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NRMRL QUALITY ASSURANCE PROJECT PLAN

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National Risk Management Research Laboratory (NRMRL)
Air Energy and Management Division (AEMD)
Energy and Natural Systems Branch (ENSB)
Distributed Source and Buildings Branch (DSBB)

Development of Emission Estimating Methodologies for Air Emissions from Animal Feeding Operations

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Distribution List

Copies of this plan and all revisions will be sent initially to the following individuals. It is the responsibility of the EPA/NRMRL/AEMD's Technical Lead Person to make copies of the plan available to all project personnel.

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Acknowledgments and Disclaimers

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Acronyms and Abbreviations

AEMD	Air and Energy Management Division (within EPA)
AFO	animal feeding operation
ATM	atmosphere(s)
β_0	intercept
β_k	regression coefficient
BLS	Backwards Lagrangian Stochastic
CAA	Clean Air Act
CERCLA	Comprehensive Environmental Response, Compensation and Liability Act
CORE	Central Operations and Resources (within EPA)
DC	direct current
DSBB	Distributed Source & Buildings Branch (within EPA)
ε	error term
EEM	emission estimating methodology
ENSB	Energy & Natural Systems Branch (within EPA)
EPA	United States Environmental Protection Agency
EPCRA	Emergency Planning and Community Right-To-Know Act
ES&P	emission source & pollutant
FAC2	fraction of predicted values within a factor of 2 of observations
FB	fractional bias
ft^3	cubic feet
ft/sec	feet per second
gal	gallon(s)
HAP	hazardous air pollutant
H_2S	hydrogen sulfide
IFSM	Integrated Farm System Model
kg	kilogram(s)
kPA	kilopascal(s)
lb	pound(s)
m	meter(s)
MB	mean bias
M&DQ QAPP	measurement and data quality assurance project plan
ME	mean error
MG	geometric mean bias
mg/g	milligram(s) per gallon

AEMD	Air and Energy Management Division (within EPA)
mg/l	milligram(s)m per liter
min	minute
MSA	manure surface area
MV	mechanically ventilated
mv	millivolt(s)
N	nitrogen
n	number
NAEMS	National Air Emissions Monitoring Study
NAS	National Academy of Sciences
NH_3	ammonia
NH_4^+	ammonium
NMB	normalized mean bias
NME	normalized mean error
NMSE	normalized mean square error
NRG	Natural Resources Group (within EPA)
NRMSE	normalized root mean square error
NO_2^-	nitrite
NO_3^-	nitrate
NRMRL	National Risk Management Research Laboratory (within EPA)
NV	naturally ventilated
OAQPS	Office of Air Quality Planning & Standards (within EPA)
OAR	Office of Air and Radiation (within EPA)
ORAU	Oak Ridge Associated Universities (contractor)
ORD	Office of Research & Development (within EPA)
P	phosphorous
pH	Measure of hydrogen ion concentration
PI	principal investigator (of study)
PM	particulate matter
$PM_{2.5}$	particulate matter, with a diameter less than or equal to 2.5 micrometers
PM_{10}	particulate matter, with a diameter less than or equal to 10 micrometers
QA	quality assurance
QAPP	Quality Assurance Project Plan
QA/QC	quality assurance/quality control
RMSE	root mean square error

AEMD	Air and Energy Management Division (within EPA)
S	sulfur
SAB	Science Advisory Board
SAS	Statistical Analysis Software
SPPD	Sector Policies and Programs Division (within EPA)
temp	temperature
TKN	total Kjeldahl nitrogen
TLP	technical lead person
TSP	total suspended particulates
USDA	United States Department of Agriculture
VG	geometric variance
VOC	volatile organic compound
VRPM	Vertical Radial Plume Mapping model
Wt.%	weight percentage
W/m^2	watt(s) per meter squared
X_k	independent or predictor variables
Y	dependent variable
%	percentage
°	cardinal directions; degrees of a compass
°C	degrees Celsius

1.0 Project Description and Objectives

1.1 Background

Animal feeding operations (AFOs) are agricultural operations where animals are kept and raised in confined areas (U.S. Environmental Protection Agency (EPA), 2017a). For over six decades, there have been movements to improve profitability within animal agriculture, resulting in fewer, but larger AFOs that are also more geographically concentrated. For example, a study by Graham and Nachman (2010) determined that since the 1950's, production of livestock and poultry have more than doubled, while the number of operations had decreased by 80%. In a recent report, the EPA estimated using U.S. Department of Agriculture (USDA) 2007 census data that there were approximately 2.2 billion livestock and poultry producing an estimated 1.1 billion tons of manure in the United States (U.S. EPA, 2013). AFOs and the associated manure emit various pollutants into the atmosphere including ammonia (NH_3), hydrogen sulfide (H_2S), volatile organic compounds (VOCs) and particulate matter (PM) (Aneja et al., 2008). Thus, there are concerns regarding these facilities due to the potential impact these compounds can have on human health and the environment.

AFOs can directly emit a significant amount of PM into the atmosphere (Takai et al. 1998). Emissions of NH_3 from AFOs can also lead to the formation of secondary PM. Atmospheric NH_3 is the dominant alkaline gas in the atmosphere and reacts with a variety of acidic atmospheric species (i.e. sulfuric, nitric and hydrochloric acid) to form ammonium (NH_4^+) PM (Seinfield and Pandis, 2006). As a particle, the NH_4^+ aerosol impacts atmospheric visibility (Seinfield and Pandis, 2006). The NH_4^+ particle also contributes a significant fraction of total $PM_{2.5}$ mass (Adams et al., 1999). The inhalation of $PM_{2.5}$ can have a number of adverse health effects including premature mortality (Pope et al., 2002). Gaseous NH_3 and NH_4^+ PM are removed through wet and dry deposition to the earth's surface, which may result in the eutrophication of terrestrial and aquatic ecosystems (Galloway, 2003). Gaseous H_2S can contribute to the formation of $PM_{2.5}$, although its primary effect is related to its odor, and has an odor characteristic described as "rotten eggs" (Schiffman et al., 2001). In addition, some VOCs are also odorous. Emissions of odorous compounds can impact people who live nearby, as they can potentially affect human health (Schiffman and Williams, 2005) and quality of life (Wing and Wolf, 2000). Additionally, many VOCs are classified as hazardous air pollutants (HAPs). HAPs are described by the EPA as "pollutants that are known or suspected to cause cancer or other serious health effects such as reproductive effects or birth defects, or adverse environmental effects" (U.S. EPA, 2017b). VOC emissions can also have regional effects. VOCs are generally reactive, and can, through a set of reactions, form ozone. Ozone can have negative impacts on the human respiratory system, and is associated with mortality (Ito et al., 2005).

Air emissions from AFOs are not regulated by any AFO specific standards within the Clean Air Act (CAA), but AFOs could emit air pollutants in sufficient quantity to trigger certain general CAA permit requirements or emission reporting requirements under two other statutes: (1) Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) and (2) Emergency Planning and Community Right-to-Know Act (EPCRA). Both CAA permitting requirements and emission reporting requirements are triggered only if a facility produces emissions over certain regulatory thresholds. In the late 1990's, the EPA recognized that they did not have adequate air emissions data from AFOs to develop reliable emission estimating methodologies (EEMs) for determining whether individual farms are subject to CAA permit requirements or emission reporting requirements (U.S. EPA, 2017c). This lack of sufficient AFO data is partly related to the difficulty in characterizing air emissions, as there is a diversity in production, management and environmental conditions at AFO sites. In 2001, the EPA and the USDA asked the National Academy of Sciences (NAS) to evaluate the current state of the science and provide recommendations on estimating air emissions from AFOs. In their 2003 seminal report (NAS National Research Council, 2003), NAS made several recommendations including a recommendation that the "EPA and USDA should initiate and conduct a coordinated research program to produce a scientifically sound basis for measuring and estimating air emissions from AFOs". Subsequently, in 2005, a voluntary Air Compliance Agreement between the EPA and the animal industries was announced. In this agreement, the industry agreed to fund a large-scale emissions monitoring study known as the National Air Emissions Monitoring Study (NAEMS). Furthermore, as part of the Air Compliance Agreement, the EPA was to use the NAEMS emissions data and other relevant data sources to develop EEMs, while the AFO industry participants agreed to use these EEMs to estimate their emissions for purposes of complying with applicable CERCLA and EPCRA reporting requirements.

The NAEMS is the most comprehensive AFO air pollution monitoring study to date, measuring emissions from representative broiler, layer, swine and dairy AFOs in the U.S. over a monitoring period of two years. The NAEMS measured emissions of NH_3, H_2S, VOCs, and PM at 27 monitoring sites. While making emission measurements, production, management and environment conditions were also monitored and/or documented.

Air monitoring for the NAEMS began in 2007 and ended in early 2010 with the data submitted to EPA by August 2010. After organizing, documenting and analyzing the data, two draft reports containing draft EEMs for NH_3, H_2S, VOC, and PM emissions from broiler houses and NH_3 emissions from swine and dairy lagoon/basins were developed. In February 2012, the EPA submitted these draft reports to the Science Advisory Board (SAB) for review and for their recommendations, which were returned to the EPA in April 2013. The SAB identified several concerns with the draft EEMs and recommended that the EEMs should not be used to estimate air emissions from AFOs on a national scale.

Currently, per the Air Compliance Agreement, the EPA is still tasked with developing EEMs, which is the subject of this QAPP.

1.2 Project Objective

To develop EEMs for air emissions from AFOs using data from the NAEMS and other relevant data sources.

2.0 Project Organization and Responsibilities

2.1 Project Personnel

This work will be conducted under the EPA's continued effort to develop and implement approaches that can be used to quantify farm-by-farm emission estimates. Project personnel for this effort will include multiple individuals from EPA/ORD/NRMRL and EPA/OAR/OAQPS. The primary personnel are described here with organization connection details contained in Figure 1.

Ian Rumsey (ORD/ENSB) is the project coordinator and principal investigator (PI) for this study. He is responsible for communicating the overall project technical direction to EPA ORD contractor (ORAU), Chelsey Fattal, as well as to the other project coordinators and NAEMS-EEM supporting investigators. Chelsey Fattal (ORD/DSBB) will provide assistance in the modeling of air emissions from AFOs as well as providing support in other areas of the project. John Walker (ORD/ENSB) and Eben Thoma (ORD/DSBB) are the leads in providing technical support and guidance to this project, however, William Yelverton (ORD/ENSB Chief) and Richard Shores (ORD/DSBB Chief) will also provide technical support and guidance. John Walker, Eben Thoma, William Yelverton and Richard Shores will review the QAPP and provide comments. William Schrock (OAR/NRG) and Allison Costa (OAR/NRG) are co-lead project coordinators in OAQPS and will provide support and guidance to this project. William Yelverton and Richard Shores will also perform personnel management roles for ORD and will communicate appropriately with other ORD supervisors as required. Robin Dunkins (OAR/NRG) will provide guidance to this project, perform personnel management roles for OAR and will communicate appropriately with other OAR supervisors as required. William Schrock, Allison Costa and Robin Dunkins will review the QAPP and provide comments.

Libby Nessley (ORD/NRMRL) is the QA Manager and QA lead for this project for activities performed within NRMRL. Ms. Nessley will formally review and approve this QAPP per NRMRL requirements. As needed, Ms. Nessley will review and approve project reporting as part of EPA ORD’s publication clearance process to verify that the project was implemented as specified in this document. Joe Elkins (OAR/OAQPS) is the QA Manager for OAQPS. Mr. Elkins will formally review and approve this QAPP per OAQPS requirements.

2.2 Project Schedule

The overall effort for this project started in January 2017. Initial project tasks involved preparing and planning for EEM development, which included determining the status of the NAEMS data set and developing this QAPP for the development of EEMs for air emissions from AFOs. The draft QAPP was submitted in November 2017. It is currently unknown how much time will be spent developing EEMs for the various emission source and pollutant (ES&P) categories, however, the plan is to determine a schedule for EEMs development in consultation with our group members in OAQPS in the third quarter of FY 2018. A summary of the project timeline and the anticipated project schedule is as follows:

- 01/8/17-03/13/18: Project preparation and planning.
- 11/27/17: Draft QAPP submitted for QA review.
- 03/13/18: Final version of initial QAPP completed.
- 06/30/18: Determine EEMs schedule for ES&P categories.

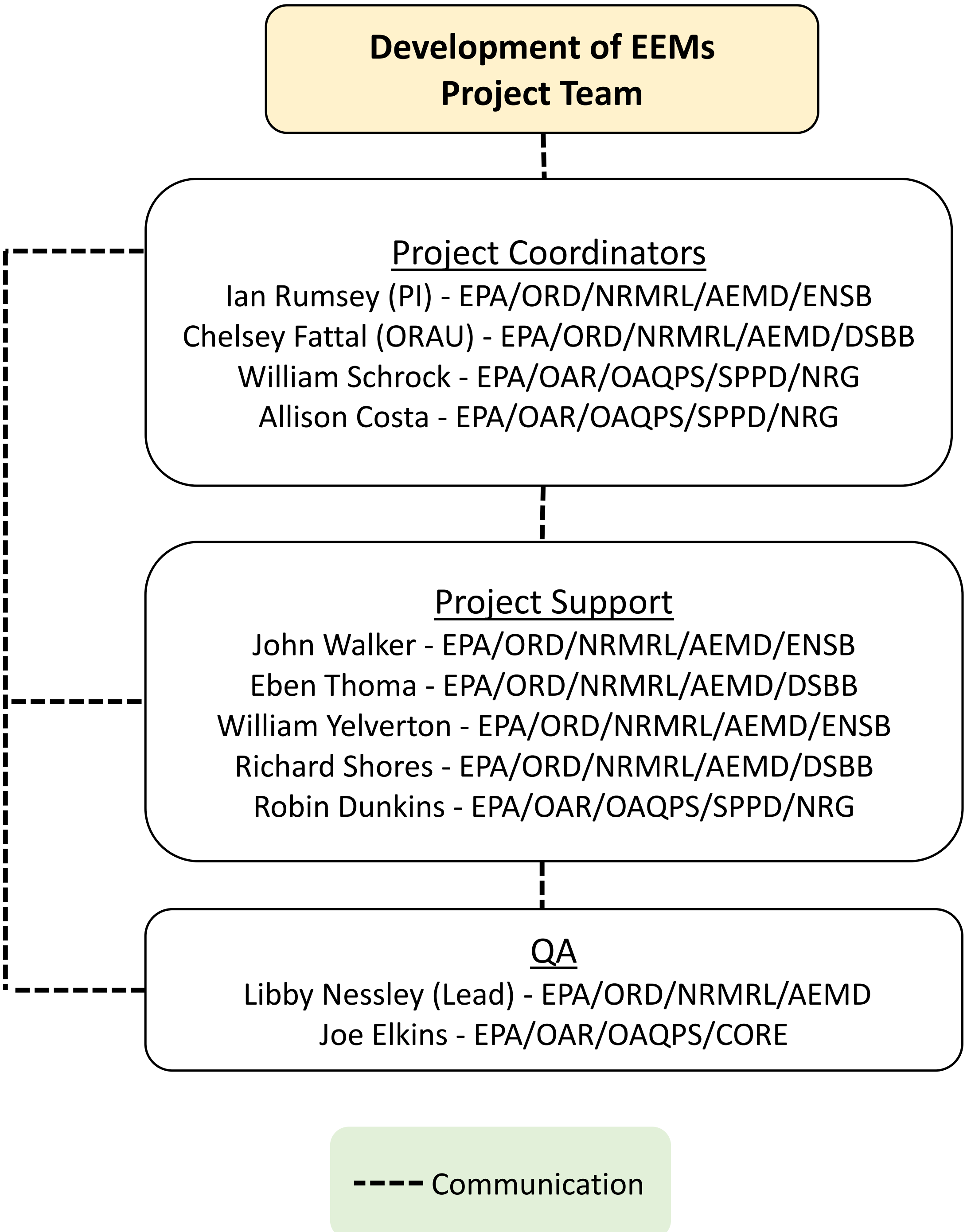

Figure 1. Organizational chart.

3.0 Emissions Database

3.1 Data Sources and Quality Metrics

EEMs will be developed using data from the NAEMS. The NAEMS data was collected under rigorous quality assurance/quality control (QA/QC) procedures that are outlined in the Measurement and Data Quality QAPPs (M&DQ QAPPs). Separate M&DQ QAPPs were developed for monitoring from barn and open/area sources associated with the project (Heber et al., 2008; Grant et al., 2008). The M&DQ QAPP was used to develop a NAEMS data set that was analyzed and used for 2012 draft EEM development reports, hereafter referred to as "2012 EEM reports". However, applying the data quality and validation procedures associated with the M&DQ QAPPs resulted in small open/area source data sets. In their review of the 2012 EEM reports, the SAB suggested two approaches that could be used to increase the amount of available data. These were to include the use of open/area source emissions determined by the Backwards Lagrangian Stochastic (BLS) method and revise the data completeness criteria. In this project, these SAB suggested changes to data quality procedures will be applied to the NAEMS dataset, thus producing a revised version of the NAEMS data set. Section 3.1.1 will discuss the rationale, methodology and application of these changes to the data quality procedures.

The potential need for additional non-NAEMS data in developing EEMs will be investigated if appropriate at a later stage of the project and addressed in a secondary data addendum to this QAPP.

3.1.1 Changes to data quality procedures

3.1.1.1 Inclusion of open/area source emissions determined by the BLS method

In the NAEMS, emissions for open/area sources could potentially have been determined using two different methodologies, the BLS method and the Vertical Radial Plume Mapping model (VRPM) method (both discussed in M&DQ QAPP (Grant et al. 2008)). However, open/area source emissions determined by the BLS method were not included in the initial NAEMS database as there were concerns with the validity of the measurement method. However, after the publication of the 2012 EEM reports, a validation study was reported by Grant et al. (2013a) (Dr. Richard Grant is the NAEMS PI for open/area sources). In the Grant et al. (2013a) study, NH_3 emissions, determined by both the BLS and VRPM methods were compared at eight NAEMS monitoring sites. In comparison, the overall BLS mean emission estimate was found to be 5% ± 25% lower than the VRPM method. Based on their findings, Grant et al. (2013a) concluded that that both the BLS and VPRM methods "can be assumed to equally represent the actual flux conditions for open waste lagoon sources". Therefore, for this project, emissions determined by the BLS method will be included in the database as suggested by the SAB, thus meaning that this project will develop EEMs using emission data determined by both the BLS and the VRPM method. The inclusion of emissions determined by the BLS method will increase the amount of data, as there were times when the BLS method produced valid emissions when the VPRM method did not. In periods, when both the BLS method and VRPM method determine valid emissions, an overall emission value will be determined based on the methodologies described in Grant et al. (2013a) and Grant et al. (2016).

3.1.1.2 Revision of the data completeness criteria

In general terms, the criteria for data completeness outlined in the M&DQ QAPPs (Heber et al. 2008; Grant et al. 2008) was to use data where ≥75% of the data was valid within a set time period, however, due to difficulties associated with open source micrometeorological measurements, this criterion resulted in a small number of valid emission days and thus limited open/area source daily data sets. As a result of the limited open/area source data sets, the SAB suggested expanding the data completeness criteria in order to increase the amount of valid data. This suggested change to data quality procedures was investigated in a recent study by Grant et al. (2013b). In the Grant et al. (2013b) study, the fraction of NH_3 emissions needed to determine an accurate daily average using NAEMS data from swine finishing and swine sow farms in Oklahoma was investigated. Using the statistical relationship between air temperature and NH_3 emissions, Grant et al. (2013b) determined that to have a daily emissions error of < 25%, at least 25 out of 48 (52%) 30-minute measurements needed to be valid (additional information on the methodology for determining daily emission error values is provided in Grant et al. (2013b)). Therefore, based on this study, the data completeness criteria for open/area source data for the updated NAEMS data set will be revised from 75% to 52%, thus meaning that daily emissions will be considered invalid if less than 52% (25) of the 48 30-minute periods recorded during that day were valid. This data quality procedure revision from 75% to 52% will increase the open/area source data set size.

It should be noted that the aforementioned M&DQ QAPP data completeness criteria value of 75% had less of an effect on the amount of valid barn emissions data. The potential need to revise this value for barn source emissions will be assessed at a later date, if appropriate.

3.2 Data Analysis, Interpretation and Management

3.2.1 Initial Data Analysis Techniques

Initial data analysis on the revised NAEMS data set (due to revisions discussed in the Section 3.1.1) will include time series analysis and composite hourly average analysis of pollutant emissions, concentrations, air flow (ventilation rate for barns and wind speed for open/area sources) and environmental parameters at each AFO site over each seasonal sampling period. In addition, summary statistics such as mean, maximum, minimum, median, standard deviation and number (of data points) values will be determined for pollutant emissions and environmental parameters over seasonal, annual and bi-annual time periods for each AFO. The animal diet (if available) and manure management practices at each AFO site will also be examined during the monitoring periods. This analysis allows a macro examination of trends in data and can be used to provide a qualitative guide to the influence of production, management and environmental conditions on emissions. This analysis can also be used to identify potential data trends that may need further investigation. This analysis may also help determine the number of EEMs that need to be developed since EEMs will be developed for different emission source categories and this analysis will help determine the appropriate emission source categories for this study (described in further detail in section 3.2.2). Progress in data analysis will be documented in informal reports (see section 7.1 for more details).

3.2.2 Determining ES&P Categories for EEM Development

Before EEM development, an initial determination of emission source categories for the NAEMS AFO sites will be completed. AFO emission source categories are typically developed where there is a significant difference in how AFO site conditions affect emission processes, however, determining when there is a significant difference in how conditions affect emissions processes can be complex and depends on the diversity of the conditions associated with each production type. AFO emission sources can be categorized by general production type (i.e. broiler, layer, dairy, swine) and general source type (i.e. barn, lagoon/basin, corral). However, within these categories, more specific determination of emission sources may be needed as differences in production type, manure management practices, and barn and manure storage type can significantly influence emission processes and thus emissions, meaning that additional emission source categories may potentially need to be developed. Table 1 presents the possible emission source categories for the NAEMS AFO sites. The first column determines the number of emission source categories based on general production type and the general source type with thick solid lines around each category, yielding seven emission source categories. The second column determines the number of emission source categories based on specific production type and specific source type that pertains to the additional differences in AFO site characteristics that may influence emission processes. These emission sources categories are indicated by dashed lines and yield thirteen emission source categories. While it is known that general production type and general source type (barn, lagoon/basin, corral) have a significant influence on emission processes and thus need separate EEMs, it is not known whether the differences in specific production type and specific source type (presented in the second column) have a significant influence on emission processes. The number of emission source categories will be initially investigated using the initial data analysis techniques described in section 3.2.1. However, the emission source categories might be revised during subsequent stages of EEM development as the influence of different site conditions are further investigated. Progress in determining emission source categories will be documented in informal reports (see section 7.1 for more details). There is currently no established criterion to determine whether an emission source warrants its own category. Any future criterion that is developed will likely consider data analysis, model characteristics and model performance, and will be decided in consultation with our project members in OAQPS, who will be responsible for approving the final report.

In terms of pollutants, there are six pollutant categories for barns including three gases NH_3, H_2S, VOCs and three sizes of PM, $PM_{2.5}$, PM_{10} and total suspended particulates (TSP). For open/area sources, there are also pollutant categories for NH_3, H_2S and VOCs, but not for PM, since PM emission measurements were not conducted at open/areas sources in the NAEMS as emissions from open/area sources are insignificant in comparison with barn emissions.

Table 1. Potential emission source categories for NAEMS AFO sites.

Emission Source Categories		
General Production Type/ General Source Type	**Specific Production Type[1]/ Specific Source Type**	**NAEMS AFO Site ID**
Broiler Barn source	Broiler Barn-MV	CA1B KY1B-1 KY1B-2
Layer Barn source	Layer High Rise Barn-MV	CA2B NC2B IN2H
	Layer Manure Belt Barn & Manure Shed-MV	IN2B
Dairy Barn source	Dairy Barn & Milking Center-MV	IN5B WI5B NY5B
	Dairy Barn-NV	CA5B WA5B
Dairy Corral Source	Dairy Corral	TX5A
Dairy Lagoon/Basin source	Dairy Lagoon	IN5A
	Dairy Basin	WI5A WA5A
Swine Barn source	Swine-Sow Gestation Barn & Farrowing room-MV	IA4B NC4B OK4B
	Swine-Finisher Barn-MV	IN3B NC3B
Swine Lagoon/Basin source	Swine-Sow Lagoon	IN4A NC4A OK4A
	Swine-Finisher Lagoon	NC3A OK3A
	Swine-Finisher Basin	IA3A

[1] Provided if applicable
MV = mechanically ventilated
NV = naturally ventilated

3.3 Data Storage

The data collected for NAEMS (discussed in sections 1.1 and 3.1) is stored using the Microsoft Access® software platform. The NAEMS database was originally developed by the Eastern Research Group under contract EP-W-12-006, Work Assignment 0-01. The database is designed to receive data submissions electronically to minimize the potential for errors introduced during data entry. The database can receive different types of data including MS excel files, text files and XML files. The NAEMS database is stored in its own designated folder on the L-drive (path:L:PRIV/NRML_AEMD/DROP/Ian Rumsey/NAEMS databases), which automatically backs up on a daily basis. The database folder will be private and will only be available to group members. The NAEMS database will contain database files for each emission source category. Database files will be stored with the version number and date in the file name. Any changes to the database files will result in creating a new version of the database with new version number (version numbering will be sequential) and appropriate date. The database folder will contain the current and all historical versions of the database.

4.0 Model Development

Broadly, there are two different types of methodologies or modeling approaches that can be used to estimate air emissions from AFOs. These are process modeling and statistical modeling. Process modeling can be defined as a "procedure by which the behavior of a system is derived from a set of functional components and their interactions with each other and the system environment through physical and mechanistic processes occurring over time." (Makela et al., 2000). As applied to this project, it means that air emissions would be estimated by using mathematical equations that describe the biological, chemical and physical processes involved in air emissions from AFOs. Statistical models are developed through statistical analysis of empirical data, which is then used to determine which factors (parameters) influence emissions and the relationship between the parameters and the emissions. From this, a statistical model is developed, which can be used to predict emissions at AFOs.

A general option available in regards to estimating emissions from AFOs is to use or modify and use a process or statistical model that has already been developed and is published in peer-reviewed journals. When selecting a model to use from literature, it is also important to consider the ease in which the models can be implemented to estimate emissions by the agricultural community, therefore the ease of implementation by the agricultural community will be evaluated for each model and will be taken into consideration when deciding if the models in these studies can be used or modified for use in EEM development in this current effort. Progress in evaluating the ease of model implementation by the agricultural community will be documented in informal reports (see section 7.1 for more details).

In selecting statistical models from literature for use, the priority is to use any statistical model that has been developed based on NAEMS data and that have been evaluated for its accuracy in predicting NAEMS emissions. An example of models in literature that fulfill this criterion are the statistical models developed by Grant et al. (2013b) and Grant et al. (2016). Grant et al. (2013b) and Grant et al. (2016) describe the development of statistical models using NAEMS data to predict NH_3 emissions from swine lagoons. In the Grant et al. (2013b) and Grant et al. (2016) studies, there are models of varying complexity, which are each evaluated for accuracy (see section 6.3 for model evaluation results for the Grant et al. (2013b) and Grant et al. (2016) studies). As mentioned, the ease of implementation by the agricultural community will also be evaluated for each model and will be taken into consideration when deciding if the models in these studies can be used or modified for use for EEM development in this current effort.

In selecting process models from literature for use, the priority is to use a process model that has accurately predicted NAEMS emissions based on NAEMS input data. An example of a model available in literature that fulfills this criterion is the dairy gas emission model, which is a process-based sub-model of the Integrated Farm System Model (IFSM) developed by USDA. In Rotz et al. (2014), the dairy gas emission model was used to estimate NH_3 emissions from NAEMS dairy barns and dairy manure storage structures. The Rotz et al. (2014) study also includes an evaluation of the accuracy of the process model in predicting NAEMS NH_3 emissions (see section 6.3 for model evaluation results for the Rotz et al. (2014) study). Similarly, the ease in which this model can be implemented by the agricultural community will be evaluated and will be taken into consideration when deciding if this model will be used or modified for use for EEM development in this current effort.

If for an emission source and pollutant category, there is no suitable model available in literature to use or use after modification, then the second option available is to develop new statistical models.

4.1 Development of New Statistical Models

4.1.1 Conceptual Model

Multivariable statistical models will be developed to estimate air emissions at AFOs. Multivariable statistical models can be defined as models that have two or more independent or predictor variables and one dependent or response variable. For this study, the dependent or response variable is emissions (for each ES&P category) and the independent or predictor variables are parameters that represent the varying conditions at an AFO. If the modeled emissions for an ES&P category are related to one predictor variable, then accordingly, a univariable statistical model will be developed.

Due to the wide variance in conditions at AFOs, developing EEMs is a complex process, therefore the first stage of EEM model development will use a focused approach to develop models based on factors (parameters) that satisfy the following conditions:

1. Known to have a major influence on air emissions from AFOs
2. Well monitored by the NAEMS
3. Can easily be monitored by the agricultural community

Some of the factors that satisfy the aforementioned conditions influence both gas and particulate emissions, while some only influence gas or particulate emissions. The reason for this differentiation is that many of the processes that generate gas and particulate emissions from AFOs are different. While gas emissions are related to the formation, generation, release and emission of chemical specie in gas form from manure, particulate emissions are caused by physical suspension (or release) of a range of different materials in barns including feed, manure, bedding, animal skin, and feathers (Cambra-Lopez et al., 2010) that are then emitted from the barn into the atmosphere.

Factors that satisfy the aforementioned conditions and influence both gas and particulate emissions include the amount of manure produced at an AFO. The amount of manure produced at an AFO is a function of the number and weight of animals at an AFO site, which therefore serves as a proxy for this factor. While the number of animals at an AFO is typically determined daily as part of the farming operation, weight is commonly estimated based on initial and final weights, which are typically recorded by the producers. The significance of the influence of animal number and weight on AFO air emissions is supported by the units used for reporting AFO emissions, which are typically reported either normalized for the number of animals or for live animal weight, which is the product of animal number and weight. The influence of both production terms will be investigated in the first stage of EEM model development for all ES&P categories. Manure surface area (MSA) is another factor that has a major influence on both gas and particulate emissions. Typically, a larger MSA results in increased emissions. The significance of this factor on manure storage is supported by lagoon emissions being typically reported in units normalized for surface area. Increased MSA in animal housing can increase emissions per animal (USDA, 2016), therefore this factor will also be investigated for barn EEM model development and thus all ES&P categories.

Gas emissions are additionally influenced by temperature as temperature affects chemical specie concentration in manure due to its influence on the decomposition of manure, the Henry's law constant and the dissociation constant. Gas emissions are also influenced by temperature due to its effect on the transfer of chemical compounds from manure into the free-air stream. The transfer occurs through two processes, diffusion, which transports chemicals through the manure to its surface and convective mass transfer, which transfers the gas from the manure surface into a free air stream (Ni, 1999). The process of diffusion is dependent on temperature (Ni, 1999) whereas the convective mass transfer is dependent on temperature and the air velocity above the manure surface (Ni, 1999 and references within; Montes et al., 2009 and references within). Increasing air velocity above the manure surface also reduces the boundary layer thickness above the manure surface, therefore lowering the resistance to volatilization (Arogo et al., 1999). The transfer rates through the manure and gas phases vary for different chemical specie and are governed by chemical specie solubility. The influence of temperature and air velocity will be investigated for all emission source and gas pollutant categories. For open/area sources AFO sites, these factors will be investigated using measurements of ambient temperature and wind speed. For barn sources, these factors will be investigated using ambient temperature and barn temperature and ventilation rate which are inter-related to ambient temperature. Ventilation rate also controls the air velocity across the manure surface in barns.

PM emissions are controlled by factors that influence the suspension of materials in the air. This process is influenced by the moisture content of the material. High moisture levels cause manure particles to aggregate together, meaning they have greater resistance to being suspended in the air. Manure moisture is influenced by temperature, relative humidity and ventilation rate as well as manure management practices. The influence of moisture content will be investigated for all barn source and PM categories using measurements of ambient temperature, barn temperature ventilation rate and ambient relative humidity.

As mentioned, statistical models will be developed to estimate air emissions at AFOs. For this method, the main goals will be to identify which parameters (that satisfy the conditions provided earlier in this section) have a significant influence (e.g. p-value) on pollutant emissions and also the relationship between the significant parameters and emissions. As mentioned, a focused approach is being used in the first stage of this study, meaning that the relationships between parameters and emissions will also be investigated by considering observed physical relationships between the parameters and emissions. Often the observed relationships between parameters and emission processes are non-linear, resulting in non-linear relationships between the parameters and emissions. An example of using the observed physical relationship between the parameter and emission processes to develop a model that predicts emissions is provided by Grant et al. (2016), in which statistical models were developed to predict NH_3 emissions at five NAEMS swine lagoon sites. In the Grant et al. (2016) study, models were developed that included the influence of air temperature on NH_3 emissions. In the models, Grant et al. (2016) related air temperature to NH_3 emissions using the Van't Hoff equation, which includes an exponential function to describe the influence of temperature. The Van't Hoff equation relates the changes of equilibrium constants such as the Henry's Law constant and the dissociation constant, which influence emissions due to the change in temperature.

The performance of these first stage statistical models will be evaluated and will serve as a guide to the level of sophistication needed in later stages of model development.

4.1.2 Model Parameters

Section 4.1.1 describes the parameters that will be investigated in the first stage of EEM development. A summary of these parameters and the associated main emission source category is provided in Table 2.

Table 2. Parameters to be investigated in the first stage of EEM development for each emission source category.

Main Emission Source Category	Parameters
Gas Open/area	n & weight of animals, MSA, ambient temp, wind speed
Gas Barn	n & weight of animals, MSA, ambient temp, barn temp, ventilation rate
PM Barn	n & weight of animals, MSA, ambient temp, barn temp, ventilation rate, ambient relative humidity

n = number
temp = temperature
MSA = manure surface area

After the first stage of EEM development, there may be additional statistical analysis conducted to determine if other parameters measured during the NAEMS have a significant influence on emissions. Model development and final model description will be documented in the informal reports (see section 7.1 for more details). A list of parameters measured during the NAEMS is provided in Table 3.

Table 3. Parameters measured during NAEMS for barns and lagoons (modified from 2012 draft EEM reports (U.S. EPA, 2012a; U.S. EPA 2012b)).

Parameter		Units
Barn Conditions	Temperature	°C
	Relative humidity	%
	Activity (personnel and livestock)	Volts DC
	Light operation	On/off
	Feeder operation	On/off
	Livestock heater operation	On/off
	Barn dimensions	m
	Ventilation rate	m^3/min
Meteorological Conditions	Ambient temperature	°C
	Ambient relative humidity	%
	Barometric/Atmospheric pressure	kPa/ATM
	Surface wetness	millivolts
	Solar radiation	Watts/m^2
	Wind speed	ft./sec
	Wind direction	Degrees
Manure Characteristics	Manure volume	Gal
	Manure loadout (Solids, N, NH_3, TKN, Ash)	Wt.%
	Layer/Surface manure (Solids, N, NH_3, TKN, Ash)	Wt.%
	Bedding / Litter (pH, Ash, NH_3, Solids, N)	Wt.%
Livestock Characteristics	Age	Days
	Livestock inventory/Mortality	n of animals
	Animal weight	Truck balance
	Average livestock mass	kg
Mass Balance Information	Feed consumption rate	lb
	Feed (Sulfur, Ash, Solids, TKN, N) content	mg/g
	Milk (TKN, N) & Eggs (Solids, N, TKN, Ash)	mg/g
	Water consumption	gal
	Incoming/new bedding addition rate	lb
	Incoming/new bedding nitrogen content	mg/g
	Litter nitrogen volume	ft^3
	Litter nitrogen content	mg/g
	Water (TKN, P, Sulfur, N, NO_3^- & NO_2^-)	mg/l
Lagoon Liquid Conditions	Lagoon Temperature	°C
	Lagoon pH	pH
	Sludge & liquid depth	m
	Lagoon appearance	coloration
	Pit liquid TAN	mg/l
	Lagoon reduction/oxidation (redox) potential	millivolts
	Lagoon dimensions	m

4.1.3 Computer Hardware/Software

The statistical models will be developed using Statistical Analysis Software (SAS v9.4, Cary, NC).

5.0 New Statistical Model Application

5.1 Use & Limitations

The developed statistical models will be used to estimate air emissions from AFOs. Statistical models are restricted by the uncertainty of the parameters used to develop them. Another limitation of statistical models is related to the data used to develop them. While the aim of the NAEMS was to measure air emissions from AFO in a wide range of conditions, it is not possible to make measurements that represent all conditions at AFOs in the U.S. For example, air emissions measurements during the NAEMS were not made during all possible air temperatures. As a result, extrapolating the model beyond the range of development (i.e. for temperature extremes) would increase the uncertainty associated with estimated air emissions.

5.2 Description

An example of a multivariable statistical model that may be developed is the multiple linear regression model, which is described as follows:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_k X_k + \varepsilon \qquad (1)$$

In equation 1, Y is the dependent variable, $X_1, X_2, \ldots, X_k$ are the independent or predictor variables, β_0 is the intercept and β_1, $\beta_{2, \ldots,}$ β_k are regression coefficients and ε is the error term. If a univariable statistical model is developed, the model is described as follows:

$$Y = \beta_0 + \beta_1 X_1 + \varepsilon \qquad (2)$$

Non-linear regression models may also be developed. A non-linear regression model takes the same form as equation 1 or 2 with the exception that at least one of the regression coefficients is non-linear.

6.0 Model Verification and Evaluation

6.1 Approach

The statistical models will be verified by using re-sampling methods. Before re-sampling methods can be applied, the ES&P datasets have to be finalized and statistically characterized. It is expected that the statistical characteristics of each ES&P category will vary and this may influence the choice of re-sampling methods. Possible re-sampling methods to verify EEMs include cross-validation, which involves dividing the ES&P data into two parts, a training set, which is used to develop the EEM and a validation set, which is used to predict the responses (James et al., 2017). There are different types of cross-validation approaches including the standard validation set approach, the leave-one-out cross-validation approach, and the k-fold cross-validation approach (James et al., 2017). Another potential re-sampling method is the bootstrap approach. The bootstrap approach allows the use of computer software to simulate the process of obtaining new data by repeatedly sampling observations from the initial data set, so the error of a predictive model can be estimated without generating additional samples (James et al., 2017). If chosen, bootstrapping would be performed using SAS. Before performing model verification, the various re-sampling methods will be evaluated for different ES&P data sets, which will aid in the process of deciding which re-sampling methods will be used. Informal reports will document the model verification approach (see section 7.1 for more details).

6.2 Model Evaluation

Agreement between observed and model predicted emissions will be evaluated using a variety of different methodologies that have been used in the evaluation of atmospheric models (Walker et al., 2014; Tong and Mauzerall, 2006), including fractional bias (FB), geometric mean bias (MG), mean bias (MB), normalized mean bias (NMB), mean error (ME), normalized mean error (NME), normalized mean square error (NMSE), geometric variance (VG) and fraction of model predicted values within a factor of two of observed values (FAC2). Root mean square error (RMSE) is a further methodology that can be used to assess a model (Bruce and Bruce, 2017) in addition to normalized root mean square error (NRMSE).

$$\text{FB} = \frac{2(\overline{E_{obs}} - \overline{E_{mod}})}{(\overline{E_{obs}} + \overline{E_{mod}})} \tag{3}$$

$$\text{MG} = \exp(\overline{lnE_{obs}} - \overline{lnE_{mod}}) \tag{4}$$

$$\text{MB} = \frac{1}{n}\sum_{i=1}^{n}(E_{mod}(i) - E_{obs}(i)) \tag{5}$$

$$\text{NMB} = \frac{1}{n}\frac{\sum_{i=1}^{n}(E_{mod}(i) - E_{obs}(i))}{\sum_{i=1}^{n}E_{obs}(i)}\ x100\% \tag{6}$$

$$\text{ME} = \frac{1}{n}\sum_{i=1}^{n}|E_{mod}(i) - E_{obs}(i)| \tag{7}$$

$$\text{NME} = \frac{1}{n}\frac{\sum_{i=1}^{n}|E_{mod}(i) - E_{obs}(i)|}{\sum_{i=1}^{n}E_{obs}(i)} x100\% \tag{8}$$

$$\text{NMSE} = \frac{\overline{(E_{obs} - E_{mod})^2}}{\overline{E_{obs}E_{mod}}} \tag{9}$$

$$\text{VG} = \exp\left[\overline{(lnE_{obs} - lnE_{mod})^2}\right] \tag{10}$$

$$\text{FB} = \frac{2(\overline{E_{obs}} - \overline{E_{mod}})}{(\overline{E_{obs}} + \overline{E_{mod}})} \tag{3}$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(E_{mod}(i) - E_{obs}(i))^2} \tag{11}$$

$$\text{NRMSE} = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(E_{mod}(i) - E_{obs}(i))^2}}{\frac{1}{n}\sum_{i=1}^{n} E_{obs}} x\ 100\% \tag{12}$$

Where $\bar{E}$ (overbar) is the average over the data set, n is the number of data points, E_{mod} and E_{obs} are the corresponding model predicted emissions and observed emissions and *i* the *i*th model-observation data points. Walker et al. (2014) and Tong and Mauzerall (2006) evaluated observed and predicted air concentrations, but the methodologies can be similarly used for emission values. These different methodologies quantify bias and/or scatter of model predicted emissions. Informal reports will document the model evaluation results (see section 7.1 for more details).

6.3 Assessment Process

There is currently no established criterion to determine whether the models are of sufficient quality for their intended use. Any future criterion for model quality that is developed will likely be decided in consultation with our project members in OAQPS, who will be responsible for approving the final report. However, model evaluation results can be examined for EEMs already developed and published in peer-reviewed journals (Grant et al., 2016; Rotz et al., 2014), although it is currently unknown how the performance of the EEMs developed in this project for the various ES&P categories will compare to those in the Grant et al. (2016) and Rotz et al. (2014) studies. Grant et al. (2016) developed statistical models to predict NH_3 emissions at five NAEMS swine lagoon sites. The most successful of the models developed by Grant et al. (2016) predicted emissions with a NRMSE ranging from 21-51% across sites with an overall site average NRMSE of 37%. Rotz et al. (2014) is another published study that describes the development and evaluation of an EEM. In the Rotz et al. (2014) study, a process-based emission model was developed for dairy NH_3 emissions and was used to predict emissions for barns and lagoons at various dairy sites including the NAEMS dairy sites. In comparison to measured NAEMS emissions, model predicted emissions had a NRMSE ranging from 29 to 75% for each site with an average NRMSE value across all sites of 49%. Model NME values reported by Rotz et al. (2014) were lower than NRMSE values with an NME ranging from 23 to 64% for each site with an average NME value of 41% across all sites. The error of the process based model developed by Rotz et al. (2014) for predicting dairy lagoon emissions at two NAEMS sites was higher with NRMSE values ranging from 85 to 105% and NME ranging from 44 to 69%.

7.0 Reporting

7.1 Project Documentation

Informal reports, which will be created at a minimum on a quarterly basis, will be used to report progress in data analysis, determining emission source categories, evaluating the ease of model implementation by the agricultural community, and model development (including any significant changes in the model). In addition, these informal reports will document final model description (including model equation(s) and specifications), model verification approach (i.e. re-sampling) and model evaluation results. The reports will be stored on the L-drive in their own designated folders, (path:L:PRIV/NRML_AEMD/DROP/Ian Rumsey/NAEMS-EEM informal reports) with the date of the report in the title. These folders will be private and will be only available to group project members.

7.2 Deliverables

The deliverables for this project are the following for each ES&P category:

- Model verification data sets, and training sets for ES&P categories where a new statistical model is developed.

- Informal reports, which will report progress in data analysis, determining emission source categories, evaluating the ease of model implementation by the agricultural community and model development (including any significant changes in the model) as well as documenting final model description (including model equation(s) and specifications), model verification approach (i.e. re-sampling) and model evaluation results.

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