Uncertainties in Benzene and 1,3-Butadiene Emissions in Houston and their Effects on Uncertainties in Concentrations Calculated by AERMOD and ISC

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Outline of presentation

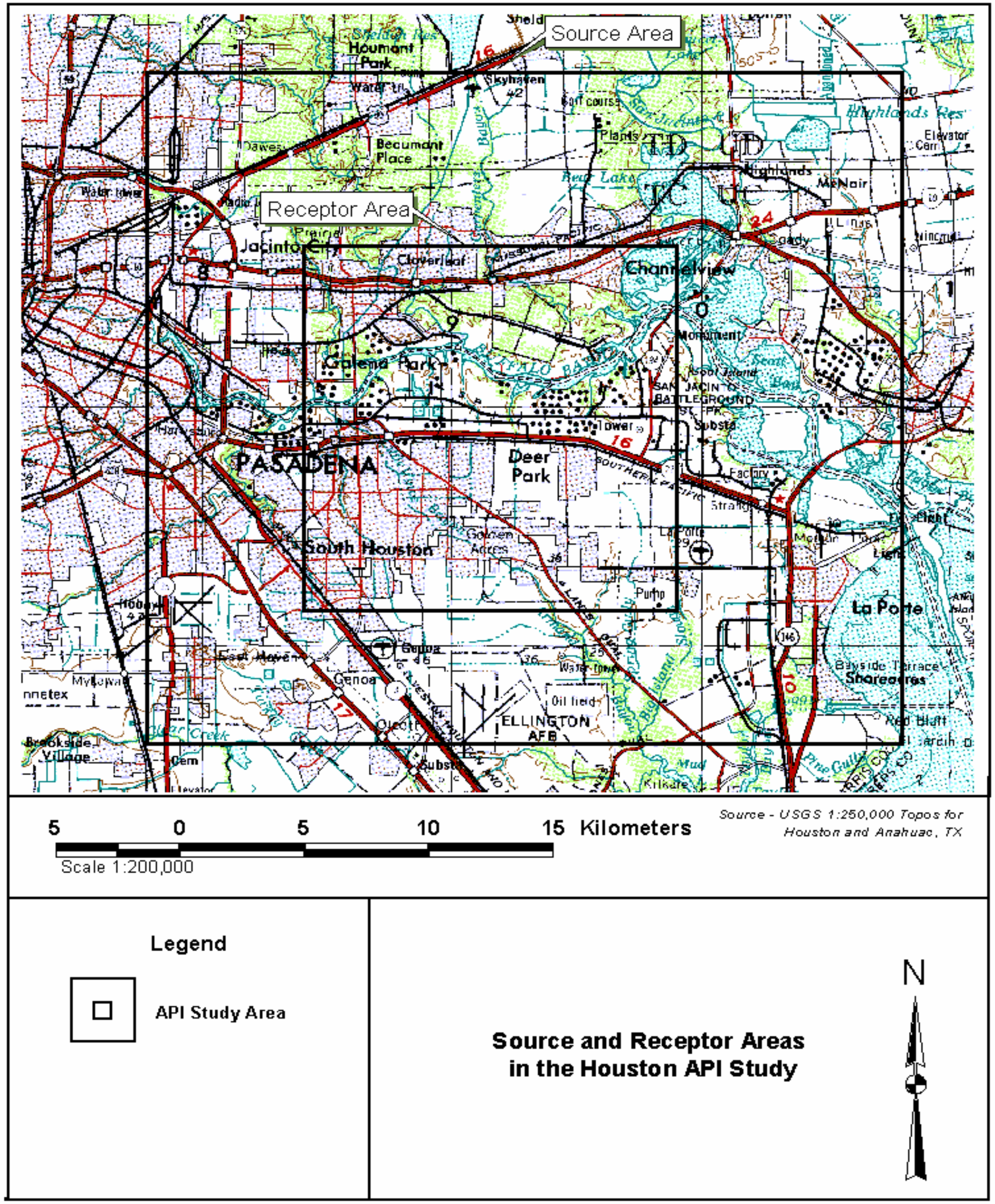
- Goals of study
- Description of overall study (emissions + air quality models)
- This study is sponsored by API but is collaborating with similar study by EPA with larger domain around Houston.
- Tables of benzene and butadiene emissions
- Uncertainty estimates

Goals of Study

- Estimate the uncertainties in predictions of modeling systems used for predicting annual averaged concentrations of toxics (benzene and 1,3-butadiene are studied as examples)
- Focus on Houston example since EPA has used that area as a test case, and is doing a probabilistic uncertainty study there at the moment
- Focus on ISC3ST and AERMOD dispersion models
- Current paper describes only emissions uncertainties

API
Study Area
(Subset of
EPA Houston
Study Area)

This domain
centers on the
Ship Channel



Questions to be addressed by study

Question 1: What is the total uncertainty in the predicted annual average maximum benzene and 1,3-butadiene concentrations in the Houston sub-domain region, and which input variables and model parameters have the most influence on this total uncertainty? How does the result vary when, instead of looking at the domain-wide maximum concentration, we look at maximum concentrations at specific receptor locations (e.g., monitor locations or population census tract centroids or on a square grid)?

Question 2: What is the relative uncertainty between the emissions and the transport and dispersion model?

Question 3: How do the total uncertainties and correlations differ for different source classes, such as mobile versus point, or major road versus minor road?

Question 4: How does uncertainty impact source apportionment conclusions? For example, what is the relative difference in uncertainties for mobile sources versus point sources?

Question 5: Do the conclusions concerning uncertainty depend on model used (e.g., ISC3ST versus AERMOD or ISC3ST with EPA rural-urban designations versus ISC3ST with all-urban?

Increasing Interest in Monte Carlo Uncertainty Studies

Now possible with fast computers with much storage, since there is a need to make 100 or more runs with a model for a given scenario.

EPA has a Guideline on Monte Carlo Modeling, which has mainly been applied to “non-air” problems such as superfund sites where water and soil contamination are the issue.

Recent examples of applications to air quality issues (emissions modeling, dispersion modeling)

Overview of Monte Carlo method

- Define modeling system and scenario
- Determine inputs (and model parameters) whose uncertainties are to be studied
- Determine outputs whose uncertainties are to be determined
- Estimate uncertainties in model inputs and parameters (median, standard deviation, distribution function)
- Run model many (100+) times with random and independent variations of inputs
- Analyze uncertainties in outputs

Define Output Variable of Interest

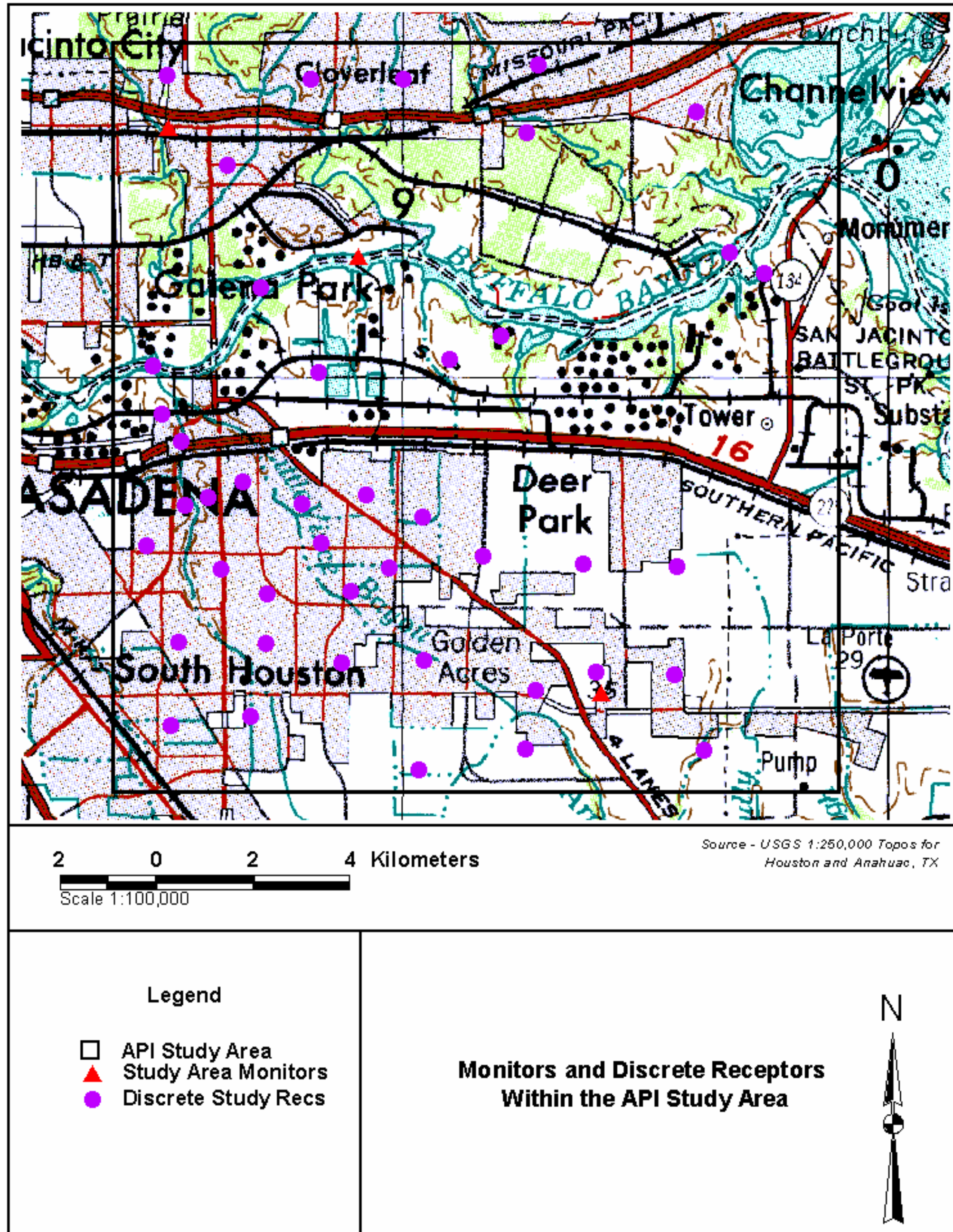
Averaging time is defined by health effects standards

In this case, the annual average concentration is of most interest

In addition, 24 hour averages are of interest to aid understanding of science

Concentrations are calculated at 46 population tract centroids and at 3 sampler (AIRS) locations

Population Centroid Receptors and Monitor Locations



Two Types of Results from Monte Carlo Studies

Estimates of **total uncertainty** in model outputs due to uncertainties in inputs and in model parameters

Estimates of **correlations** between variations in model outputs and variations in individual model inputs, allowing the inputs to be identified whore uncertainties have the largest effect on the model output uncertainties.

EPA and API are conducting collaborative Monte Carlo uncertainty studies in Houston

The modeling system has three parts – 1) emissions, 2) transport and dispersion, and 3) exposure, dose, and risk.

The current projects are now concerned about only parts 1 and 2. Part 3 will come later.

Major difficulties

> determining uncertainties in emissions categories, since little information is available

> accounting for hour-to-hour versus site-to-site variations in meteorological and dispersion model inputs

August 2004 Emissions Uncertainty Workshop for Houston Toxics Study

25 specialists on toxics emissions (e.g., benzene) met in Houston

The goal was to obtain information from experts on methods of estimating emissions and their uncertainties of benzene and 1,3-butadiene in the Houston area

The information was be used in EPA and API Monte Carlo probabilistic studies of uncertainties in model predictions due to uncertainties in inputs.

Implications of long (annual) averaging time

There is little need to define uncertainties from hour-to-hour in emissions

Similarly, hour-to-hour uncertainties in wind speed and other variables have little effect on the annual average.

We need to define exactly what is meant by the "uncertainty" in emissions that we are asking for.

Emissions categories

1 - Major Point (petroleum refineries, chemical and allied products, power plants, other)

2 - Major Volume (fugitives from oil refineries, tanks, treatment facilities)

3 - Area and Other (oil and natural gas production, gas distribution stages 1&2, natural gas storage and transfer, fires, chemical and allied products, other)

4 - Mobile

4.1 On Road Major (emissions are assigned to long thin rectangles covering interstate, US, and state highways)

4.2 Non Road Area – includes off-road vehicles and all types of gas engines, marine engines, loco-motives, plus on-road mobile sources on minor highways such as local streets and county roads

Methods for estimating emissions uncertainties

- Use emissions data and categories developed for previous EPA and API studies of Houston toxics
- Under EPA support, and for the larger EPA domain, Dr. Chris Frey developed a draft set of “top 24” categories for benzene and estimated their uncertainties based on data and literature reviews
- This benzene list was discussed and refined at the Houston workshop
- The benzene list was revised based on emissions in the API Houston ship channel domain
- We used a similar approach to developing a list of “top 13” categories for 1,3-butadiene

Some decisions

- At the Houston workshop, it was decided that there was not enough information available to distinguish differences in uncertainties between Emissions Factors and Activity Factors
- It was also decided that there was not enough information available to come to firm recommendations about mean biases
- Similarly, there was insufficient information to allow correlations between variations in emissions uncertainties to be determined (other than a strong correlation between LDGT and LDGV, which were combined into one category)

Assumed Uncertainties for API Study

- Because most of the uncertainties for the 24 benzene categories in Chris Frey's draft table were close to each other (e.g. ± factor of 2 or 3), it was decided to assume that all benzene and butadiene emissions categories had uncertainty ranges of ± factor of three (covering the 95 % range)
- All PDFs are assumed to be log-normal
- No mean biases and no correlations

Industrial Sources by Category

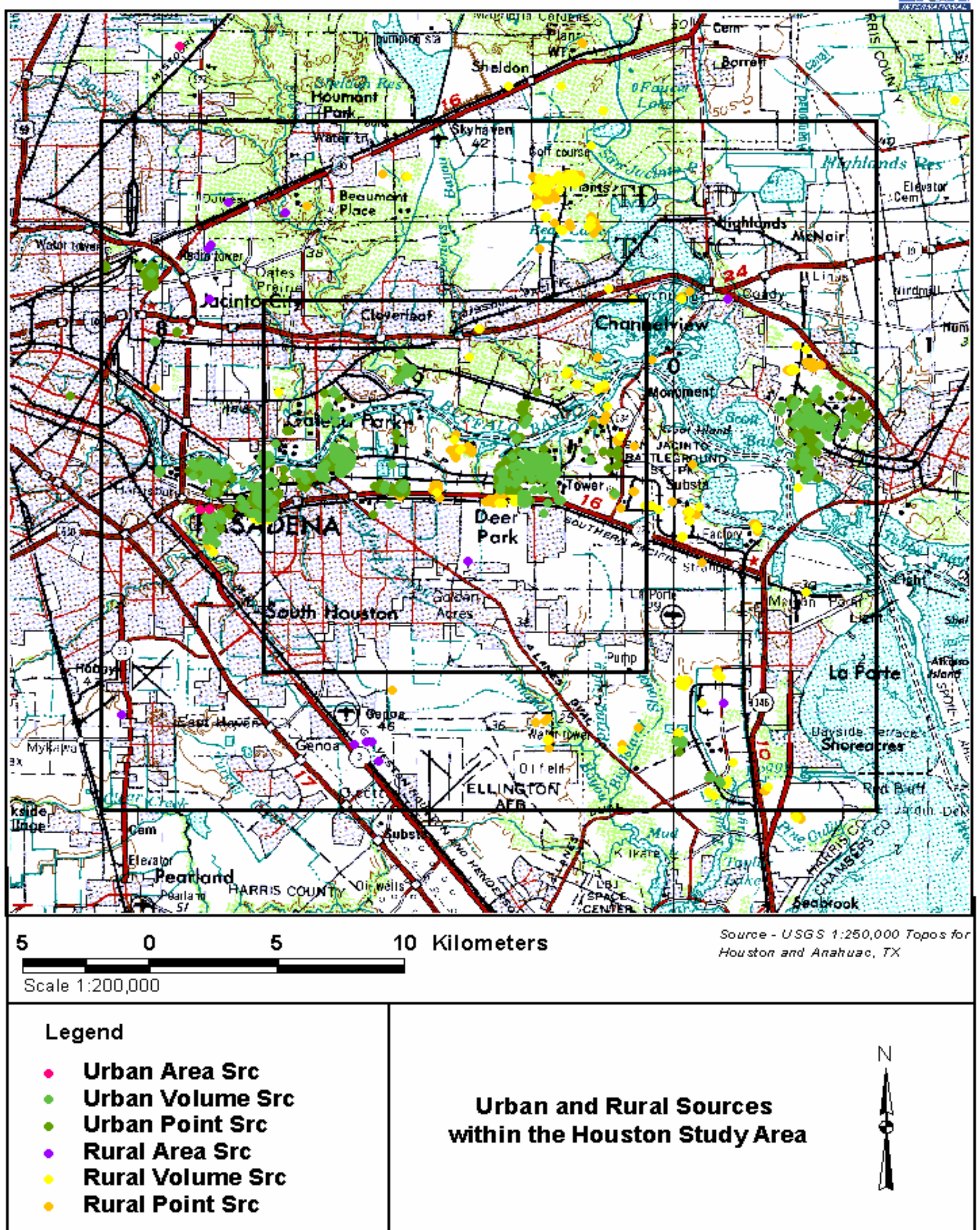


Table 1. Emission categories used for benzene in the uncertainty assessment

Cate-Gory	Description	TPY	% of Total	Emissions Type and Source
1	Light Duty Gas Vehicles (LDGV), Light Gas Trucks (LDGT), Road Segments	475.0	28.5	On-Road - HDDV, HDGV, LDGT, LDGV, MC, and All Road Segments
2	Petroleum refineries	412.7	24.7	Point - Petr Refineries, Catalytic Cracking, and Sulfur Plants; Non-Point - Petr Refining-Nat Gas Support
3	Non-road 4-stroke gas engines, Internal Combustion Engines	145.8	8.7	Non-Road - Res. Heat-Distillate Oil; Point - Internal Comb Engines; Non-Pt - Station Inter. Comb. Eng. Diesel & Nat. Gas
4	Non-rd 2-stroke gas engines	34.3	2.1	Non-Road - Off Highway Gas. 2-stroke
5	Non-road diesel (construction, farm, and industr)	26.2	1.6	Non-Road - Off Highway Diesel
6	Oil and gas production	10.2	0.6	Non-Pt Oil & Nat. Gas Prod and support
7	Natural gas transmission and marine transport	63.7	3.8	Non-Point - Nat Gas Transmission & Storage; Marine Cargo Handling
8	Forest wildfires, Municipal Landfills	5.8	0.4	Non-Point - Open Burning-Scrap Tires, Forests & Wildfires, POTWs,; Point - Municipal Landfills
9	Solid waste disposal (sewage treatment, aeration tanks)	59.2	3.5	Point - Waste Disposal and Solid Waste Disposal
10	Acetylene prod (butylenes, ethylene, propylene, olefin)	47.8	2.9	Point - Acetylene Production

11	Fuel oil external combustion, External Combustion Boilers	37.9	2.3	Point - Fuel Oil External Comb, External Comb Boilers; Non-Point - POTW Digest Gas, Res. Heat. Distillate Oil,
12	Typical ethylene plant	17.0	1.0	Point - Ethylene Plant
13	Gas service stations stage 1	9.6	0.6	Non-Point - Gasoline Distribution Stage I & II
14	Petroleum industry fugitives	26.8	1.6	Point - Petroleum Industry Fugitives
15	Managed burning, prescribed	0.6	0.04	Non-Point - Open Burning: Prescribed
16	Chemical manufacturing; fugitive emissions	16.7	1.0	Pt - Chem Manuf: Fug Emis; Non-Pt - Indus Org & Inorg Chem Manuf, Misc. Org Chem Proc; On-Rd - LDDV
17	Aircraft	6.5	0.4	Point – Aircraft
18	Petr ind; fug emis; misc. Petr & Solvent Evap.	121.8	7.3	Point - Petroleum and Solvent Evaporation
19	Process vents in refinery production	15.0	0.9	Point - Process Vents in Refinery Production
20	Loading, ballasting, transit losses from marine vessels	21.6	1.3	Point - Loading, Ballasting, Transit Losses from Marine Vessels; Non-Road - Commercial Marine Vessels
21	Industrial Processes	113.3	6.8	Pt - Ind Proc; Non-Pt - Consumer Prod Usage, Architect Surface Coatings, Asphalt Concrete and Roofing Manuf
	Total Emissions	1667.6	100.0	

Table 2. 1,3-butadiene emissions source categories

Category	Description	TPY	% of Total
1	Fuel oil external comb, petr and solvent evap, organic solvent evap, fuel fired equip, natural gas, flares, indust proc, petr ind, process gas	271.8	40.1
2	Styrene-butadiene rubber and latex production, nitrile butadiene rubber production	105.8	15.6
3	Chemical manuf fugitive emis, industl processes, general processes, fabricated metal products fugitive emissions, plastics production	118.8	17.5
4	Industrial processes, chemical manufacturing, butadiene fugitive emissions	17.1	2.5
5	Ethylene plant, industrial processes chemical manufacturing butylenes. Ethylene propylene, olefin production fugitives emissions	26.3	3.9
6	Loading, ballasting, transit losses from marine vehicles	10.7	1.6
7	Indust proc, petr industry cooling towers and fugitive emissions from flanges and all streams	13.9	2.0
8	Aircraft	5.1	0.8
9	Unknown	6.4	0.9
10	Road Segments	42.4	6.3
11	On-road Gridded	30.0	4.4
12	Non-road	17.6	2.6
13	Non Point	12.6	1.9
	Total Emissions	**678.4**	**100.0**

Current Status – Just beginning MC runs with ISC3ST and AERMOD

- There is a need to check inputs and assumptions carefully before beginning multiple model runs
- Results will be available in about 3 months
- We will be able to compare with results of EPA MC runs on larger Houston domain (they have a preliminary draft report available)