

# Methods for Estimating Meteorology-Based Emissions Temporal Profiles for Livestock and Residential Wood Combustion Sources

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# **Executive Summary**

Models that relate ambient meteorology and pollutant observations can be used to simulate the temporal patterns of air emissions sources. The implementation of these models in software that uses simulated, rather than observed, meteorology data enables the estimation of temporal variations due to local weather for different locations and time periods. This approach has an advantage over the standard emissions temporal allocation process that uses static profiles because it supports the estimation of spatially and temporally dynamic temporal variability in emissions sources. The University of North Carolina at Chapel Hill's Institute for the Environment (UNC-IE) developed software to estimate temporal profiles for residential wood combustion (RWC) and livestock ammonia emissions sources. UNC-IE conducted research to seek an empirical relationship between observed meteorology and wood smoke emissions and to implement this relationship as a step in the emissions processing sequence to calculate daily and hourly RWC emissions from annual, seasonal, or monthly emissions estimates in the National Emissions Inventory (NEI). Using a statistical model of the relationship between an ambient wood smoke chemical tracer and ambient temperatures at rural air quality monitors in the Pacific Northwest, UNC-IE developed an algorithm for computing daily temporal profiles for RWC emissions. UNC-IE also adapted an equation from the peer-reviewed literature to use countyaverage meteorology to estimate hourly emissions from county-total monthly agricultural livestock ammonia inventories. These algorithms are implemented in a new Sparse Matrix Operator Kernel Emissions (SMOKE) processor called GenTPRO that reads hourly, simulated meteorology data to produce temporal profiles for use in preparing emissions inputs to air quality models.

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### 1 Overview

Models that relate ambient meteorology and pollutant observations can be used to simulate the temporal patterns of air emissions sources. The implementation of these models in software that uses simulated, rather than observed, meteorology data enables the estimation of temporal variations due to local weather for different locations and time periods. This approach has an advantage over the standard emissions temporal allocation approach that uses static profiles because it supports the application of spatially and temporally dynamic profiles. A barrier to implementing meteorology-based temporal profiles is the spatial incommensurability between model-ready meteorology data and emissions inventories. This document summarizes approaches developed by the University of North Carolina at Chapel Hill's Institute for the Environment (UNC-IE) in collaboration with the U.S. EPA for coupling gridded, hourly meteorology data to county-based emissions inventories that support the calculation of meteorologybased temporal profiles. UNC-IE developed or implemented algorithms to estimate temporal profiles for two specific inventory sectors: residential wood combustion (RWC) and livestock ammonia (LNH3). In addition, we developed a process to estimate temporal profiles based on any user-defined meteorology variable, such as temperature or wind speed. Adelman et al. (2009; 2010a; 2010b) presents the development and testing of the temporal profile models described here and is considered a supplemental reference for this research.

# 2 Emissions Temporal Profile Algorithms

#### 2.1 RWC: Residential Wood Combustion Profile Algorithm

Establishing a quantitative relationship between RWC activities and meteorology can provide a way to use the temporal variability in predicted meteorology data to estimate the temporal patterns in RWC emissions. If a quantitative relationship between a monitored chemical tracer of wood smoke emissions and an observed meteorology field, such as temperature, could be established, this relationship could be used to estimate the daily or hourly variability in simulated RWC emissions using predicted hourly meteorology. UNC-IE conducted research to seek an empirical relationship between observed meteorology and wood smoke emissions and to implement this relationship as a step in the emissions processing sequence to calculate daily and hourly RWC emissions from annual, seasonal, or monthly emissions estimates in the National Emissions Inventory (NEI) (http://www.epa.gov/ttn/chief/net/2008inventory.html). Figure 1 is a basic schematic of the hourly RWC emissions model we developed.



Figure 2. Conceptual model for estimating hourly RWC emissions from meteorology

Figure 1 shows that we used observed meteorology and RWC tracer data to develop regression equations implemented in a SMOKE preprocessor. Our model estimates a daily RWC inventory using RWC emissions in the NEI and hourly, predicted meteorology. The daily RWC inventory is converted to hourly RWC emissions with SMOKE using hourly temporal profiles (Hourly TPRO).

In this conceptual model, the two input data components to the statistical model (observed meteorology and observed RWC tracer data) are the complicating components of this approach; the rest of the input data (annual RWC emissions inventory and hourly predicted meteorology) are readily available. Although levoglucosan (LG) is a conservative chemical tracer for wood combustion that might provide a way to relate ambient pollutant concentrations to RWC emissions (Fraser and Lakshmanan, 2000), the specialized analysis techniques required for collecting LG from particle filters limit its availability to a small number of ambient monitoring campaigns. Further, some of the studies that do provide LG measurements were conducted to assess the air quality impacts of forest and agricultural fires and so are not appropriate for studying the impacts of RWC emissions. The limited number of LG measurements in the U.S. inhibits the development of a nationally extensible and statistically significant model relating a wood smoke tracer and meteorology.

In an attempt to circumvent the problem of limited LG measurements, UNC-IE explored the use of alternative chemical tracers of wood smoke. Relevant tracers that are routinely monitored include organic carbon (OC) and elemental carbon (EC). Unlike LG, however, these pollutants are not unique to wood combustion and often include signals from other combustion sources, such as the combustion of transportation fuels. Because these alternative compounds are not unique to wood smoke emissions, we tried to target analysis of these data to the times of the year and the PM monitoring locations that have strong RWC signals.

Quantifying the relationship between potential wood smoke chemical tracers and meteorology is also complicated by the complexity of the atmospheric processes that influence ambient pollutant

concentrations. While temperature plays a role in the magnitude of RWC activity, with lower temperatures corresponding to higher activities, other factors, such as the extent of atmospheric mixing, significantly influence ambient pollutant concentrations. To use ambient measurements of RWC chemical tracers as proxies for emissions activity, it is necessary to consider the various meteorology parameters affecting both the emissions activities and ambient concentrations of RWC pollutants. While ambient temperature measurements are commonly co-located with the PM chemical measurements, indicators of atmospheric mixing or stability are typically not measured and must be derived from simulated meteorology. Factors in the calculation of atmospheric stability may include vertical temperature gradients, planetary boundary layer (PBL) heights, cloud cover, wind speeds, and the Monin-Obukhov length. Atmospheric stability parameterizations have been developed to consider combinations of these factors, and include the ventilation index (Hardy et al., 2001) and the atmospheric dispersion index (Lavdas, 1986). Both of these indices are defined in terms of numeric ranges that correspond to different classes of atmospheric stability. Table 1 defines the categories for both the ventilation index (VI) and the atmospheric dispersion index (ADI).

Mixing	Classification VI (m <sup>2</sup> /sec)		ADI (m <sup>2</sup> /sec)	
Extensive mixing	Very Good	_	>100	
	Good	Good >7,050		
	Generally Good –		41-60	
Stagnation with low wind speeds	Fair	4,700-7,050	21-40	
	Generally Poor	Generally Poor 2,350-4,700		
	Poor	_	7-12	
None Very Poor		< 2,350	1-6	

 Table 1. Classification schemes for two stability indices, VI and ADI

UNC-IE used multiple data sources to research the relationship between chemical tracers of wood smoke and meteorology. The Puget Sound Clean Air Agency (PSCAA) distributes daily PM<sub>2.5</sub> and LG observations from 2005 to present for sites around Seattle, WA (<u>http://trend</u> graphing.pscleanair.org/). Field campaign data collected for particulate matter (PM) source apportionment studies that included LG were available for sites in the southeastern U.S. for 2007 and the Great Lakes region for 2004 (Marc Houyoux, EPA, personal communication, 2009). We downloaded OC and EC data from the Speciation Trends Network (STN) (http://www.epa.gov/ttnamti1/slams.html) for multiple years for sites throughout the country. Many of the chemical observation sites also included ambient temperature measurements that could be used in these analyses. We used simulated temperatures, wind speeds, PBL heights, and

derived ventilation indices from meteorology data provided by EPA. They provided meteorology modeling results at 12-km resolution for 2005 and 2006 for the western U.S., 12-km resolution for 2006 for the eastern U.S., and 36-km resolution for the continental U.S. (Patrick Dolwick, EPA, personal communication, 2009).

Investigation of the PSCAA LG data showed a fairly strong relationship with ambient temperatures at suburban and rural sites in the area (Onstad and Simpson, 2008). A series of five monitors with LG observations covers a range of locations from rural to urban around Puget Sound. Figure 2 shows regression curves relating ambient LG and temperatures at the PSCAA sites for the years 2006 and 2007. We compared daily average LG and temperatures at the five PSCAA sites and fitted the data with regression lines and calculated R<sup>2</sup> values for each site.

The regressions in Figure 2 demonstrate that without any corrections for atmospheric stability, there appears to be an exponential relationship between ambient LG and temperature. The strongest relationship occurs at the rural Darrington site, with weaker relationships at the suburban Marysville and Tacoma sites. The urban sites, Duwamish and Beacon Hill, show an insignificant relationship between LG and temperature. The rural and suburban sites have high wintertime concentrations of LG due to a high prevalence of wood-burning devices used in residences for wintertime heating. Roadways and industry heavily impact the urban sites, with little influence from woodstove use (Onstad and Simpson, 2008). The higher LG concentrations in the rural and suburban monitors, relative to the urban sites, are also seen in the plots in Figure 2. These plots indicate that rural monitors in areas that have a high level of woodstove use could be used to establish an empirical relationship between RWC activity and meteorology.

Investigation of the LG data collected at southeastern U.S. sites showed less compelling relationships with temperature than at the Puget Sound sites. Figure 3 shows the locations of five sites in the Southeast that reported LG observations, and regression plots of daily average LG and daily minimum temperatures.

Given the limited number of sites in the U.S. that collect LG observations, we decided to explore other chemical tracers of wood smoke emissions. In the STN database there are OC and EC measurements for several years and dozens of sites. Although OC and EC are not unique tracers for wood smoke and RWC, we filtered the STN data to identify sites that are affected by RWC emissions. To isolate periods when RWC activity is high, we applied a maximum-temperature restriction of 10°C, excluding all observations collected at temperatures above this threshold. We assumed that this temperature threshold would also be a proxy for excluding the wildfire season, which occurs during warmer months of the year. To identify what we call "RWC monitors"—those monitors most likely affected by RWC sources—we used the ratio of OC to EC. By assuming that higher OC/EC ratios may indicate a wood smoke signal (Ward et al., 2011), we identified potential RWC sites as the 80<sup>th</sup> percentile of the median OC/EC ratios across all STN monitors. We applied an additional filter by including only those monitors with negative correlation between temperature and measured OC. Table 2 shows the results from this analysis for the year 2006.



Figure 3. Regressions for the five PSCAA monitoring sites



Figure 4. Regressions for five southeastern U.S. monitoring sites

Obs	State_name	County_name	Unique_ID	Mean	Median	No. of Obs	Corr
1	California	Plumas Co	6-63-1009	16.4542	15.0000	58	-0.66155
2	Oregon	Lane Co	41-39-60	22.6467	8.4076	38	-0.65874
3	California	Butte Co	6-7-2	12.9292	10.8000	36	-0.62111
4	Oregon	Jackson Co	41-29-133	14.6109	13.0085	41	-0.61450
5	Montana	Lincoln Co	30-53-18	63.9475	12.5759	48	-0.41110
6	Idaho	Canyon Co	16-27-4	63.1415	9.9390	47	-0.39716
7	Oregon	Union Co	41-61-119	15.3529	13.4674	43	-0.37476
8	North Carolina	Buncombe Co	37-21-34	11.2095	9.4103	33	-0.27715
9	Montana	Missoula Co	30-63-31	12.1630	9.0000	81	-0.18745
10	South Carolina	Greenville Co	45-45-9	44.5487	9.4490	48	-0.18711
11	Massachusetts	Hampden Co	25-13-8	14.2456	9.2365	34	-0.15018
12	Georgia	Floyd Co	13-115-5	19.9213	9.5082	30	-0.12476
13	Virginia	Henrico Co	51-87-14	31.5479	8.7162	45	-0.08493
14	Indiana	Vanderburgh Co	18-163-12	17.6479	8.1405	34	-0.06512
15	Minnesota	Hennepin Co	27-53-963	11.5916	8.1673	66	-0.04818
16	Tennessee	Lawrence Co	47-99-2	32.6421	11.1330	31	-0.01946

Table 2. STN RWC monitors for the year 2006; mean and median measured organic carbon ( $\mu g/m^3$ )

NOTE: "Corr" (final column) is the value of the correlation between temperature and measured OC.

For the initial attempt at developing a statistical model for RWC emissions, we focused on data from the year 2006 because of readily available meteorology and ambient monitoring data for that year. Some of the STN monitors that we identified through these analyses are known locations of high RWC activity and air quality impacts (e.g., Missoula, MT). Using these sites, we experimented with different meteorology predictors (temperature, wind speed, PBL height, ventilation index), time averaging (day, week, month, year), and spatial aggregation (site ID, state, region, quadrant) in an attempt to find statistically significant relationships with the observed OC concentrations. We used both monitored and predicted temperatures, which are highly correlated with each other, and simulated wind speeds and PBL heights as proxies for atmospheric mixing. Covariance in the meteorology variables inhibited their use as interaction terms in a model and required us to explore models that treated the variables separately.

Figures 4 through 6 illustrate comparisons between OC observations at the 16 STN RWC monitors listed in Table 3 and various simulated meteorology variables: daily average temperature in Figure 4, daily average PBL height in Figure 5, and daily average wind speed in

Figure 6. The purpose of these comparisons was to explore associations between a wood smoke proxy and various atmospheric conditions.



Figure 5. Scatterplots comparing measured OC ( $\mu$ g/m<sup>3</sup>) and simulated daily average temperatures (°C) at STN RWC sites in 2006



Figure 6. Scatterplots comparing measured OC ( $\mu$ g/m<sup>3</sup>) and simulated daily average PBL heights (m) at STN RWC sites in 2006



Figure 7. Scatterplots comparing measured OC (μg/m<sup>3</sup>) and simulated daily average wind speeds (m/s) at STN RWC sites in 2006

Of all the possible predictors for OC in the STN data for 2006, we found that the site location was the best predictor of variance in the data. We explored aggregation of the data from single sites to general locations/regions (e.g., northeastern U.S. sites, southwestern U.S. sites) and from days to week/season/month in attempts to develop extensible relationships between OC and meteorology. We also tried filtering the data by different temperature ranges, PBL heights, and wind speeds to explore whether relationships existed in different categories of meteorology conditions. Table 3 presents results from various models we developed from the STN OC data. These results confirm that of all the variables we tested, the site location was the best predictor of variance in the observed OC. As site location is not a useful model parameter for the simulation of temporal variability in RWC emissions, we decided against further analysis of the STN data and opted instead to revisit the PSCAA monitoring data.

Model	Variables Controlled in the Model	R <sup>2</sup>
#1	Date, temperature, PBL height, wind speed, and all possible interactions among these variables	0.15
#2	Same as #1 + month-specific variable	0.16
#3	Same as #1 + site-specific variable	0.35
#4	Same as #1 + location-specific variable	0.20
#5	Same as #1 + all possible interactions of site variable with other predictors	0.51

Table 3. STN model development experiments

To expand the number of data points available for developing a statistical model relating meteorology and wood smoke, we compared LG observations at the PSCAA sites to other, more routinely measured PM data. Nephelometer  $PM_{2.5}$  has been measured by the PSCAA from 2004 to the present and shows a strong correlation in both space and time with measured LG at several monitors. Figure 7 shows comparisons between LG and nephelometer  $PM_{2.5}$  at two sites in the PSCAA monitoring network. Due to the strength of these correlations, we decided that nephelometer  $PM_{2.5}$  could be used to increase the sample size of observations for developing an RWC emissions model.



Figure 8. PSCAA site comparisons between daily levoglucosan (LG) and PM<sub>2.5</sub> nephelometer measurements

Figure 8 compares time series of daily temperatures and nephelometer  $PM_{2.5}$  at the PSCAA monitoring sites from 2004 to 2010. Qualitatively this plot indicates a negative correlation between the two variables. To explore this apparent correlation further, we developed regressions between  $PM_{2.5}$  and temperature at the PSCAA sites. Figures 9 and 10 summarize these regression results. Figure 9 shows the relationship between  $PM_{2.5}$  and temperature for all data points collected from 2004 to 2010. Although the  $R^2$  values for these relationships are low (not shown), there is a distinct elbow in the fitted regression line, indicating that there is a temperature below which the correlation between the two variables switches from being positive to negative. To explore this trend further, we filtered the PSCAA data to exclude temperatures greater than 50°F (>10°C) and outliers (90<sup>th</sup> percentile of  $PM_{2.5}$  measurements). Figure 10 shows the filtered scatterplots and regression lines, and indicates that despite these refinements, the correlation between these variables is still fairly weak.







Figure 10. PM<sub>2.5</sub> nephelometer (µg/m<sup>3</sup>) vs. temperature (°F); no restrictions on any variables



Figure 11. PM<sub>2.5</sub> nephelometer (µg/m<sup>3</sup>) vs. temperature (°F); removed observations above 10°C and upper 10% of PM<sub>2.5</sub> measurements

UNC-IE tested the hypothesis that observed  $PM_{2.5}$  at monitors with strong RWC signals would be inversely correlated to ambient temperatures. Despite promising qualitative relationships, statistical analysis of the chemical and meteorology data failed to produce a statistically significant model. We finally developed a basic regression equation from the three sites in the PSCAA network that were most strongly associated with RWC sources. Details of the regression equations used to relate ambient PM to temperatures are included below:

- PSCAA monitoring sites: Darrington, Marysville, Tacoma South
- Years: Observed temperature and nephelometer PM<sub>2.5</sub> from 2004 to mid-2010
- Predictors: (1) daily minimum temperature, (2) weekly averaged temperature, and (3) monthly averaged temperature; note that all predictors included a restriction for temperatures ≤50°F (i.e., all measurements associated with temperatures >50°F were excluded)

Table 4 summarizes the three regression equations we developed. The intent of these equations is not to predict ambient  $PM_{2.5}$  concentrations but to simulate the temporal variability in ambient concentrations, which would then be used as a proxy for RWC emissions' temporal emission patterns.

Model	Averaging	Equation	Number of Observations	$\mathbf{R}^2$
#1	Daily	$PM_{2.5} = 42.12 - 0.79T$	2,008	0.258
#2	Weekly	$PM_{2.5} = 38.03 - 0.68T$	305	0.260
#3	Monthly	$PM_{2.5} = 36.52 - 0.64T$	71	0.354

Table 4. RWC emissions regression equations

We adapted these equations to estimate temporal variability from RWC emissions sources. Equation 1a uses estimates of daily  $PM_{2.5}$  emissions to build annual-to-daily emission profiles for application to RWC sources. The algorithm uses county-average daily minimum temperatures to estimate the percentage of RWC emissions allocated to each day of the year, including a maximum temperature cutoff to prevent RWC emissions from being allocated to days too warm to have much (if any) RWC emissions. The outputs from this algorithm are temporal profiles that convert annual RWC inventories to daily emissions for every county in the modeling domain.

$$PE_{i,d} = \frac{(42.12 - 0.79 * T_{i,d})}{\sum_{d=1}^{365} (42.12 - 0.79 * T_{i,d})}$$
(Equation 1a)

where

 $PE_{i,d}$  = Percentage of annual emissions in county *i* on day *d*.  $T_{i,d}$  = Daily minimum ambient temperature (°F) in county *i* on day *d* (maximum temperature of 50°F)

Equation 1a could be adapted to estimate weekly or monthly emissions from an annual inventory by replacing linear regression model #1 from Table 4 with model #2 or #3, respectively. After converting an annual inventory to daily emissions using Equation 1a, a uniform diurnal profile can be applied to estimate hourly emissions for input to an air quality model.

Figure 11 shows hypothetical RWC emissions calculated with standard U.S. and Canadian profiles compared to the meteorology-based algorithms we developed. These plots show emissions for a 1,000 ton/yr inventory. Year 2006 meteorology was used to compute emissions for the five counties shown in Figure 11. The weekly and daily plots show several points where the emissions drop to zero. These occur because the algorithm calculates RWC emissions only for periods when the minimum temperature in the county is  $\leq 50^{\circ}$ F. For weeks or days when the minimum temperature never goes below 50°F, the RWC emissions are calculated as zero.

To provide flexibility in the way that the RWC emissions algorithm is activated, we implemented a temperature threshold override. A temperature threshold ( $T_t$ ) variable sets a maximum temperature cutoff by either state or county. By default the algorithm activates RWC emissions at temperatures below 50°F. If the user sets the temperature threshold variable, RWC emissions will instead be activated below  $T_t$ . A lookup table of state/county FIPs codes and temperatures (°F) can be input to the algorithm if the user needs to set different temperature thresholds across a modeling domain. The temperature threshold override is used to control when RWC emissions are activated in regions where the 50°F cutoff may not be appropriate. For example, counties in southern Florida may experience only one or two days in an entire year when the minimum temperature dips below 50°F. Without using the threshold override, all of the RWC emissions for these counties would be allocated to those one or two days, producing large emissions spikes that might not be realistic. By increasing the temperature threshold, these spikes can be avoided by activating the RWC algorithm on other days.



Figure 12. Sample RWC emissions computed with regression models #1, #2, and #3 from Table 4; comparison of standard profiles with modeled profiles

A more detailed implementation of Equation 1a, including the conditions for the temperature threshold, is included below in Equation 1b.

If 
$$T_{i,d} \le 50$$
  
 $PE_{i,d} = \frac{(42.12 - 0.79 * T_{i,d})}{\sum_{d=1}^{365} (42.12 - 0.79 * T_{i,d})}$ 

If  $T_{i,d} > T_t$  $PE_{i,d} = 0$ 

(Equation 1b)

If 
$$50 < T_{i,d} \le T_t$$
  
 $PE_{i,d} = \frac{(42.12 - 0.79 * 50)}{\sum_{d=1}^{365} (42.12 - 0.79 * 50)}$ 

where

 $T_{i,d}$  = Daily minimum ambient temperature (°F) in county *i* on day *d* (maximum temperature of 50°F)

 $PE_{i,d}$  = Percentage of annual emissions in county *i* on day *d*.  $T_t$  = Temperature threshold (default = 50°F)

Note:  $T_{i,d}$  can be replaced by  $T_{i,m}$  = monthly minimum ambient temperature in county *i* during month *m*.

UNC-IE and EPA developed a second RWC temporal algorithm as an ad hoc approximation of the original equation to broaden its application by removing the intercept term. With this term removed, Equation 1b will not produce negative emissions when the temperature threshold is increased above 53.3°F. Equation 2 shows the ad hoc, alternative RWC equation.

If 
$$T_{i,d} > T_t$$
  
 $PE_{i,d} = 0$ 

If  $T_{i,d} \leq T_t$ 

$$PE_{i,d} = \frac{0.79 * (T_{i,t} - T_{i,d})}{\sum_{d=1}^{365} 0.79 * (T_{i,t} - T_{i,d})}$$

where

 $T_{i,d}$  = Daily minimum ambient temperature (°F) in county *i* on day *d* (maximum temperature of 50°F)

 $T_t$  = Temperature threshold for the state or county (default = 50°F)

(Equation 2)

 $PE_{i,d}$  = Percentage of annual emissions in county *i* on day *d*.  $T_{i,t}$  = Temperature threshold (°F) in county *i* 

Note:  $T_{i,d}$  can be replaced by  $T_{i,m}$  = monthly minimum ambient temperature in county *i* during month *m*.

The alternative RWC algorithm can be selected using the environment variable RWC\_ALT\_EQ\_YN.

RWC\_ALT\_EQ\_YN = N  $\rightarrow$  Use Equation 1 to calculate RWC temporal profiles RWC\_ALT\_EQ\_YN = Y  $\rightarrow$  Use Equation 2 to calculate RWC temporal profiles

Recommended spatial surrogates for computing the county-average meteorology for the RWC profile algorithm include home heating-wood, housing, and population.

#### 2.2 LNH3: Agricultural Livestock Ammonia Profile Algorithm

Russell and Cass (1986) developed a theoretical equation based on investigations of ammonia (NH<sub>3</sub>) emissions from animal waste decomposition conducted by Muck and Steenhuis (1982) to predict diurnal NH<sub>3</sub> emission variations as a function of daily meteorology. UNC-IE, with support from ENVIRON International Corporation (Mansell et al., 2009), adapted the Russell and Cass equation to create Equation 3, which uses county-average meteorology to estimate hourly emissions from county monthly agricultural livestock NH<sub>3</sub> inventories.

$$E_{i,h} = [(2.36^{\frac{T_{i,h}-273}{10}}) \bullet V_{i,h}]$$
(Equation 3)

where

 $E_{i,h}$  = Emissions rate in county *i* at hour *h*.  $T_{i,h}$  = Ambient temperature (Kelvin) in county *i* at hour *h*.  $V_{i,h}$  = Wind speed (m/s) in county *i* at hour *h* (minimum wind speed of 0.1 m/s)

UNC-IE applied Equation 3 to estimate hourly temporal allocation factors by using the derived  $E_{i,h}$  values in Equation 4:

 $PE_{i,h} = \frac{E_{i,h}}{\sum_{h=1}^{24} E_{i,h}} \bullet A$  (Equation 4)

where

 $PE_{i,d}$  = Percentage of daily total emissions rate in county *i* at hour *h*.  $A_i$  = Monthly emissions in county *i*.

Equation 4 outputs temporal profiles that are used to convert monthly livestock inventories to hourly emissions for every county in the modeling domain. For an emission modeling applica-

tion, annual livestock inventories are converted to monthly inventories using county-specific monthly temporal profiles.

Recommended spatial surrogates for computing the county-average meteorology for the livestock ammonia profile algorithm include agricultural land area, rural land area, and total land area.

### 2.3 MET: Generic Meteorology Profile Algorithm

UNC-IE also implemented an algorithm to compute annual-to-hourly temporal profiles based on hourly time series of a selected meteorology variable (Equation 5):

$$PE_{i,h} = \frac{m_{i,h}}{\sum_{h=1}^{8760} m_{i,h}}$$
(Equation 5)

where

 $PE_{i,d}$  = Percentage of annual emissions in county *i* at hour *h*.  $m_{i,h}$  = Meteorology variable in county *i* at hour *h* 

This is a simple algorithm that computes the percentage of emissions to allocate to each hour based on the hourly fractional contribution of a selected meteorology variable relative to the annual sum of all hourly values for that variable. While the fractional contribution of county-average wind speed for each hour of the year is somewhat meaningless, it does provide a way to build a time series that can be applied to an annual emission inventory to estimate hourly values.

# 3 Temporal Profile Generator: GenTPRO

For use as a processor in the Sparse Matrix Operator Kernel Emissions (SMOKE) system, UNC-IE developed a temporal profile generator that implements the meteorology-based temporal profile algorithms described in Section 2. This processor, called GenTPRO, reads in hourly meteorology data from the Meteorology-Chemistry Interface Processor (MCIP) and a gridded spatial surrogate (commonly used in SMOKE) to produce temporal profiles and cross-reference data in a comma-delimited (CSV) format and a temporal data binary netCDF file. Annual MCIP data are required to calculate temporal profiles with GenTPRO. The spatial surrogate defines the grid cells that will be used to compute county averages of the required meteorology variables. Equation 6 and the corresponding Figure 12 illustrate the calculation that GenTPRO uses to compute county-average meteorology. The figure shows an example of 16 grid cells that overlay a polygon (the shape outlined with the blue line) representing a county. The two solid blue shapes in the county represent a particular land cover or land use category in the county, such as agricultural land. The pink shaded areas are the cells with which the land cover intersects and would contain nonzero values in the gridded spatial surrogate data. If agricultural land were selected as the surrogate to use to compute county-average temperatures, GenTPRO would use the temperature values in the pink shaded cells in Figure 12 to compute the county average and would ignore the blank cells. The averages are arithmetic means based on a simple intersection between the surrogate and the meteorology data grid, with no weighting. Equation 6 is an example of how the county average temperatures would be computed for the situation represented in Figure 12.

$$T_{avg,i} = \frac{T_2 + T_3 + T_4 + T_{10} + T_{11} + T_{12} + T_{14} + T_{15} + T_{16}}{n}$$
(Equation 6)

where

 $T_{avg,i}$  = average temperature in county *i*  $T_x$  = temperature in grid cell *x* (e.g., T<sub>2</sub> = temperature in grid cell 2) *n* = number of grid cells that intersect the selected surrogate (*n* = 9 in this example)



Figure 13. Schematic of county-average temperature approach

GenTPRO provides an option to specify a "profile method," which can be set to generate temporal data for residential wood combustion (RWC) sources, agricultural livestock ammonia sources (LNH3), or generic meteorology-based (MET) profiles. Additional operational details of GenTPRO, including input and output files and environment variables, are available in the *SMOKE v3.0 User's Manual* (http://www.smoke-model.org).

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