Incorporating Biogenic Hydrocarbon Emission Inventories into Mesoscale Meteorological Models

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ABSTRACT

Isoprene flux measurements have been collected since 1996 at the AmeriFlux site located at the University of Michigan Biological Station (UMBS) as part of the Program for Research on Oxidants: Photochemistry, Emissions, and Transport (PROPHET). The isoprene flux data show that there is a very strong linear correlation between daily isoprene emissions and sensible heat fluxes for the predominantly aspen/oak stand located in northern Michigan. Our hypothesis is that the surface energy flux is a better model parameter for estimating isoprene emissions at the canopy scale than temperature and light levels, and the link to the surface energy budget will provide an improvement in isoprene emission models. Since surface energy budgets are an integral part of mesoscale meteorological models, this correlation could potentially be a useful tool for incorporating biogenic emissions explicitly into regional atmospheric modeling systems. The correlation can also be useful as a diagnostic tool for current biogenic emission inventory models, to determine if we are correctly predicting isoprene for the right reasons. Because sensible heat flux is a surrogate for the integration of temperature and light through the depth of the canopy, heat flux is potentially another predictor of isoprene fluxes based on physiological/biological control mechanisms. In this paper, correlations between observed sensible heat flux and isoprene flux are presented along with the results of a multiple linear regression for predicting isoprene flux as a function of sensible heat flux and maximum daily heat flux. We also examine the performance of the Biogenic Emission Inventory System (BEIS) canopy model for isoprene.

INTRODUCTION

The importance of isoprene at urban, regional, and global scales of atmospheric chemistry is well established (Fehsenfeld et al., 1992; Guenther et al., 1995; Cowling et al., 1998; Guenther et al., 2000; Fuentes et al., 2000). In rural areas, isoprene is almost always the dominant reactive hydrocarbon. In order to understand the chemistry of rural atmospheres, it is essential that the emissions of isoprene be well characterized. However, the details of how much isoprene, from what ecosystems, and under what conditions, remain troublesome aspects of accurately portraying isoprene in chemical cycles. In many cases, our ability to model isoprene and other biogenic hydrocarbons is limited to an accuracy of approximately a factor of two.

We know that isoprene is emitted at high rates from oak, aspen, poplar and at lower rates from other deciduous vegetation and from spruce (Guenther et al., 1994; Geron et al., 1994; Guenther et al., 1996; Kempf et al., 1996). We know that isoprene is emitted in the presence of sunlight and exhibits an exponential increase with temperature to a maximum level near 40^oC (Guenther et al., 1993). At the same time, we know that isoprene is not directly tied to photosynthesis; isoprene emissions can increase while photosynthesis ceases—at least in the short term (minutes to hours) (Monson and Fall, 1989). Yet, it has also been theorized that there is long term (few days) control of isoprene emissions linked to the average temperature and PPFD over the previous 48 hours (Sharkey et al, 1999). We know that the basal isoprene emission rate can be different from sunlit leaves in the top of a canopy compared to shady leaves deep in a canopy (Harley et al., 1996, 1997). We know that the onset of isoprene emissions is delayed for several weeks after bud break in the spring and that isoprene emissions decrease in the fall at the approach of leaf senescence (Monson et al., 1994; Goldstein et al., 1998; Fuentes et al., 1999).

However, our understanding of the biological or physiological controls on the emission of isoprene is limited, in particular when incorporating isoprene emissions into atmospheric chemical cycles.

Biogenic emission models, such as BEIS (Biogenic Emission Inventory System) rely on above canopy environmental parameters and below canopy scaling factors to estimate canopy scale biogenic hydrocarbon fluxes. Other canopy models such as CANVEG (Baldocchi and Harley, 1995) incorporate dynamic micrometeorological and physiological modules to simulate the canopy environment for predicting biogenic emissions. Continuous eddy covariance flux measurements of isoprene from several forested canopies show considerable variability in the emission pattern from day to day and even from one hour to the next; a significant portion of the variability cannot be explained using temperature and/or light effects as given in the current emission models. Second, at some sites, there is considerably rapid decay of isoprene concentration from afternoon into evening, with patterns that can be quite different from one evening to the next. In an effort to more accurately predict the isoprene fluxes, alternative model parameters for isoprene emissions are being explored, with the hope that this will provide some insight into the short-term physiological control of the emissions.

Seasonal eddy covariance flux data from a site in northern Michigan for the previous 3 years have shown strong linear correlations on a daily basis between sensible heat fluxes and isoprene fluxes (Westberg et al., 2001). The strong correlation suggests that sensible heat flux may be an excellent parameter to use in modeling isoprene fluxes. If this tie between isoprene and sensible heat flux can be determined, using the surface energy flux as a model parameter for isoprene emissions could be a very useful tool. Surface energy flux is an inherent surface layer parameter predicted in all mesoscale meteorological models and global circulation models. Thus, it is readily available for modeling isoprene on regional and global scales.

This paper presents correlations between measured eddy covariance isoprene flux data and surface energy flux data, with the intent that these correlations can be used within the framework of mesoscale meteorological models. The correlations presented are for a deciduous forest located in northern Michigan.

MODELING APPROACH

Currently isoprene and other biogenic hydrocarbons are incorporated into atmospheric models using a variety of methods that are all quite similar to the Biogenic Emission Inventory System (BEIS) developed by Lamb et al. (1993), revised by Geron et al. (1994) and, more recently, significantly expanded and updated as GLOBEIS by Guenther et al. (2000) (see also Greenberg et al. (1999)). The BEIS models generate hourly emission estimates of biogenic VOCs. Plant species composition and foliar density distributions are characterized using satellite derived databases and vegetation inventories. Above canopy meteorological conditions (e.g., photosynthetic photon flux density (PPFD), wind speed, temperature, and humidity) are scaled for each layer within the canopy according to a simple canopy model. Leaf temperature is calculated using an iterative method to solve a leaf energy budget for each canopy layer. The vertical profiles of leaf temperature and PPFD are then used to drive empirical equations to estimate genus specific biogenic emission rates (Geron et al. 1994). Additional factors are also included in the above-canopy flux equation to account for the different processes that affect emission activity behavior (e.g., leaf age, phenology, and past leaf temperature) and the landscape escape efficiency (canopy ventilation). Other models, such as CANVEG, are coupled micrometeorological and physiological modules that incorporate the feedback mechanisms present in a canopy environment (Baldocchi and Harley, 1995; Baldocchi et al., 1995; Baldocchi et al., 1999). This kind of dynamic canopy model provides more realistic simulation of the canopy environment, but evaluations of BEIS and CANVEG show that model performance is not substantially different in comparison to observed isoprene emissions (Lamb et al., 1996).

An alternative approach proposed in this paper estimates hourly isoprene emissions based on an empirical model involving sensible heat flux. Instead of using vertical profiles of leaf temperature and PPFD, the surface energy flux of sensible heat is used to drive the estimate of isoprene flux. Sensible heat flux is a parameter available from mesoscale models and it is a canopy scale surrogate of the canopy integrated leaf level temperature and PPFD that drive emissions in the BEIS type models. Physiologically sensible heat flux reflects the transfer of heat out (or in) of the canopy, presumably the heated air mass from within the canopy that is driving the isoprene emissions.

There are many mesoscale models available for regional applications, but the modeling system used at WSU consists of the Fifth-generation Pennsylvania State University-National Center for Atmospheric Research Mesoscale Model (MM5) (Grell et al. 1994; Anthes and Warner 1978) and the CALMET-CALGRID modeling package (Yamartino et al. 1992; Scire and Robe 1997; Robe and Scire 1998). A recent application of this modeling package has used BEIS type emission inventories (Barna et al 2000), and work is currently underway to link the latest version of BEIS (GLOBEIS) directly to MM5. Future work also involves applying the empirical equation presented here to sensible heat flux data generated from MM5.

EXPERIMENTAL DATA

With the introduction of a fast isoprene analyzer (FIS) by Hills and Zimmerman (1990), it is now possible to make eddy covariance flux measurements for isoprene using:

Equation (1) $$F = \overline{w'C'}$$

where

w' = fluctuating component of vertical velocity
C' = fluctuating component of ambient isoprene concentration

Guenther and Hills (1998) employed a FIS with eddy covariance methodology to measure isoprene fluxes over a mixed deciduous forest in North Carolina. They noted that this system has the capability to make eddy covariance flux measurements in an automated mode on a continuous basis for extended periods of time. Since these measurements can be obtained simultaneously with sensible and latent heat fluxes and CO_2 fluxes, the foundation now exists for exploring isoprene emissions with respect to the dynamics of a forest ecosystem.

Seasonal eddy covariance isoprene flux data have been collected from a deciduous forest within the University of Michigan Biological Preserve during the past 3 years (1998 – 2000) as part of the PROPHET atmospheric chemistry program. Results from 1998 are presented in Westberg et al. (2001). The site is located near Pellston, MI (45°30' N, 84°42' W, elevation 238 m) and it is part of DOE's AmeriFlux network of research sites in North America. The AmeriFlux tower is 50 m tall and is used to study biosphere-atmosphere carbon exchange in a northern hardwood forest regime. The forest, with an average canopy height of 22 m, contains a mix of aspen, beech, birch, maple and oak, with a strong under story component of white pine. The primary isoprene emitters are aspen and oak, with aspen accounting for approximately 90% of the isoprene emitting biomass in the prevailing westerly upwind direction. Biomass surveys completed at the site yield a relatively uniform distribution of isoprene emitters around the tower. The average isoprene-emitting biomass is estimated to equal 153 g m^{-2}. The cumulative leaf area index for the site is 3.9.

Instrumentation located on the AmeriFlux tower at 31 m above ground level includes a 3-dimensional sonic anemometer (Applied Technologies, Inc.), and an open path infrared CO_2/H_2O gas analyzer (IRGA, Auble and Meyers, 1992). Located at the base of the tower is a fast isoprene sensor

(FIS, Hills Scientific, Inc., Hills and Zimmerman, 1990; Guenther and Hills, 1998). Teflon tubing and a pump provide sample air from the 31 m level near the sonic anemometer to the FIS. Using eddy covariance sampling techniques, continuous isoprene, sensible heat, latent heat, and CO_2 fluxes were obtained for approximately two weeks in 1998 and throughout the growing season (May - Oct) in 1999 and 2000.

EMPIRICAL RELATIONSHIP

Using the 30-minute average observed isoprene flux and sensible heat flux from the site in northern Michigan; correlations between the two measurements were identified. On a daily basis, the correlations are very strong. As shown in Figure 1, three days from the summer of 2000 all have strong correlations, however, the slope ranges from 0.02 to 0.04. With few exceptions, correlation coefficients range between 0.73 and 0.98 for other days throughout 2000. In 1998, we observed a series of days with a slope near 0.025 and then after a rainy day, another series of days occurred when the slope was changed to 0.013. This is shown in Figure 2 in terms of the daily slope and correlation coefficients for the linear regressions between sensible heat flux and isoprene flux. At this point, the cause for the differing slopes from day to day is not well understood, but analyses indicate a correlation between the slope and the daily maximum heat flux.

To further explore the possible correlations, a multiple regression analysis was done with the observed isoprene fluxes and other parameters including sensible heat flux, maximum daily sensible heat flux, latent heat flux, and above canopy air temperature and PPFD. As previously mentioned, sensible heat flux combines the effects of both temperature and PPFD along with the physical transport of energy in and out of the canopy. The theory associated with using the maximum daily sensible heat flux is physiological in nature. The rate of production and therefore emission of isoprene does respond quickly (within seconds to minutes) to changes in temperature and light for the short term, however, for longer time periods (hours to days) isoprene emissions seem to be more variable. Recently, Singsaas and Sharkey (2000) have shown some of the variability is caused by the rate at which leaf temperature increases. The maximum daily heat flux is a measure of the limit with respect to temperature that the leaf encounters during a 24-hour period. Thus, including maximum daily heat flux in the regression provides a mathematical measure of the difference between hourly heat flux and the maximum daily heat flux.

Many regression analyses were performed with various combinations of the previously mentioned parameters. The most complex regressions (with 5 degrees of freedom) were the best predictors for isoprene flux (compared to the observed isoprene flux), however, in order to keep it less cumbersome, a simple regression was favored. The simple regression only uses heat flux and maximum daily heat flux, and the correlation is still significant (0.70 with 694 observations for the 2000 data). The same regression equation for 2000 was tested using the 1998 data and a correlation of 0.65 with 472 observations was obtained. Figures 3 and 4 show the comparison between observed isoprene fluxes using the eddy covariance technique and the predicted isoprene fluxes using the multiple regression equation as follows:

Equation (2) $$[\text{isoprene flux}] = 0.672 + .0211\ H - 4.057 \times 10^{-5}\ MaxH$$

where

[isoprene flux] = predicted flux (mgC m^{-2} h^{-1})
H = observed sensible heat flux (W m^{-2})
MaxH = daily maximum sensible heat flux (W m^{-2})

Figures 5 and 6 show the time series of observed isoprene fluxes and predicted fluxes for selected days in 1998 and 2000, respectively.

DISCUSSION AND CONCLUSIONS

The regression equation (2) used to predict isoprene fluxes (shown in Figures 5 and 6) does a relatively good job at capturing the sometimes-large fluctuations between each 30-minute period. There is also very good temporal correlation between the observed and predicted isoprene fluxes. However, as shown, there are certain days that isoprene is overestimated (August 11, 1998 and July 10, 2000) and there are days when isoprene is underestimated (August 8, 1998 and July 12, 2000). Again, this inability to predict day-to-day (long term) changes in emissions appears to be the problem with almost all of the current emission inventory models. The robustness of the regression equation is promising; meaning the application of the equation (based on the 2000 data) with the 1998 data was favorable. Additional work will include testing the regression equation with observational data from other sites, including a poplar plantation in Oregon and an AmeriFlux site in Oak Ridge, TN, both of which have different species composition.

The predicted isoprene fluxes presented in Figures 5 and 6 are on par with predicted isoprene fluxes from models such as BEIS. Figure 7 compares observed with predicted daily isoprene fluxes using both BEIS and the multiple regression. The BEIS terms E_S, C_L, and C_T correspond to the canopy scale standard emission rate, a light correction term and a temperature correction term. Once again, BEIS predictions compare favorably with observational data for some days, but not for every day.

However, the correlations and the predicted isoprene fluxes do not explain the physiological control mechanism that is driving the emission of isoprene. Does BEIS predict isoprene fluxes for the correct reasons? One way to consider this is to compare the BEIS predicted sensible heat fluxes with the observed heat fluxes. Figure 8 shows a comparison between these two variables, and the correlation is good except that BEIS overestimates the heat flux by a factor of two. Based on the strong correlation between sensible heat flux and isoprene flux, the BEIS predicted fluxes are accurately estimating isoprene flux for another reason. Deeper explorations into these types of questions may help to unravel the mystery behind isoprene emissions. The regression equation presented here provides a diagnostic tool for testing canopy models such as BEIS. We know there is a strong correlation between sensible heat flux and isoprene flux for this particular site, but does it hold true for different sites with different species composition? If so, then sensible heat flux could be a very useful surrogate for modeling isoprene emissions in current mesoscale meteorological models. Not only is sensible heat flux inherently available in surface meteorological models, but is also provides a basis for atmosphere/biosphere feedbacks (by coupling isoprene emissions with meteorological parameters) in regional models.

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KEYWORD

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