Next Generation Ammonia Inventory for the San Joaquin Valley of California

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ABSTRACT

A team of contractors including ENVIRON International Corporation (ENVIRON) and E.H. Pechan & Associates, Inc. (Pechan) is developing a state-of-the-science ammonia emission inventory for the San Joaquin Valley (SJV) in California. This gridded ammonia inventory will be used for data analysis and grid-based aerosol modeling for the California Regional $PM_{10}/PM_{2.5}$ Air Quality Study (CRPAQS). The ammonia inventory will have 1-hour temporal resolution and 1-kilometer by 1-kilometer spatial resolution. The inventory will be developed using the best available ammonia emissions information for the study domain, including several ongoing studies in California. Through incorporation of information from these and other new studies, the project team anticipates that the best characterization to date of important ammonia source categories in the SJV will be accomplished. In particular, significant improvements will be made in temporal and spatial allocation of emissions for fertilizer application, livestock operations, biomass burning, and on-road mobile sources. A thorough assessment of natural soil/plant canopy systems will also be made to better characterize these emissions (i.e., whether they are sources or sinks for ammonia). The project team will adapt ENVIRON's Global Biosphere Emissions and Interactions System (GLOBEIS) model to handle ammonia emissions modeling.

INTRODUCTION

CRPAQS is a multi-year program to study particulate matter (PM) air pollution in central California and consists of meteorological and air quality monitoring, emissions inventory development, data analysis, and air quality modeling. The primary objectives of the study are to:

- provide an improved understanding of emissions and atmospheric processes that influence particle formation and transport;
- develop methods useful to planning agencies in formulating and assessing candidate control strategies for attaining the federal and state PM standards in central California; and,
- provide reliable tools for estimating the impacts of control strategies for PM on visibility, air toxics, and acidic aerosols and on attainment strategies for other pollutants, specifically ozone.

Chemical reactions of ammonia emissions with airborne oxides of sulfur and nitrogen produce fine ammonium sulfate and ammonium nitrate particulate matter. These reactions, especially those leading to ammonium nitrate, represent a significant percentage of wintertime $PM_{2.5}$ in the SJV. Thus, ammonia plays a major role in determining secondary aerosol concentrations within the SJV study area. The modeling domain for the study area covers much of the state (see Figure 1).

As part of the overall CRPAQS, grid-based aerosol models are to be applied to simulate particulate matter concentrations in the SJV and to investigate the sensitivity of secondary particulate matter formation to various parameters. A first step in the successful application of air quality models to investigate proposed control strategies is the demonstration of acceptable model performance through comparison of modeled estimates and field study observation data. A key requirement for the credible application of air quality models

are accurate input data specifying three dimensional meteorology and ground-level emission rate estimates. Ideally these inputs are to be developed with adequate spatial and temporal resolution in order to accurately represent the complex chemical and transport processes occurring in the atmosphere which contribute to the formation of PM.

Thus, the development of a state-of-the-science ammonia emission inventory for the SJV study area is the subject of this project. Accurate emission inventories based on the best available ammonia emissions information and processing methodologies will be critical in supporting numerous aspects of CRPAQS activities over the coming years including ambient data analysis and photochemical modeling.

The primary goal of the project is to develop a draft, ground-level, gridded ammonia emission inventory for use in data analysis and grid-based aerosol modeling for the CRPAQS. The study will place emphasis on important sources within the SJV. The draft inventory is to be used to assess the sensitivity of aerosol model estimates to changes in such variables as spatial and temporal resolution, and emissions magnitude for various ammonia source categories. The ammonia inventory is to be developed at a spatial resolution of 1-km by 1-km with a temporal resolution of 1-hour. The geographic extent of the gridded inventory will cover the SJV study area (see Figure 1), although where feasible, data will be collected for the entire state of California. In addition, another objective of the project is to develop a standard input data library and processing procedures in order to facilitate future in-house refinements or revisions to the inventory in a programmatic way.

A secondary goal of the study is the development of an ammonia-capable GIS-based emissions modeling system. For many ammonia emission source categories, emission estimates are intimately linked to land cover/land use (LULC) characteristics and environmental variables. Hence, an emissions model which combines the GIS data on LULC distributions with LULC specific emission factors to calculate gridded emissions in a single processing step would be ideal. In addition, the increased efficiency with which the inventory is generated within the GIS-based emissions model will facilitate future updates and revisions with minimal processing effort. A focus of this paper is on important SJV ammonia source categories where GIS-based emissions modeling can play an important role in improving emissions estimates and spatial and temporal resolution.

METHODS

Source Category Prioritization

Through an extensive review of existing ammonia emission inventories, relevant literature and data sources, and information from ongoing studies, the most promising processing methodologies and data sources have been identified for use in the development of a gridded ammonia emission inventory for the SJV study area. Since all of the relevant data needed to quantify the relative contribution of each source category in the complete emission inventory has either not yet been collected or is not yet available, a source category prioritization based on emissions magnitude is not yet possible. Table 1 summarizes the methodologies and sources of emissions/activity data, and temporal and spatial allocation proposed for important source categories in the SJV. The table entries are ordered as to reflect our understanding of the relative importance of each source category as well as to reflect the importance of each emission source with respect to potential improvements that may be realized.

Finally, it should be noted that there are several common sources of temporal and spatial allocation data that have been used in the past for the development of emission inventories. These include the default temporal allocation profiles used in common emission models such as EPS2.0, EMS-95 and SMOKE, as well as the standard U.S. Geological Survey (USGS) LULC databases derived from 1:100,000 scale (~200 meter resolution) LULC data. However, for the prioritized emission source categories presented in Table 1, we do not believe that any of these do a very good job of allocation, and therefore alternate methods and data sources are described in subsequent sections of this paper.

Methods for Improving Emission Estimates for Significant Source Categories

Fertilizer Application

Significant agricultural activity, including a wide variety of crops and livestock, occurs in the SJV. The primary objectives for this source category are to better spatially and temporally allocate the emissions. We are also evaluating new emissions data (i.e., emission factors) as they are made available from the Potter et al study[1], as well as any new information found in the literature search conducted during this project. We will default to the use of the existing emission factors[2], as needed.

The primary source of information for activity data and spatial allocation will be the GIS shape files produced by Potter et al[1.] These data should be available in the Spring of 2001. We have developed a set of CARB Emission Inventory Classification (EIC) codes specific to primary crop types. The proposed classification scheme is shown in Table 2.

The advantages of having the fertilizer application loss emissions disaggregated as shown in Table 2 include:

1) the ability to incorporate new emissions data (i.e., emission factors) which may be crop-specific;
2) the ability to allocate emissions temporally based on fertilizer application schedules, specific to different crop types (as described below);
3) the availability of crop-specific spatial coverages with the high level of spatial resolution needed for this study[1].

Another source of information relative to both activity (mass of fertilizer applied per acre) and temporal allocation is a study being conducted for the California Department of Food and Agriculture (CDFA). This study is expected to be completed by the end of Spring 2001 and is referred to as a crop calendar for the SJV. This study will provide information on the timings of fertilizer application to major crop types in the SJV. The study should also provide information on the amounts and possibly types of fertilizer applied.

We will evaluate application schedule information from the CDFA study and other ongoing work in order to develop temporal allocation factors for each crop type. This information will be combined with data collected during a literature search to develop temporal allocation to at least the monthly level. If sufficient data are found to justify a higher level of temporal resolution (e.g., down to specified weeks of the year), then these factors will be developed.

Another source of information for both temporal and spatial allocation will be surveys that we will conduct to fill in any data gaps found in the information sources described above. These surveys will be conducted with both county agricultural offices and university researchers.

The final source of activity data are fertilizer sales statistics from the CDFA. These are the same data used in the existing SJV inventory (and EPA's national inventory) with the emission factors from Battye et al.[2] Reports of fertilizer sales (over 100 tons) by county are issued twice per year. The entire state is covered. It is not clear how well fertilizer sales data represent actual application, however. Given the availability of the other data sources mentioned above that can be used to estimate fertilizer application from the bottom up, the sales data will likely be used to perform a quality assurance (QA) check (e.g., by comparing annual sales in the domain to the estimated mass of fertilizer applied that was calculated from the bottom up). Potter et al conducted such a QA check on fertilizer usage in California[1]. At a regional level (e.g., the SJV), the analysis showed good agreement (see Table 3). However, significant differences exist at the county level, which indicate that an allocation of emissions to the county level via fertilizer sales data may provide poor spatial allocation for use in photochemical modeling.

An example GIS crop coverage is shown in Figure 2. A primary objective of this project is to incorporate these data (from the California Department of Water Resources) into a GIS-based emissions modeling system. Such a system is described later in this paper. The important issue to note here is the significant increase in the accuracy of spatial allocation achievable through the use of refined GIS data. Combined with the information

noted above on fertilizer application schedules by crop type and emissions data, emission estimates that with a high spatial and temporal resolution will be developed. For comparison, in modeling inventories, county-level fertilizer application emission estimates (based on sales data) have typically been allocated to a single land use coverage (e.g., agricultural crops).

Agricultural and Natural Soil/Plant Canopy Systems

The primary objective here is to determine whether emissions from natural soils should continue to be included in the inventory. Secondary objectives include determining what adjustments should be made to the emission estimating methods and temporal/spatial allocation.

It is highly uncertain whether natural soils (treated here as a part of soil/plant canopy systems) are net emission sources over annual time frames. Studies conducted in Europe have shown that the systems studied can be net sources or net sinks of ammonia. This issue is complicated by the interactions of ammonia within the soil/plant canopy system, and should not be simplified by only considering emissions from the soil surface. For example, depending on the system, the plant canopy can take up gaseous ammonia directly.

Given the contribution of emissions from this category, it is important to determine whether the state of the science supports the modeling of various systems as net sources. For example, it could be that some systems are sources only during certain seasons (e.g., when no plant canopy exists). Objectives of this project will be to determine where there is sufficient weight of scientific evidence to treat a system as a net source of ammonia and under what conditions (e.g., seasons). Table 4 presents a suggested source categorization scheme for soil/plant canopy systems. By treating each system separately, future refinements to the inventory will be easier to make (e.g., plugging in new emission factors, adjusting temporal allocation factors).

Biomass Burning (Prescribed Burning/Wildfires, Agricultural Burning, and Residential Burning)

Each of these categories could be significant during certain episodes (e.g., wildfires in summer, agricultural burning in the fall). Emissions data are lacking for ammonia from this category, which explains their absence from the current SJV inventory. Work done by researchers in the early 1990's on wildfires reported NH_3 to NO_x ratios of 5:1 using remote sensing methods[3]. We are assessing the available literature to determine the feasibility of estimating ammonia emissions for the biomass burning categories with the use of emission ratios. We will also incorporate the results of other ongoing studies in California, as they are available during the study period. These include the development of an agricultural burn permit database covering portions of the modeling domain, a survey of residential wood burning, and a GIS-based inventory for wildfires and prescribed burns. The GIS crop coverages described above for fertilizer application serve as valuable input to the development of emission estimates for agricultural burning.

Livestock

We will focus attention on improving the spatial and temporal allocation of livestock emissions. In the SJV, cattle (both dairy and beef) and poultry operations are significant contributors of ammonia emissions.

One of the primary sources of information on emission rates for dairy cattle will be an analysis performed during the development of the South Coast Air Quality Management District's (SCAQMD's) ammonia inventory[4]. Although this analysis was conducted for the South Coast Air Basin (SCAB), it includes an analysis of data from throughout California and around the world. We will consult with the California Cattleman's Association and the Western Dairy Association to assess any differences in management practices between operations in the SJV and SCAB, which could affect ammonia emissions.

Theoretical models to temporally allocate dairy and beef cattle emissions are being reviewed. These models use environmental variables (e.g., temperature, wind speed, relative humidity) to estimate hourly and

seasonal emission rates. Current inventories generally allocate emissions evenly throughout the day and year. Other temporal variations may occur because of management practices regarding manure removal, feed cycles and seasonal population fluctuations.

For spatial allocation, we will pursue data from California Cattleman's Association, Western Dairy Association, local Regional Water Quality Control Boards (RWQCBs), county vector control offices and/or county health departments, and the Department of Water Resources land use database. We will identify as many dairy facilities, with populations, as possible, filling in data from multiple data sources, as required. These facilities will be distributed as point sources. If spatial location data is not available from the relevant data source it will be determined by geo-coding the facility address. We will focus on identifying the largest facilities, especially large poultry facilities, in order to pinpoint the majority of these emissions. The balance of the livestock populations will be treated as area sources and assigned to appropriate land use coverages.

Other Significant Categories

Additional refinement to the SJV inventory will be made for emissions from publicly-owned treatment works (POTWs) and composting operations. We will identify a preliminary list of POTWs from the California State Water Resources Control Board (SWRCB) database of waste dischargers. Because past researchers have noted that not all POTWs are listed on the SWRCB database, we will contact local sanitation districts within the study area to identify any additional facilities. We will survey POTWs within the SJV to determine the extent to which sludge drying occurs at the facilities or off-site and to determine flow rates if not available from the SWRCB database. Emission rates will be assigned specific to sludge drying for those facilities where sludge drying occurs. Emissions data for sludge drying and waste water treatment will be taken from previous studies conducted in the SJV and SCAB. The activity data (i.e., flow rates) will be taken from the SWRCB database or telephone survey for other facilities in the SJV. Facility addresses will be geo-coded and the emissions allocated as point sources.

We have reviewed the Solid Waste Information System (SWIS) database of the California Integrated Waste Management Board to determine the extent of current composting operations in the San Joaquin Valley and throughout the State. The database includes almost 200 composting facilities statewide. The database does not contain the relevant activity data (amount of waste composted) to develop ammonia emissions estimates for significant portion of these facilities. We will attempt to fill the data gaps via a telephone survey facilities within the SJV. Emission factors developed for the SCAQMD from source tests of facilities composting several different waste types will be used to estimate emissions[5].

Composting emissions will be allocated as point sources based on the latitude/longitude information from the SWIS database. Known emissions information from composting operations is insufficient to develop a temporal profile for this source category.

Ammonia Emissions Model Development

The need for a separate area source emissions model depends upon the amount of detail to be included in the emission relationships. In the simple case where ammonia emissions are estimated from land area multiplied by an emission factor, there is no need for a separate model because: (1) the calculation is simple to accomplish within the GIS (e.g., ARC/Info); and (2) since there are no day specific effects on emissions the calculation need only be performed once.

This simple approach neglects environmental impacts (e.g., temperature dependence, seasonal dependence) on ammonia emissions. Incorporating environmental effects is a superior approach provided that information on environmental effects is available. One result is likely to be a need to prepare day specific inventories (similar to biogenic emissions modeling) which means that the emissions calculation must be repeated several times and efficiency becomes important. This suggests a different calculation approach, similar

to that used in biogenic emissions preparation. Under this approach, the landcover data are pre-processed using GIS into a gridded landcover database. This operation need only be performed once. An emissions model then combines the gridded landcover data with the emission factors and makes adjustments to account for environmental effects. There are several advantages to this approach:

- Improved efficiency because the landcover data are gridded only once;
- Improved efficiency because emissions calculations are performed at the resolution of the modeling grid, which is generally lower than the resolution of the raw landcover data; and
- Improved usability because the emissions modeling step is separated from the GIS processing, therefore expensive GIS software is not required to prepare new emission inventories.

A prototype emissions modeling system of this type already exists in the GLOBEIS model. GLOBEIS, the Global Biosphere Emissions and Interactions System, was developed for modeling biogenic VOC and NO_x emissions, but also includes ammonia. The ammonia emission algorithms in the current version of GLOBEIS are very simple and so improvements will be required for this study. The development of GLOBEIS is described in Yarwood et al[6]. The GLOBEIS model runs under Microsoft Access® on Windows based personal computers. The main input data for GLOBEIS are:

- GIS data on gridded LULC distributions;
- Plant species distributions for each LULC category (internal data table);
- Emission factors by plant species (internal data table);
- Gridded environmental data (temperature, solar radiation or cloud cover); and
- Seasonal biomass adjustments (satellite data based).

Data processing tasks for GLOBEIS have been divided to make the best use of the capabilities of GIS and database software tools. The LULC data for GLOBEIS are prepared using GIS tools such as ARC/Info or ARCView. This data preparation step is a straightforward application for the GIS software. The emission calculations are performed in GLOBEIS, which is based on the Microsoft Access® database, because this step is essentially a data synthesis and cross-referencing application and is well suited to a modern database program like Access®. The reporting capabilities available within Access also provide strong QA/QC capabilities to be built into GLOBEIS. The system is easy to maintain and upgrade because it is based on widely used software tools.

A significant advantage of GLOBEIS is the ease with which an emission inventory can be regenerated with alternate assumptions. For example, all of the emission factor data are readily accessible in data tables within the model, so an alternate emission factor can be used and the inventory regenerated in a single step.

The output from GLOBEIS includes a gridded, temporally allocated, speciated emissions file ready for use in photochemical modeling. An example emission inventory for the Houston area is shown in Figure 3. This figure demonstrates the ability of a GIS based system (like GLOBEIS) to accurately resolve areas of high and low emissions density without introducing artifacts related to geopolitical boundaries.

GLOBEIS was designed as a biogenic emissions processing system but support for ammonia was built into the model. Several simple improvements to GLOBEIS are anticipated to allow maximum use of available ammonia emissions information and improve the efficiency of the system for processing ammonia emissions.

- Switch to turn off the biogenic emissions calculations if they are not being used. This would reduce unnecessary computational and data requirements;
- Add the ability to specify seasonal and temporal profiles by source category; and
- Add environmental relationships between ammonia emission factor and environmental factors (e.g., dependence on temperature) to provide day specific emissions. This would be analogous to the current built-in emission relationships between isoprene emission factors and sunlight/temperature. GLOBEIS already reads gridded hourly temperature and radiation data, and other environmental data inputs can be added if needed.

RESULTS

This work is currently ongoing. The draft ammonia inventory is scheduled to be completed by March of 2002. Data to be used in developing the inventory is scheduled to be completed by September of 2001.

CONCLUSIONS

Although it is too early to draw conclusions for this ongoing study, we anticipate that the results of the work will be the most highly-resolved ammonia inventory produced for regional PM modeling. For others interested in developing ammonia inventories for regional modeling purposes, we suggest the adoption of similar approaches to those described above. In particular, for areas where high contributions of ammonia emissions come from agricultural crops, identification or development of detailed GIS crop coverages is extremely important. Not only do these GIS data serve as a basis for the refinement of ammonia emissions for fertilizer application, but also ammonia emissions from crop soil/plant canopy systems, ammonia and other pollutant emissions from agricultural burning, biogenic VOC emissions, and PM emissions from agricultural tilling and harvesting practices.

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KEYWORDS

ammonia
emission inventories
area sources

Table 1. Important source categories and associated inventory parameters being revised in this project.

Source Category	Emissions/Activity	Temporal Allocation	Spatial Allocation
Fertilizer Application	Incorporate new emissions data from recent studies in the SJV. Use detailed crop land cover data to scale up the inventory.	Monthly – via incorporation of crop calendars developed for the SJV.	Allocate to specific crop coverages developed for the SJV.
Livestock	Emissions data from recent studies in the SJV and South Coast Air Basin. For cattle, incorporate methods to differentiate confined and unconfined operations. Activity data from Calif. Cattlemens Assoc., Western Dairymans Assoc., USDA; Regional Water Quality Control Boards; American Horse Council Foundation	Diurnal based on Wilkinson et al. and James et al. Seasonally - as data exist to support to these factors.	Geocode large confined operations (dairies, feedlots, poultry operations). Remaining populations to existing LU/LC data.
Natural Soils/Plant Canopies	Primary objective is to determine whether the existing scientific evidence supports the use of the existing emission factors.	Seasonally - as data exist to support these factors.	To existing land use/land cover data (e.g., DWR, USGS).
Agricultural Burning	Use emission ratios of NH_3 to either NO_x or CO from biomass burning studies in Europe and the U.S. Activity data from recent surveys of local agricultural extension offices.	Monthly – using the activity calendar developed by Fife and/or the Team.	Allocate using the same shape crop coverages developed above for fertilizer application.
Prescribed Burning/Wildfires	Use biomass burning emission ratios as mentioned above for agricultural burning. Activity data from the U.S.F.S. and CA state agencies.	Monthly - as data exist to support these factors.	Coverages developed from CDFFP and NIFC data
Residential Burning	Estimates based on EPA's EIIP alternative methods using data from Energy Information Administration's State Energy Data Report and Residential Energy Consumption Survey; other source to be determined through further literature reviews	Seasonally - as data exist to support these factors.	Residential land use/land cover and Census data
On-Road Mobile Sources	Apply a ratio of NH_3 emissions to direct PM emissions in a gridded inventory for the study area. Update the emissions to calendar year 2000, as needed with VMT growth factors.	Allocate based on the underlying gridded mobile source inventory (e.g., CCOS).	Allocated base on the underlying gridded mobile source inventory (e.g., CCOS).
Industrial sources	Emission factor data developed for SCAQMD by ATC; Activity data from major ammonia suppliers in the state.	Existing default temporal allocation for industrial sources.	Zip Code coverages
Sewage Treatment Plants	Emission and activity data from SWRCB database; local surveys of POTWs.	Existing default temporal allocation for industrial sources.	Point
Composting	Emissions data from Solid Waste Information System database, if available; emission factors developed for SCAQMD inventory.	Existing default temporal allocation for industrial sources.	Point

Table 2. Suggested emission inventory codes (EIC) for fertilizer application.

EIC Description[1]	EIC
Existing Code	
Misc. Agricultural Losses	420-418-6000-0000
Proposed Codes	
Fertilization Losses – Grain and Hay	420-418-6001-0001
Fertilization Losses – Truck Crops	420-418-6001-0002
Fertilization Losses – Citrus	420-418-6001-0003
Fertilization Losses – Rice	420-418-6001-0004
Fertilization Losses – Pasture	420-418-6001-0005
Fertilization Losses – Vineyards	420-418-6001-0006
Fertilization Losses – Deciduous Fruit and Nuts	420-418-6001-0007
Fertilization Losses – Field Crops	420-418-6001-0008

[1] Crop names and number of categories taken from Potter et al.[1]

Table 3. Comparison of county-level fertilizer usage based on sales data versus a bottom-up approach.

County	Fertilizer Usage (metric tons)		% Difference
	CDFA Sales (1999)	Bottom-up Method	
San Joaquin	77,701	25,360	**67**
Stanislaus	16,169	15,233	**6**
Madera	4,540	10,835	**-139**
Merced	17,008	22,782	**-34**
Fresno	47,546	60,625	**-28**
Kern	41,296	41,108	**0**
King	22,983	26,420	**-15**
Tulare	20,144	31,877	**-58**
San Joaquin Valley Total	**247,386**	**234,240**	**5**

Source - preliminary draft information from Potter et al.[1]

Table 4. Suggested source classification for soil/plant canopy systems.

EIC Description[1]	EIC
Existing Codes	
Agricultural Biogenics – Day Time	910-910-0250-0001
Agricultural Biogenics – Night Time	910-910-0250-0002
Non-Agricultural Biogenics – Vegetative	910-912-0250-0000
Proposed Codes	
Soil/Plant Canopy Systems – Cropland and Semi-Agricultural Land	910-910-0250-0010
Soil/Plant Canopy Systems – Evergreen Needleleaf Forest	910-912-0250-0010
Soil/Plant Canopy Systems – Mixed Forest	910-912-0250-0011
Soil/Plant Canopy Systems – Open Shrubland and Desert	910-912-0250-0012
Soil/Plant Canopy Systems – Grassland	910-912-0250-0013
Soil/Plant Canopy Systems – Bare Soil	910-912-0250-0014
Soil/Plant Canopy Systems – Deciduous Broadleaf Forest	910-912-0250-0015
Soil/Plant Canopy Systems – Woodlands/Wooded Grasslands	910-912-0250-0016

[1] System names and number of categories taken from Potter et al.[1]

Figure 1. The CRPAQS modeling domain.

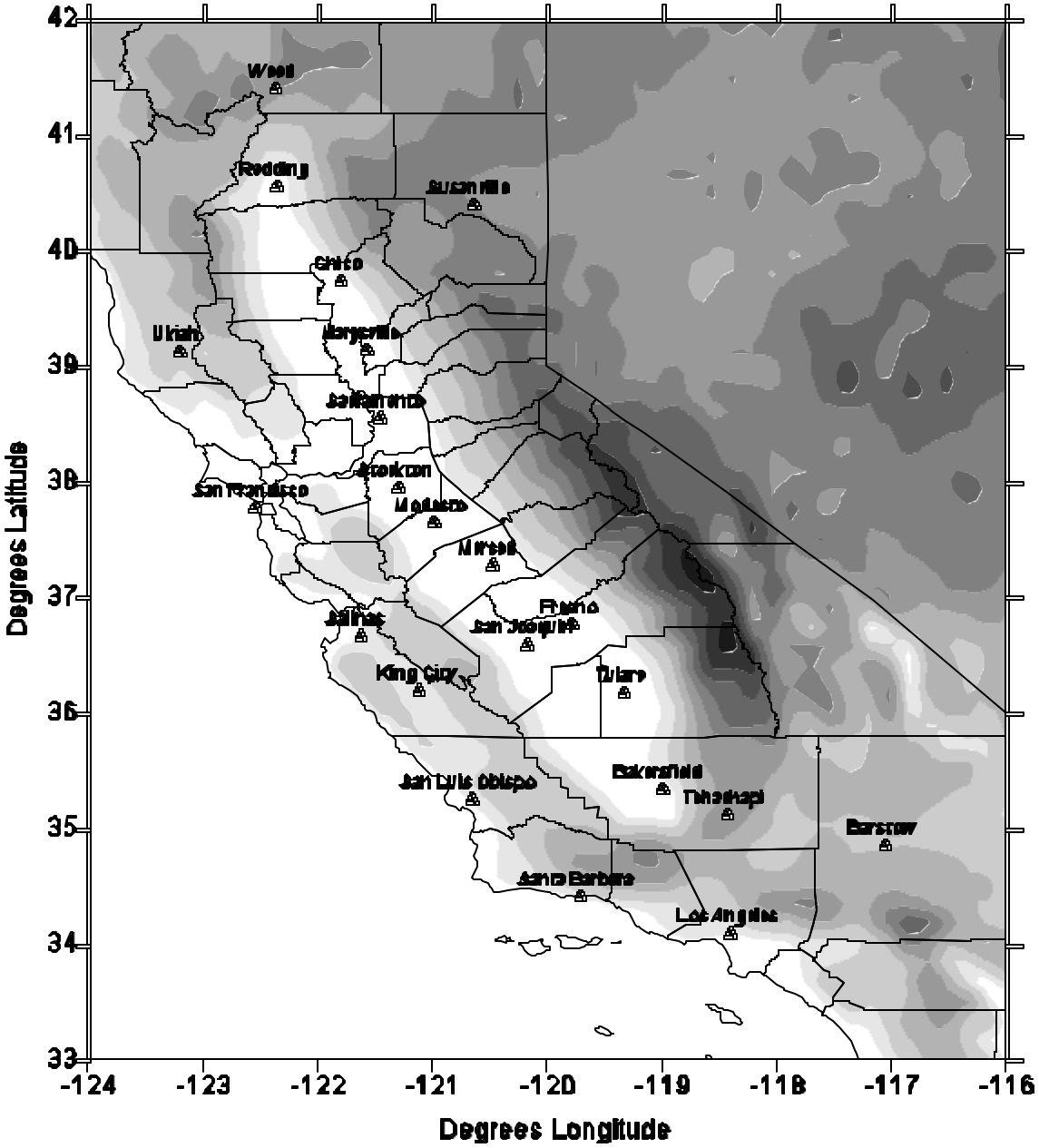

Figure 2. Crop coverages for Kern County from the California Department of Water Resources.

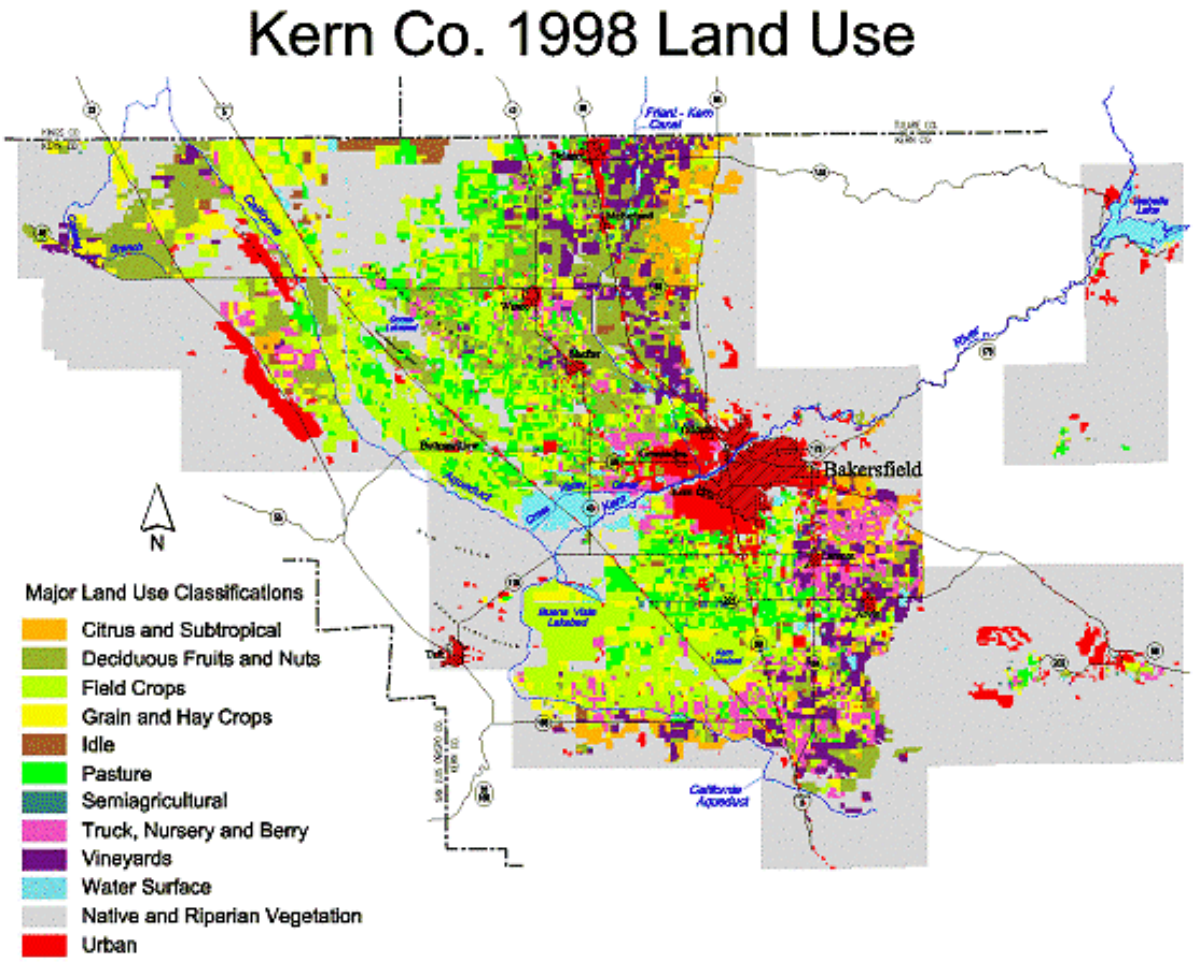

Figure 3. Isoprene emission inventory for the Houston area prepared with GLOBEIS.