Delete LAI Header" and "Make LAI" and module "5a Import LAI" were created).
2. Added a new feature to the "Simple Inputs" utility to create a constant LAI table. The "Make Inputs" module and "Enter Constant Values" form were modified accordingly.
3. Deleted tables, "link days seasons" and "seasonal foliage.

Task 4. Estimating leaf temperature using leaf energy balance

1. The banner page was modified to allow user to select to input wind speed and humidity files (Form "banner" and associated class object were modified, modules "5b Import Wind", "5c Import Humidity", and Queries "Delete Wind Header", "Make Wind", "Delete Humidity Header" and "Make Humidity" were created).
2. New features for creating constant humidity and wind tables were added to the "Simple Inputs" utility. The queries "Make Constant Humidity" and "Make Constant Windspeed" were created, the module "Make Inputs" was modified, and the form "Enter Constant Values" and associated class object were modified accordingly.
3. Significant modifications were made to the emissions code module, "7 Make EMISSIONS," and substantial amounts of code were added to the "Procedures: Canopy MicroClimate" module that calculate leaf temperature as a function of solar radiation, ambient temperature, humidity, wind speed, canopy type and drought index.

Task 5. Characterize influence of prolonged high leaf temperatures

1. The banner page was modified to allow the user to import an antecedent temperature file. The "Banner" form and associated class object were modified. The "Delete AnTemp Header" query and module "4f Import Antecedent T" were created.
2. A new utility called "Antecedent temperatures" was added. This utility calculates the three antecedent temperatures (18 hour, 48 hour and 360 hour average temperature) using the data in the temperature table. The "Make Temperature Sorted" query, "Calculate Antecedent Temperatures" form, and associated class objects were created. The "Make Inputs" (replacing "Make Constant Inputs") module and "Main_Utilities" macro were modified accordingly.
3. The "Model Parameters" screen was modified to include new fields for the location of antecedent temperatures, LAI, Drought Index, humidity, and wind speed input files.
4. The "7 Make EMISSIONS" and "Procedures: 2001" modules were modified to estimate isoprene emission variations associated with the average temperature of 1) the past 18 hours, 2) the past 48 hours, 3) the past 360 hours and 4) a combination of all three.

Changes not related to a specific task

1. The "Model Parameters" form was modified to clarify the purpose of the factor previously referred to as the "Isoprene EP ratio". This factor was replaced by the two factors that it is based on: "Database Max. Iso. EF" and "Revised Max. Iso. EF". The "Database" value refers to the maximum isoprene emission factor used for isoprene in the "vegCode char" table (this can be calculated by dividing "iso" in this table by "LMD"). If BEIS2 emission factors are used to generate vegCode char then "Database Max. Iso. EF" is equal to 79.3 micrograms compound per gram per hour. The "Revised Max. Iso. EF" represents the maximum isoprene emission factor that the user would like to use. A value of 113.3 micrograms compound per gram per hour (equivalent to 100 micrograms carbon per gram per hour recommended by Guenther et al. 2000) is recommended. The "7 Make EMISSIONS" module, "Model Parameters" table, and "Model Parameters" form and associated class object were modified accordingly.
2. The "Model Parameters" form was modified so that the user can select to run a range of days in addition to a range of hours. The queries, "Make PAR" and "Make Temperature", the form "Model Parameters" and associated class object were modified.
3. The "Model Parameters" screen was modified so that the user can choose "BEIS2" or "modified BEIS2" (which continue to operate the same as GLOBEIS2) as well as a new option to select "GloBEIS3" which provides ability to include specified LAI, variable leaf age, drought index, leaf temperature and antecedent temperature. The queries "Input AnTemp", "Input AnTemp Dindex", "Input Antemp Dindex HumWind", "Input AnTemp Dindex HumWind LAI", "Input AnTemp Dindex LAI", "Input AnTemp HumWind", "Input AnTemp HumWind LAI", "Input AnTemp LAI", "Input Dindex", "Input Dindex HumWind", "Input Dindex HumWind LAI", "Input Dindex LAI", "Input HumWind", "Input HumWind LAI", "Input LAI" were all created.
4. The new import modules were named "5a Import LAI," "5b Import Wind," "5c Import Humidity," "5d Import Drought Index," and "5e Import Antecedent T." Incremented the module numbers for all remaining modules by one. The remaining modules are now "6

QA," "7 Make Emissions," "8 Make Emissions CB4," "9 Export CB4 Emissions," and "10 Cleanup."

5. The QA module was enhanced to 1) verify the completeness of all inputs for each hour and domain cell over the range of days specified in the "Model Parameters" screen and 2) ensure there are no duplicate records in the input files upon import.
6. The model year is now forced to a four digit year to ensure that there is no inconsistency between inputs and what the user specifies in the "Model Parameters" screen. Every two digit year imported from an input file is now automatically converted to a four digit year. Two digit years entered in the "Model Year" fields of the "Model Parameters" and the "Simple Inputs" screens are also automatically converted to four digit years. The conversion convention for two digit years is that if the year is less than 50, it is converted to 2000 + model year, otherwise, it is converted to 1900 + model year.