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Abstract:

Photochemical modeling supporting ozone State Implementation Plans (SIPs) is evaluated by its ability to replicate ozone events. This modeling relies on emissions inventories (EIs) reported by regulated entities, which may be ozone-season-day (OSD) estimates, or more typically, annual estimates. In the Houston-Galveston-Brazoria nonattainment area (HGB) of Texas, recent air quality studies, such as the 2006 Texas Air Quality Study (TexAQS II), have provided an abundance of ambient measurements of air quality constituents to use in evaluating the photochemical modeling. These measurements indicated the need for a higher temporal resolution of EIs. The Texas Commission on Environmental Quality (TCEQ) plans to use episodes which occurred during the TexAQS II study for modeling supporting future ozone SIP revisions. In order to acquire a higher temporal resolution of EIs for this modeling, TCEQ requested an hourly, chemically-speciated "Special Inventory" (SI) from selected industries in HGB that operated continuous emissions monitors (CEMs) during the TexAQS II study period. Unlike the SIs TCEQ has requested in the past, this request was accompanied by the development of new collection and processing procedures. In addition to those developed to support the SI, new processing procedures to generate hourly, chemically-speciated emissions were also developed for at least three other "emission event" databases compiled by TCEQ. The standard hourly emissions from the EPA Acid Rain Program were combined with these four datasets to develop photochemical model-ready emissions. This paper describes these five emissions datasets and the procedures used to generate hourly, chemically-speciated, episodic EIs for modeling.

Development of an Hourly Modeling Emissions Inventory from Several Sources of Regulatory Speciated Hourly Data for the Houston-Galveston-Brazoria Ozone Nonattainment Area

Distinctions in Terms

- *"Regulatory"*
  - Data sources are regulatory (State-mandated by rules or State-collected)
  - Used in SIP Attainment Demonstration modeling
  - As opposed to "research grade"
- *"Hourly"*
  - Bottom-up (measured) or one step from bottom
  - As opposed to processed into hourly via default profiles
- *"Speciated"*
  - Individual chemical constituents
  - As opposed to mixtures or lumped species

Background & Motivation

- **History**
  - Used Hourly emissions for SIP modeling since COAST
    - (Coastal Oxidant Assessment for Southeast Texas), 1993
  - Incorporated hourly Acid Rain data into SIP attainment demonstration modeling, 1999
  - Striving for higher resolution in all parts of the EI
    - e.g., time and pitch of airport take-offs and landings
- **TexAQS 2000**
  - Corroborating field studies (aircraft, monitoring) showed that reported VOC EIs were underestimated by 10-100x
  - Highly-reactive VOC (HRVOC) species were found to be in larger proportion than expected at locations not expected
  - HRVOC process flow monitoring implemented, 2005
- **TexAQS II (2005-06)**
  - Intensive field study campaign
    - July 15 – October 15, 2006
  - 2006 Special Inventory (SI)
    - August 15 – September 15, 2006
    - Requested from 141 accounts (plants) in 24 counties
    - Expected to capture ozone modeling episodes

Emissions Modeling Databases

Sources of Hourly Data used by TCEQ Emissions Modelers

National Databases

EPA's National Emissions Inventory (NEI)

(1) EPA's Acid Rain Program

Texas (TCEQ) Databases

State of Texas Air Reporting System (STARS)

(2) Special Inventory (SI)

(3) Consolidated Compliance and Enforcement Data System (CCEDS)

(4) Tank Landing Losses (TLL)

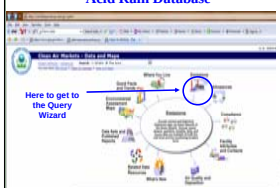
National Databases

- NEI (not hourly, VOC not speciated)
- EPA's Acid Rain Program (ARP)
  - Download hourly CEM data from Clean Air Market's Query for all states in modeling domain
  - Replace annual or seasonal data in NEI
  - Assume EPA SCC-specific speciation for those outside of Texas
  - Replace Texas ozone season daily (OSD) records from STARS for all ARP Electric Generating Units (EGUs)
  - Ratio the VOC and CO to the hourly NOx
  - Use Texas point-specific VOC profiles

Texas-Specific Databases

- STARS (State of Texas Air Reporting System)
  - Annual
  - OSD (ozone season daily avg.) – TCEQ modeling
  - Hourly (only after a Special Inventory Request)
- Special Inventory (SI) via HEIRS
  - HEIRS (Hourly Emissions Inventory Reporting System), 2005, 2006
  - SI is requested from select companies on an as-needed basis
  - HEIRS data uploaded into STARS
- CCEDS (Consolidated Compliance and Enforcement Data System)
- TLL (Tank Landing Losses)

Acid Rain Database



Then choose "Unit Level Emissions", "Hourly", and a month from the Query Wizard.

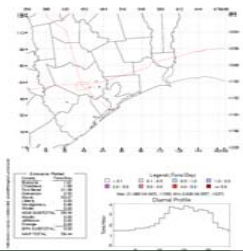
TCEQ downloads entire modeling domain.

http://canddataandmaps.epa.gov/gdm/

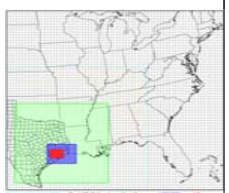
Hourly Acid Rain NOx in HGB

Tileplot (2 km grid cells) QA

Note diurnal profile – follows the electrical demand of the Houston area



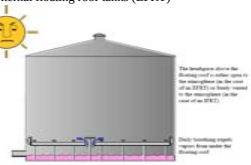
CAMx Modeling Domain



Tank Landing Losses (TLL)

- Tanks in specific service in the Houston Ship Channel (HSC) area were found to be landing their tanks on their legs and not reporting those vapor space losses
- Discovered as a result of a Remote Sensing VOC project in July 2005 (part of TexAQS II)
- As a result, new TCEQ rule that limits the number of permissible "convenience" roof landings
- In the meantime, we had to model the real world emissions, as a portion of the "under-reported" VOC in HGB for internal floating roof tanks (IFRT) and external floating roof tanks (EFRT)

Standing Idle Losses – Floating Roof Tank with a Liquid Heel



TLL Emissions Modeling

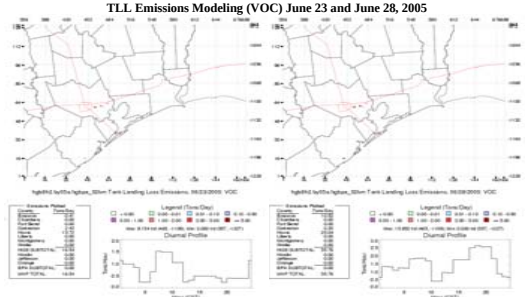
- Hourly distribution
  - Survey respondents provided date/time of tank landing operations, as well as tank breathing and refilling loss rates.
  - Tank breathing losses allocated to eight hours between 9 AM and 5 PM (sunny hours)
  - Refilling losses allocated to time/date and duration detailed in the survey
- Speciation
  - Breathing vapor composition based on composition of tank heel
  - Refilling based on new tank inventory
  - Tank contents not very reactive

TLL Emissions Modeling – Spreadsheet Excerpt

Company	Account #	FIN	EPN	Type of Floating Roof Tank	Landing Start Date and Time	Landing End Date and Time
TEPPCO	BL0571U	SW02TANK01	SW02TANK01	External Floating Roof Tank	6/27/2005 2:26	6/27/2005 11:08
TEPPCO	BL0571U	SW02TANK01	SW02TANK01	External Floating Roof Tank	6/27/2005 20:37	6/28/2005 14:03

Landing Product Contaminant Name	Refilling Start Date and Time	Refilling End Date and Time	Refilling Pollutant Contam Code	Refilling Vapors - Pollutant Name	Standing Idle Losses (lb/hr)	Refilling Losses (lb/hr)
Crude Oil	6/27/2005 11:08	6/27/2005 14:46	59001	Crude Oil	37.5197	1572.9691
Crude Oil	6/28/2005 14:03	6/28/2005 17:41	59001	Crude Oil	31.9739	1572.9691

TLL Emissions Modeling (VOC) June 23 and June 28, 2005



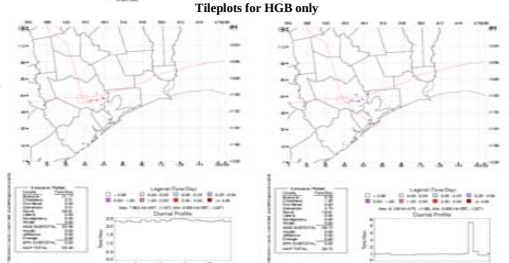
2006 Special Inventory (SI)

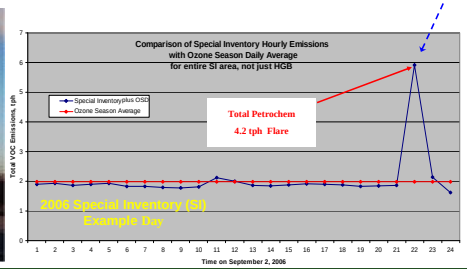
- Part of the TexAQS II (2005-06) Intensive campaign, August 15 – September 15, 2006
  - Requested from 141 accounts (plants) in 24 counties
  - Mainly for units that have regulatory monitoring
  - 49 of those accounts were in HGB, and requested hourly emissions from 405 paths (process unit–emission point combinations)
  - HRVOC, other VOC, NOx, but requested all species for all hours during this 32-day period
  - Modelers generated a record for each path-hour-contaminant (species) combination
  - Replacement for reported OSD records

Speciation

- Improved speciation procedure
  - Object is to have companies report as much detail as possible
  - Each path can report any number of contaminants in any given hour
  - A unique chemical speciation profile is generated for every hour for every path
  - Previous SIP modeling used an episode average

Tileplots for HGB only



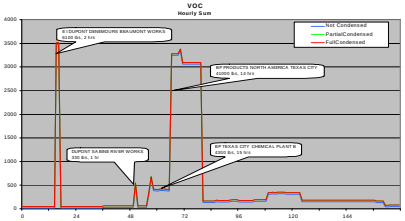


Consolidated Compliance and Enforcement Data System (CCEDS)

TCEQ database of Emission Events

- Emissions in excess of permit allowable
  - Upsets, maintenance, startups, shutdowns
- Self-reported, but followed-up

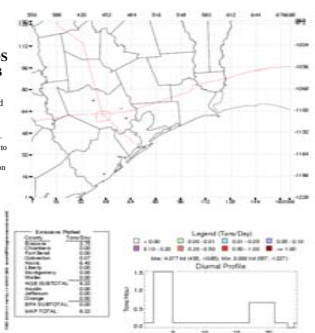
- Hourly representation after assumptions
- Majority of reports include speciation detail
- Excerpt of database query
  - One account with two emission points
  - VOC emissions here (HRVOC and NOx analyzed in separate files)
  - Assumptions
    - Flat temporal distribution during event
    - "best match" when path not well defined



Hourly CCEDS VOC in HGB

Tileplot (2 km grid cells) QA

Note diurnal profile – this data is in addition to other modeled data sources for the Houston area



REG_ENT_NUM	CITY	COUNTY	FIN_EPN_NUM	EVENT_START_DT	EVENT_START_TM	EVENT_END_DT	EVENT_END_TM	DurationHours	CONTAMINANT	QUANTITY RELEASED (lbs)
RN102535077	TEXAS CITY	GALVESTON	S01	7/28/2005	18:00	7/29/2005	8:00	14.00	Propane	636
RN102535077	TEXAS CITY	GALVESTON	S01	7/28/2005	18:00	7/29/2005	8:00	14.00	Pentane	1101
RN102535077	TEXAS CITY	GALVESTON	S01	7/28/2005	18:00	7/29/2005	8:00	14.00	Hexane, n	2036
RN102535077	TEXAS CITY	GALVESTON	S01	7/28/2005	18:00	7/29/2005	8:00	14.00	Butane, N-	456
RN102535077	TEXAS CITY	GALVESTON	S01	7/28/2005	18:00	7/29/2005	8:00	14.00	Isopentane	76
RN102535077	TEXAS CITY	GALVESTON	S01	7/28/2005	18:00	7/29/2005	8:00	14.00	Isobutane	91
RN102535077	TEXAS CITY	GALVESTON	F-480	7/28/2005	18:00	7/29/2005	8:00	14.00	Butane	6401
RN102535077	TEXAS CITY	GALVESTON	F-480	7/28/2005	18:00	7/29/2005	8:00	14.00	Isobutane	2891
RN102535077	TEXAS CITY	GALVESTON	F-480	7/28/2005	18:00	7/29/2005	8:00	14.00	Pentane	3716
RN102535077	TEXAS CITY	GALVESTON	F-480	7/28/2005	18:00	7/29/2005	8:00	14.00	Propane	13513
RN102535077	TEXAS CITY	GALVESTON	F-480	7/28/2005	18:00	7/29/2005	8:00	14.00	Isopentane	2435
RN102535077	TEXAS CITY	GALVESTON	F-480	7/28/2005	18:00	7/29/2005	8:00	14.00	Hexane, n	5829

Conclusions

- Where there were overlapping data between databases, there was decent agreement
  - CCEDS events during modeled episodes were also generally reported in the SI
- Tank landing losses are a newly-discovered significant VOC source, but not of HRVOC
- Hourly Acid Rain NOx emissions precisely account for many (e.g., peaking) EGUs
- Special Inventory (SI) data is an upgrade that captures emissions fluctuations during requested episodes
- CCEDS data complement an EI, by including atypical excursions, but have a minor contribution
- Average ozone season daily EI is generally adequate for modeling most non-EGU point sources, especially those that operate continuously or near-continuously; a move to even-higher resolution modeling may note more immediate benefit

Final Statement

Generally the more detailed (i.e., temporally, spatially, and chemically resolved) the input data, the more likely the model will appropriately replicate ozone episodes, especially as modelers push the resolution envelope.

References

TCEQ Emission Sources and Inventories webpage (for TexAQS II, contracts and general inventory documents and data)
http://www.tceq.state.tx.us/nav/eq/eq_airdata_sources.html

TCEQ General Air Quality Research Projects:
http://www.tceq.state.tx.us/nav/eq/eq_aq_research.html

TCEQ TexAQS II webpage
http://www.tceq.state.tx.us/nav/eq/texaqsII.html

TCEQ Emissions Modeling:
http://www.tceq.state.tx.us/implementation/air/airmod/overview/am_ei.html

Acknowledgments

TCEQ Emissions Assessment Section
TCEQ Data Analysis/Field Study Team
TCEQ Air Modeling Team
TCEQ Air Quality Division Managers
TexAQS Participating Researchers

June 2008