Uncertainty in Emissions Estimates

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Reasons for Needing Emission Inventories

• Implementation Plan or Control Strategy Development
• Emission Cap and Trade Activities
• Early Reduction Program Design
• Emission Trends Analysis and Projections
• Permit Limit Determination
• Information for Public
• Emission Statement/Fee Collection
• International Treaty Reporting
• Environmental Impact Modeling and Assessment
• Field Study Design
• Compliance Determination
• Real-time Air Quality Forecasting
• Conformity Analysis
• Exposure and Risk Analysis
• Prioritizing Data Needs
• Accountability Assessments

Emission Inventory

\[ EI = \sum_{i} (EF_i \times AF_i) \]

\( EI \) = Emission Inventory
\( EF_i \) = Emission factor for source category, i
\( AF_i \) = Activity factor for source category, i

Questions that Decision-Makers and Stakeholders Typically Ask

• How well do we know these numbers?
  – What is the precision of the estimates?
  – Is there a systematic error (bias) in the estimates?
  – Are the estimates based upon measurements, modeling, or expert judgment?
• How significant are apparent trends over time?
• How effective are proposed control or management strategies?
• Emissions for a population vs. individual source?
• Determination of permit limit or trade allowance?
• What is the key source of uncertainty in these numbers?
• How can uncertainty be reduced?
Recommendations for Quantification of Uncertainty in Emissions

- National Research Council
  - 1992, Rethinking the Ozone Problem in Urban and Regional Air Pollution
  - 1994, Science and Judgment in Risk Assessment
  - 2000, Modeling Mobile Source Emissions
- NARSTO Emission Inventory Assessment (2005)
- Intergovernmental Panel on Climate Change
  - 2000, Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories
  - 2006 IPCC Guidelines for National Greenhouse Gas Inventories

Current Practice for Qualifying Uncertainty in Emission Factors and Inventories

- Qualitative ratings for emission factors (AP-42)
- Data Attribute Rating System (DARS) (not really used in practice)
- Both methods are qualitative
- No quantitative interpretation
- Some sources of uncertainty (i.e. non-representativeness) difficult to quantify
- Qualitative methods can complement quantitative methods

EPA Emission Test Rating

<table>
<thead>
<tr>
<th>Rating</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Tests are performed by a sound methodology and are reported in enough detail for adequate validation.</td>
</tr>
<tr>
<td>B</td>
<td>Tests are performed by a generally sound methodology, but lacking enough detail for adequate validation.</td>
</tr>
<tr>
<td>C</td>
<td>Tests are based on an unproven or new methodology, or are lacking a significant amount of background information.</td>
</tr>
<tr>
<td>D</td>
<td>Tests are based on a generally unacceptable method, but the method may provide an order-of-magnitude value for the source.</td>
</tr>
</tbody>
</table>

EPA Emission Factor Rating

<table>
<thead>
<tr>
<th>Rating</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>A (Excellent)</td>
<td>Factor is developed from A or B rated test data taken from many randomly chosen facilities in the industry population. The source category population is sufficiently specific to minimize variability.</td>
</tr>
<tr>
<td>B (Above Average)</td>
<td>Factor is developed from A or B rated test data from a reasonable number of facilities. Although no specific bias is evident, it is not clear if the facilities tested represent a random sample of the industry. As with an A rating, the source category population is sufficiently specific to minimize variability.</td>
</tr>
<tr>
<td>C (Average)</td>
<td>Factor is developed from A, B, or C rated test data from a reasonable number of facilities. Although no specific bias is evident, it is not clear if facilities tested represent a random sample of the industry. As with an A rating, the source category population is sufficiently specific to minimize variability.</td>
</tr>
<tr>
<td>D (Below Average)</td>
<td>Factor is developed from A, B, or C rated test data from a small number of facilities, and there may be reason to suspect that these facilities do not represent a random sample of the industry. There may also be evidence of variability within the source population.</td>
</tr>
<tr>
<td>E (Poor)</td>
<td>Factor is developed from C and D rated test data, and there may be reason to suspect.</td>
</tr>
</tbody>
</table>

Trends in Quantity and Quality of Emission Factors

<table>
<thead>
<tr>
<th>Factor Rating</th>
<th>Qualitative Description</th>
<th>As of March 1996</th>
<th>As of September 2004</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Factors</td>
<td>Percent of Total</td>
<td>Number of Factors</td>
<td>Percent of Total</td>
</tr>
<tr>
<td>A Excellent</td>
<td>1,270</td>
<td>14</td>
<td>2,135</td>
</tr>
<tr>
<td>B Above Average</td>
<td>1,190</td>
<td>13</td>
<td>1,829</td>
</tr>
<tr>
<td>C Average</td>
<td>1,513</td>
<td>17</td>
<td>2,619</td>
</tr>
<tr>
<td>D Below Average</td>
<td>2,077</td>
<td>24</td>
<td>4,740</td>
</tr>
<tr>
<td>E Poor</td>
<td>2,798</td>
<td>32</td>
<td>5,787</td>
</tr>
<tr>
<td>Total</td>
<td>8,833</td>
<td>17,110</td>
<td></td>
</tr>
</tbody>
</table>


Aggregated Assessment of Confidence in U.S. Emission Inventories

<table>
<thead>
<tr>
<th>Source</th>
<th>Estimated Confidence Levels in Overall Inventory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities</td>
<td>SO2</td>
</tr>
<tr>
<td>Other Point</td>
<td>M</td>
</tr>
<tr>
<td>Onroad Mobile</td>
<td>M</td>
</tr>
<tr>
<td>Nonroad Mobile</td>
<td>M</td>
</tr>
<tr>
<td>Stationary Nonpoint</td>
<td>L</td>
</tr>
<tr>
<td>Biogenic</td>
<td>L</td>
</tr>
<tr>
<td>Other Anthropogenic (non-combustion)</td>
<td>L</td>
</tr>
</tbody>
</table>

Source: NARSTO (2005)
Variability and Uncertainty

- **Variability**: refers to the certainty that
  - different emission sources will have different emissions (inter-unit variability)
  - emissions will vary over time for a given source (intra-unit variability)
- **Uncertainty**: refers to lack of knowledge regarding
  - True value of a fixed but unknown quantity
  - True population distribution for variability
- Both depend on averaging time

Sources of Variability
(Example of a Process Technology)

- Design
- Feedstocks
- Ambient Conditions
- Maintenance Practices
- Operational practices and occurrences (e.g., load following, baseload, transients, process upsets)
- Seasonality/Periodicity

Sources of Uncertainty

- Random sampling error for a random sample of data
- Measurement errors
  - Systematic error (bias, lack of accuracy)
  - Random error (imprecision)
- Non-representativeness
  - Not a random sample, leading to bias in mean (e.g., only measured loads not typical of daily operations)
  - Direct monitoring versus infrequent sampling versus estimation, averaging time
  - Omissions
- Surrogate data (analogies with similar sources)
- Lack of relevant data

How Good are the Emission Factors? NOx From Coal-Fired Power Plants

- Compilation of Air Pollutant Emission Factors, AP-42, U.S. Environmental Protection Agency
- Example: Bituminous coal, Wall-fired, dry bottom boilers
  - Data Quality Rating of A
  - 28 data points
  - 9.5 to 44.5 lb NOx/ton
  - Average = 21.1 lb NOx/ton, std dev = 8.2
  - 95% Confidence Interval on the mean: 17.9 ± 24.1 (±15%)
- Uncertainty: Depends on context
  - ±15% of the average of many plants
  - A factor of two for a randomly selected individual plant
- The Rating of an AP-42 emission factor does not translate into a quantitative estimate of uncertainty

Methods for Quantifying Uncertainty

- Bottom-Up Approaches
  - Statistical Methods Based Upon Empirical Data
  - Statistical Methods Based Upon Judgment
  - Sensitivity Analysis
- Top-Down Approaches

Quantifying Uncertainties in Emission Inventories: Conceptual Bottom-Up Approach

- Input Uncertainties
- Emission Factor
- Activity Factor
- Output Uncertainty
- Total Emissions

**Table:**

<table>
<thead>
<tr>
<th>Source Category</th>
<th>Input Uncertainties</th>
<th>Emission Factor</th>
<th>Activity Factor</th>
<th>Output Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>k</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Statistical Methods Based Upon Empirical Data

- Frequentist, classical
- Statistical inference from sample data
  - Parametric approaches
    - Parameter estimation
    - Goodness-of-fit
  - Nonparametric approaches
- Mixture distributions
- Censored data
- Dependencies, correlations, deconvolution

Propagating Variability and Uncertainty

- Analytical techniques
  - Exact solutions (limited applicability)
  - Approximate solutions
- Numerical methods
  - Monte Carlo
  - Latin Hypercube Sampling
  - Other sampling methods (e.g., Hammersley, Importance, stochastic response surface method, Fourier Amplitude Sensitivity Test, Sobol’s method, Quasi-Monte Carlo methods, etc.)

Monte Carlo Simulation

- Probabilistic approaches are widely used
- Monte Carlo (and similar types of) simulation are widely used.
- Why?
  - Extremely flexible
    - Inputs
    - Models
  - Relatively straightforward to conceptualize

Methods Based Upon Expert Judgment

- Expert Elicitation
  - Heuristics and Biases
  - Availability
  - Anchoring and Adjustment
  - Representativeness
  - Others (e.g., Motivational, Expert, etc.)
- Elicitation Protocols
  - Motivating the expert
  - Structuring
  - Conditioning
  - Encoding
  - Verification
- Documentation
- Individuals and Groups
- When Experts Disagree

An Example of Elicitation Protocols: Stanford/SRI Protocol

- Motivating (Establish Rapport)
- Structuring (Identify Variables)
- Conditioning (Get Expert to Think About Evidence)
- Encoding (Quantify Judgment About Uncertainty)
- Verify (Test the Judgment)

Statistical Methods Based Upon Expert Judgment

- Bayesian methods can incorporate expert judgment
  - Prior distribution
  - Update with data using likelihood function and Bayes’ Theorem
  - Create a posterior distribution
- Bayesian methods can also deal with various complex situations:
  - Conditional probabilities (dependencies)
  -Combining information from multiple sources
- Appears to be very flexible
- Computationally, can be very complex
- Complexity is a barrier to more widespread use
Sensitivity Analysis

- Objectives of Sensitivity Analysis (examples):
  - Help identify key sources of variability (to aid management strategy)
    » Critical control points?
    » Critical limits?
  - Help identify key sources of uncertainty (to prioritize additional data collection to reduce uncertainty)
  - What causes worst/best outcomes?
  - To assist in process of model development
- Local vs. Global Sensitivity Analysis
  - Global sensitivity analysis in combination with probabilistic analysis
- Model Dependent vs. Model Independent Sensitivity Analysis
- Applicability of methods often depends upon characteristics of a model (e.g., nonlinear, thresholds, categorical inputs, etc.)

Local Sensitivity Analysis

\[
\frac{\partial z}{\partial x} = s_{x,b} \\
\frac{\partial z}{\partial y} = s_{y,b} \\
\frac{\partial z}{\partial y} = s_{y,a} \\
\]

Summary of Probabilistic Emissions Case Studies at NCSU

- Case Studies (examples):
  - Point sources
    » Power Plants
    » Natural gas-fired engines (e.g., compressor stations)
  - Mobile sources
    » On-Road Highway Vehicles
    » Non-Road Vehicles (e.g., Lawn & Garden, Construction, Farm, & Industrial)
  - Area sources
    » Consumer/Commercial Product Use
    » Natural Gas-Fueled Internal Combustion Engines
    » Gasoline Terminal Loading Loss
    » Cutback Asphalt Paving
    » Architectural Coatings
    » Wood Furniture Coatings
- Pollutants
  - NO\textsubscript{x}
  - VOC
  - Urban air toxics (e.g., Houston case study)

Example of Benzene Emission Factor for Summer Storage Losses at a Storage Tank: Empirical Distribution

Example of Benzene Emission Factor: Fitted Lognormal Distribution

Bootstrap Simulation Process
Example of Benzene Emission Factor: Confidence Interval for the Fitted Distribution

Example of Benzene Emission Factor: Uncertainty in the Mean

Uncertainty in mean - 73% to +200%

Using AuvTool to Fit a Distribution for Variability

Using AuvTool for Bootstrap Simulation

Using AuvTool to Quantify Uncertainty in the Mean

Uncertainty in Total Emission Inventory: AUVEE Prototype Software
### Summary of Probabilistic Emission Inventory

#### Table: Summary of Probabilistic Emission Inventory

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Engine and Load Range</th>
<th>AP-42 Emission Factor</th>
<th>Engine and Load Range</th>
<th>AP-42 Emission Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOx</td>
<td>2SLB, 90-105%</td>
<td>3.17</td>
<td>2SLB, 90-105%</td>
<td>3.17</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.05</td>
<td></td>
<td>-24 to +24</td>
</tr>
<tr>
<td></td>
<td>4SLB, 90-105%</td>
<td>4.08</td>
<td>4SLB, &gt;90%</td>
<td>0.847</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.06</td>
<td></td>
<td>-39 to +49</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.61</td>
<td></td>
<td>-65 to +120</td>
</tr>
<tr>
<td></td>
<td>2SLB all load</td>
<td>1.84</td>
<td>4SLB all load</td>
<td>1.47</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.48</td>
<td></td>
<td>-16 to +16</td>
</tr>
<tr>
<td></td>
<td>4SLB all load</td>
<td>1.12</td>
<td></td>
<td>-45 to +57</td>
</tr>
</tbody>
</table>

#### Notes:
- Units are lb/10^6 BTU.
- MLE is used for 2SLB engine, MoMM is used for 4SLB engine.
- W = Weibull distribution, G = Gamma distribution.
- Calculated based upon bootstrap simulation results.

### Identification of Key Sources of Uncertainty in an Inventory

#### Figure: Identification of Key Sources of Uncertainty

### Probabilistic AP-42 Emission Factors for Natural Gas-fueled Engines (July 2000 Version)

<table>
<thead>
<tr>
<th>Engine and Load Range</th>
<th>AP-42 Emission Factor</th>
<th>No. of Data / Engines</th>
<th>Fixed Distribution</th>
<th>Mean of Bootstrap sample mean</th>
<th>Relative 95% CI of mean (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOx</td>
<td>2SLB, 90-105%</td>
<td>3.17</td>
<td>34 / 11</td>
<td>W</td>
<td>3.05</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.05</td>
<td>-24 to +24</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4SLB, 90-105%</td>
<td>4.08</td>
<td>12 / 4</td>
<td>G</td>
<td>4.06</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.06</td>
<td>-39 to +49</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4SLB, &gt;90%</td>
<td>0.847</td>
<td>13 / 5</td>
<td>W</td>
<td>1.81</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.81</td>
<td>-65 to +120</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TOC</td>
<td>2SLB all load</td>
<td>1.64</td>
<td>37 / 16</td>
<td>W</td>
<td>1.48</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.48</td>
<td>-16 to +16</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4SLB all load</td>
<td>1.12</td>
<td>37 / 16</td>
<td>G</td>
<td>1.12</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.12</td>
<td>-45 to +57</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Notes:
- Units are lb/10^6 BTU.
- MLE is used for 2SLB engine, MoMM is used for 4SLB engine.
- W = Weibull distribution, G = Gamma distribution.

### Summary of Probabilistic Emission Inventories for Selected Air Toxics

#### Table: Summary of Probabilistic Emission Inventories for Selected Air Toxics

<table>
<thead>
<tr>
<th>City</th>
<th>Pollutant</th>
<th>95% Probability Range Relative to the Mean Estimate, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Houston</td>
<td>Benzene</td>
<td>(-46, 108)</td>
</tr>
<tr>
<td></td>
<td>Formaldehyde</td>
<td>(-35, 67)</td>
</tr>
<tr>
<td></td>
<td>Chromium</td>
<td>(-20, 34)</td>
</tr>
<tr>
<td></td>
<td>Arsenic</td>
<td>(-69, 203)</td>
</tr>
<tr>
<td></td>
<td>1,3-butadiene</td>
<td>(-46, 108)</td>
</tr>
<tr>
<td></td>
<td>Mercury</td>
<td>(-25, 30)</td>
</tr>
<tr>
<td></td>
<td>Arsenic</td>
<td>(-83, 243)</td>
</tr>
<tr>
<td></td>
<td>Benzene</td>
<td>(-56, 146)</td>
</tr>
<tr>
<td></td>
<td>Formaldehyde</td>
<td>(-42, 89)</td>
</tr>
<tr>
<td></td>
<td>Lead</td>
<td>(-54, 175)</td>
</tr>
<tr>
<td>Jacksonville</td>
<td>1,3-butadiene</td>
<td>(-46, 108)</td>
</tr>
<tr>
<td></td>
<td>Mercury</td>
<td>(-25, 30)</td>
</tr>
<tr>
<td></td>
<td>Arsenic</td>
<td>(-31, 143)</td>
</tr>
<tr>
<td></td>
<td>Benzene</td>
<td>(-56, 146)</td>
</tr>
<tr>
<td></td>
<td>Formaldehyde</td>
<td>(-42, 89)</td>
</tr>
<tr>
<td></td>
<td>Lead</td>
<td>(-54, 175)</td>
</tr>
</tbody>
</table>

### Key Sources of Uncertainty

#### Table: Key Sources of Uncertainty

<table>
<thead>
<tr>
<th>City</th>
<th>Pollutant</th>
<th>Key Sources of Uncertainty (number of dominant sources)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Houston</td>
<td>Benzene</td>
<td>Gasoline onroad mobile sources (1)</td>
</tr>
<tr>
<td></td>
<td>Formaldehyde</td>
<td>Onroad mobile sources, Nonroad mobile sources (2)</td>
</tr>
<tr>
<td></td>
<td>Chromium</td>
<td>Chemical manufacturing-fuel fired heaters (1)</td>
</tr>
<tr>
<td></td>
<td>Arsenic</td>
<td>External utility coal combustion boilers (1)</td>
</tr>
<tr>
<td></td>
<td>1,3-butadiene</td>
<td>Onroad mobile sources (1)</td>
</tr>
<tr>
<td></td>
<td>Mercury</td>
<td>External coal combustion boilers (1)</td>
</tr>
<tr>
<td></td>
<td>Arsenic</td>
<td>External coal combustion boilers (1)</td>
</tr>
<tr>
<td></td>
<td>Benzene</td>
<td>Onroad mobile source (1)</td>
</tr>
<tr>
<td></td>
<td>Formaldehyde</td>
<td>Onroad mobile source, Aircraft (2)</td>
</tr>
<tr>
<td></td>
<td>Lead</td>
<td>External coal combustion boilers, Fuel oil external combustion, Waste oil external combustion (3)</td>
</tr>
</tbody>
</table>

### Case Study of Emissions Uncertainty and Predicted Air Quality

- Charlotte modeling domain
- 32 units from 9 different coal-fired power plants
- 1995 and 1998 data used
- Propagation of uncertainty investigated using July 12 – July 16 1995 meteorological data
- Data available for emission and activity factors
- Vector autoregressive time-series modeling of emissions from each unit
H. Christopher Frey  
North Carolina State University  
September 2010  
Presented at MARAMA

**PROBABILISTIC MODELING**

- **Input Uncertainties**
  - Emissions
  - Meteorology
  - Initial & Boundary Conditions
- **Output Uncertainties**
  - Peak Ozone
  - Local Ozone
  - Local NOx
  - Local VOC

**Time Series and Uncertainty**

- Different uncertainty ranges for different hours of day

**Probability of Exceeding NAAQS: Comparison of 1-hour and 8-hour Standards**

- Analysis of Correlation in Emissions versus Ozone Levels in a Specific Grid Cell Can Detect Influence of a Specific Plant

**Location of Power Plant Impact**

- Correlation Coeff = 0.87
- Emissions (t/hr)

**Top-Down Methods: Identify Major Biases**

- Comparison of Inventories Developed Using Independent Methods and Data
- Comparison of Air Quality Model Predictions to Monitoring Data
- Comparison of Source-Oriented vs. Receptor-Oriented Modeling Approaches
- Comparison of Inventories and Ambient Monitoring Data

**Comparison of Fuel-Based Versus Mileage-Based Mobile Source Inventories**

- Source: NARSTO (2005)
Example: Comparing Trends in Estimated Emissions and Ambient Monitoring Data

Source: NARSTO (2005)

Answering Decision-Maker Questions

• How well do we know these numbers?
  – What is the precision of the estimates?
  – Is there a systematic error (bias) in the estimates?
  – Are the estimates based upon measurements, modeling, or expert judgment?
• How significant are apparent trends over time?
• How effective are proposed control or management strategies?
• Emissions for a population vs. individual source?
• Determination of permit limit or trade allowance?
• What is the key source of uncertainty in these numbers?
• How can uncertainty be reduced?

Emission Factors and Inventories: Findings (1)

• Data visualization is highly informative
• Original data:
  – Typically poorly documented
  – Time consuming to recreate databases
  – Time to quantify uncertainty typically small compared to time to compile data
• Real world data and/or expert judgment are necessary

Emission Factors and Inventories: Findings (2)

• There is a need for systematic reporting of the precision and accuracy of measurement/test methods
• Uncertainties in emission factors are typically positively skewed.
• Uncertainty attributable to random sampling error should be accounted for

Emission Factors and Inventories: Findings (3)

• Variability and uncertainty increases as the averaging time decreases
• Uncertainty in future estimates can be informed by analysis of historical data
• Prototype software makes probabilistic analysis more convenient
• Often, just a few key emission sources drive overall uncertainty

General Recommendations (1)

• Use uncertainty and sensitivity analysis:
  – prioritize scarce resources toward additional research or data collection
  – make choices among alternatives,
  – evaluate trends over time.
• Include uncertainty and sensitivity analysis from the beginning into model and input data development
• Provide data for uncertainty (e.g., summary statistics such as mean, standard deviation, sample size)
### General Recommendations (2)

- Allow flexibility. Choose approach according to assessment objective.
- Commit necessary resources
  - Adequate time and budget
  - Adequate training and peer review
  - Workshops and other training, and periodic authoritative compilations, and recommended practice

### General Recommendations (3)

- Develop appropriate software tools
- Research – best techniques for communication, real-world information needs for decision makers
- Compile relevant case studies and insights
- Ensure uncertainty and sensitivity analysis are transparent