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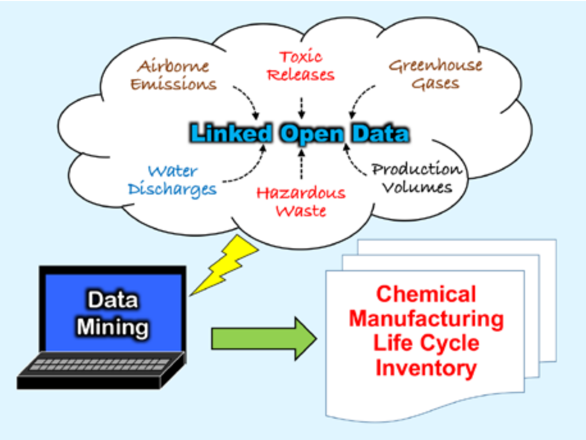
Agency

Rapid Life Cycle Inventory Modeling of Chemical Manufacturing Using the US EPA's Emissions Inventories

David E. Meyer*, Sarah Cashman (Eastern Research Group), John Abraham, Scott Unger, Wesley Ingwersen

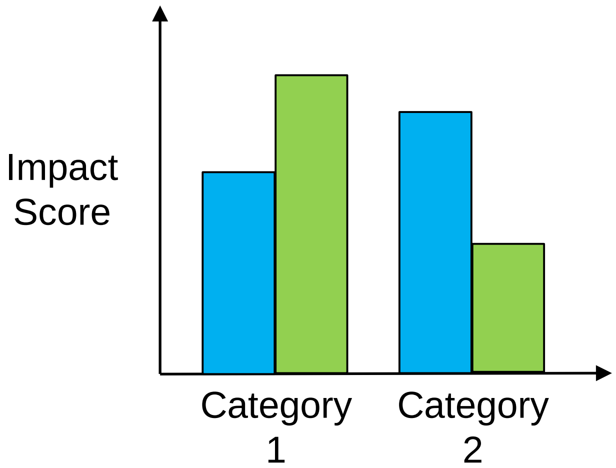


International Emissions Inventory Conference - August 16, 2017
Baltimore, Maryland

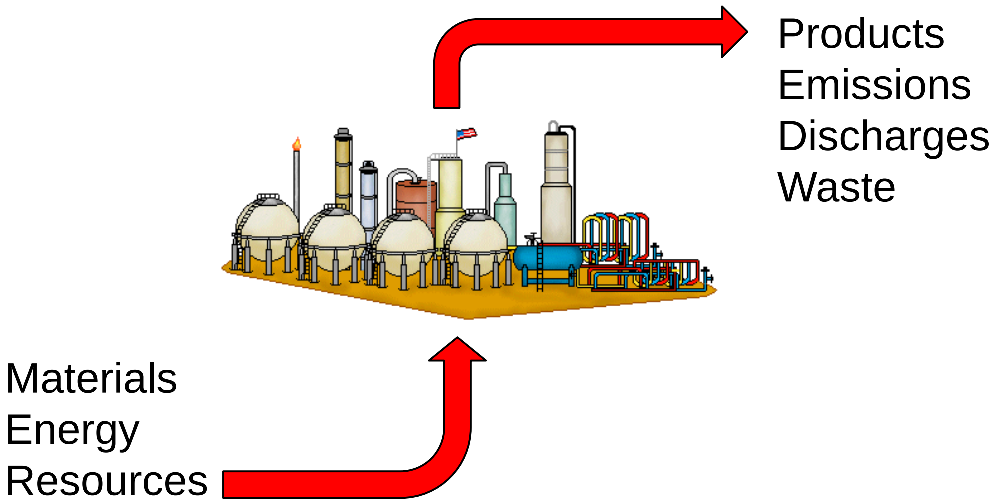
Office of Research and Development
National Risk Management Research Laboratory
Life Cycle Assessment Center of Excellence

Life Cycle Assessment and Inventory Modeling

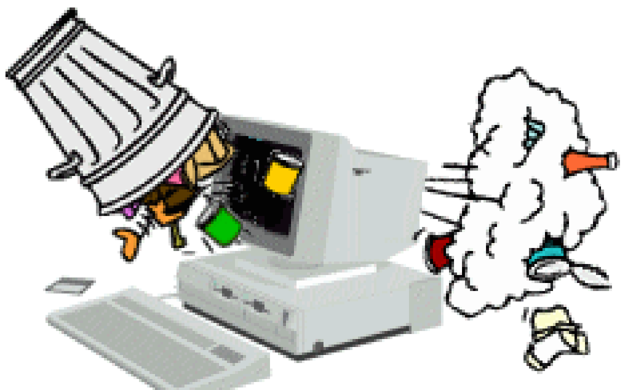
You can’t get this…



… without this!



- **The success of an LCA is highly dependent on the Life Cycle Inventory (LCI).**

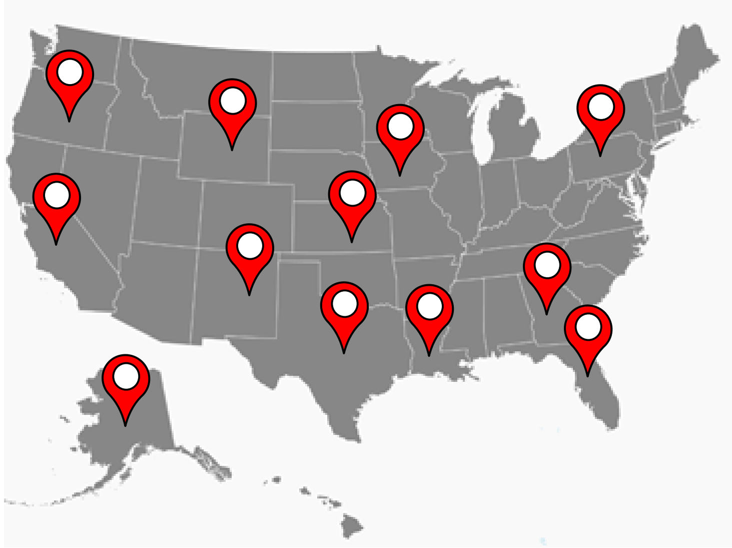


Garbage In = Garbage Out

http://www.lovemytool.com/blog/2010/06/avoid-garbage-in-garbage-out-in-network-analysis-by-peter-hage.html

Inventories of Scale

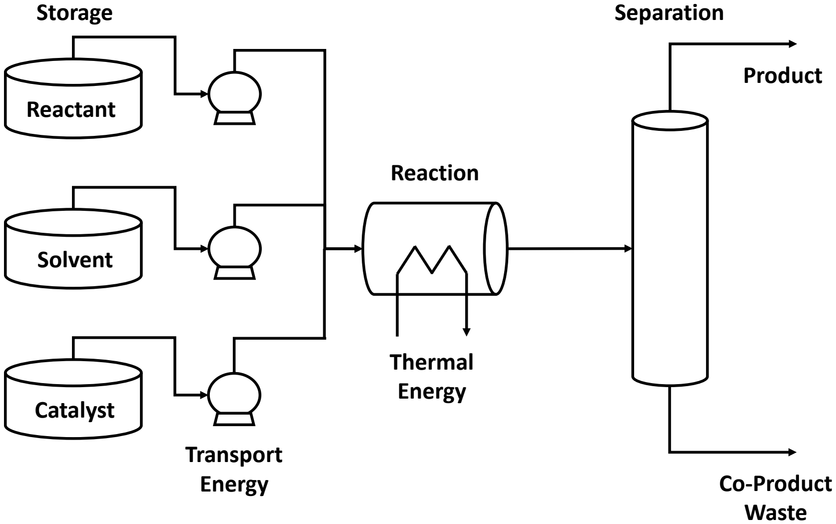
Sector



- Develop LCI by NAICS classification
- ***Uses:*** Input-Output LCA; Policy Analysis
- ***Challenges:*** millions of data points; multi-NAICS facilities; aggregate products and functional unit

Vs.

Process



- Develop LCI for a specific chemical
- ***Uses:*** Process LCA; Sustainable chemistry and engineering
- ***Challenges:*** multi-product facilities; CBI data; unknown production volumes

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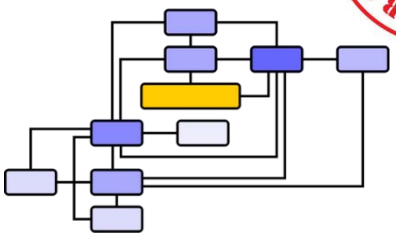
Rapid and Reliable LCI: the Issues

- Field data = the best = resource intensive
- Most chemical process data for the US are proprietary
- Cradle-to-gate chemical LCI may involve hundreds of processes
- EPA has a trove of data that could be useful for LCA
- EPA is both a consumer and provider of LCA data
- EPA data needs to be reproducible, reusable and publically available

Emissions

Discharges

Waste

United States Environmental Protection Agency

Data Mining EPA Data Sources

DOI: 10.1021/acs.est.6b02160
Environ. Sci. Technol. 2016, 50, 9013−9025

Environmental Science & Technology
Policy Analysis
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Mining Available Data from the United States Environmental Protection Agency to Support Rapid Life Cycle Inventory Modeling of Chemical Manufacturing

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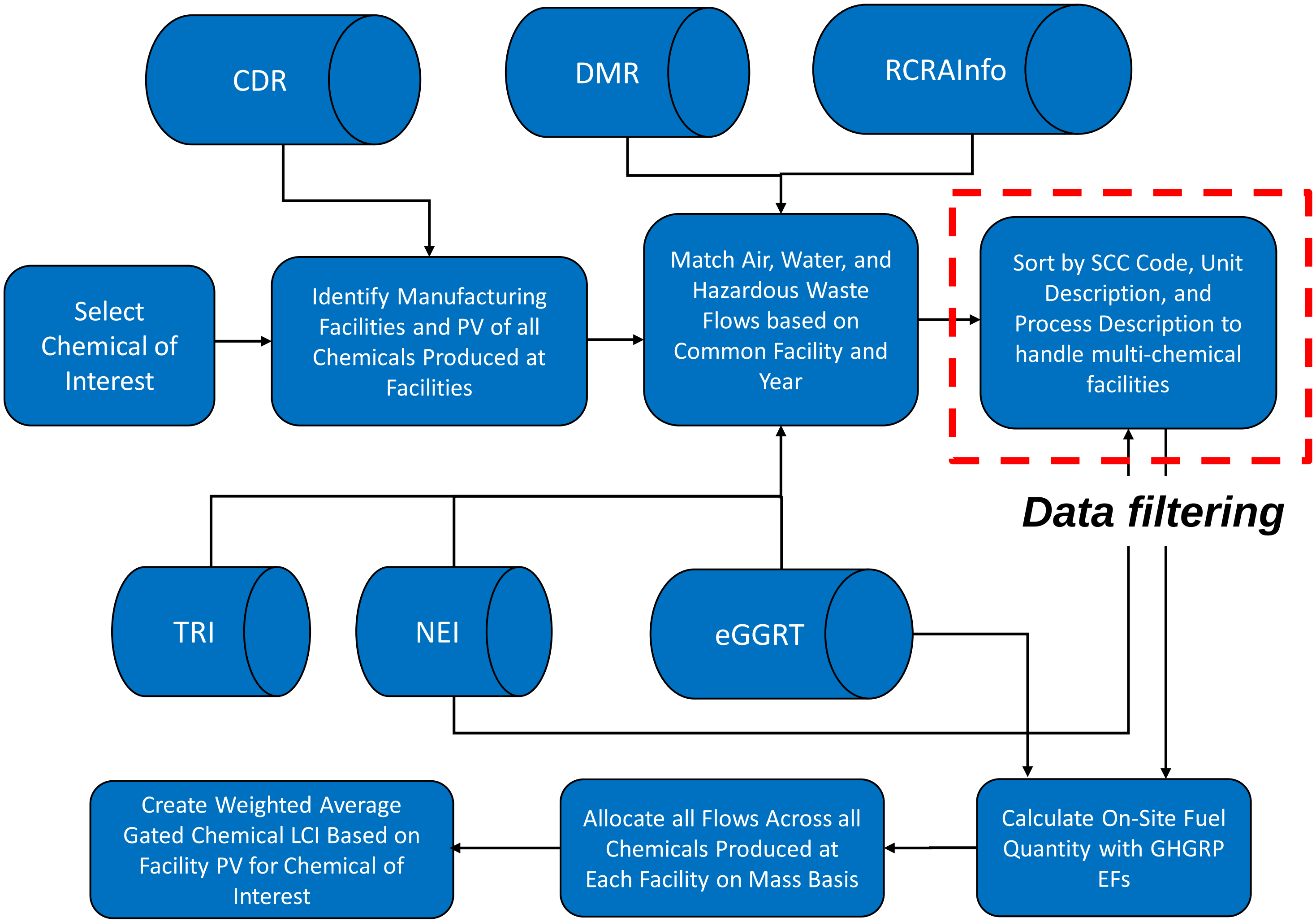
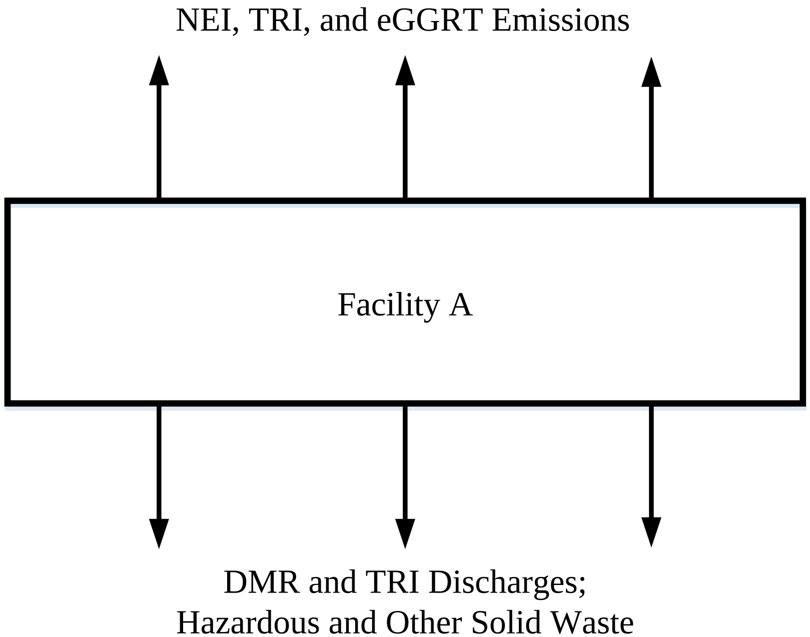
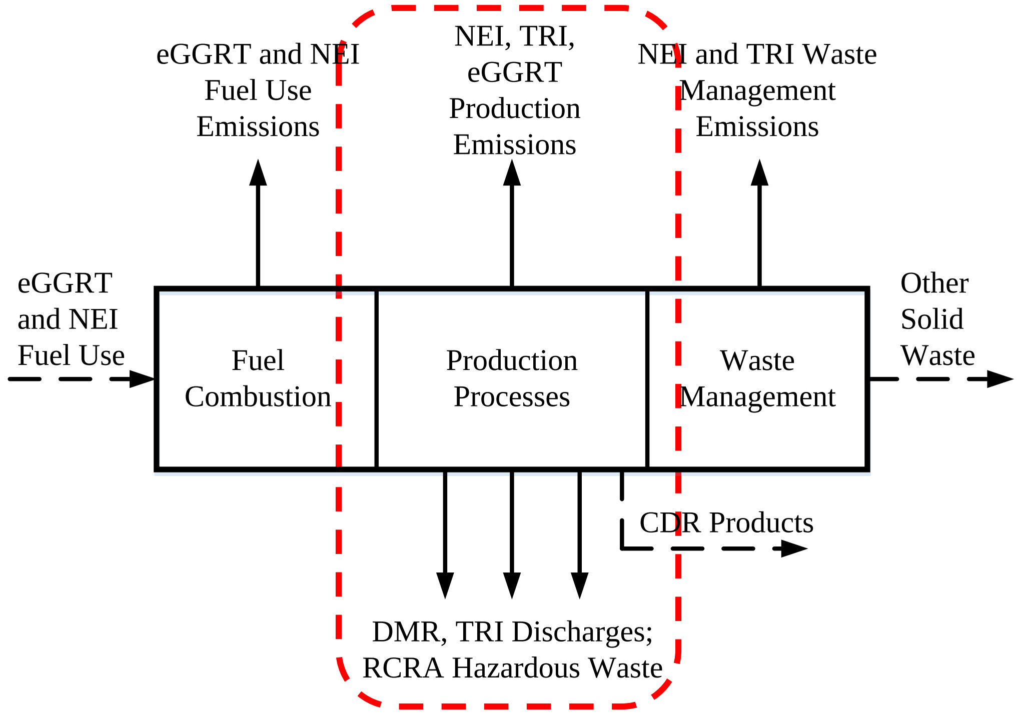
- A method developed with semantic data management in mind
  - 6 publically available data sources
  - Builds on EPA efforts to develop linked open data (LOD)
  - 12 discrete steps that can be translated into Simple Protocol and RDF Query Language (SPARQL) queries
  - repeatable
- Automating the method could lead to rapid and more efficient inventory modeling

Gated Chemical LCI Data Mining Method



Facility vs. Process Modeling





- For process LCA, need emissions by chemical and process.
- Ancillary processes (energy, waste treatment) are modeled separately to allow flexibility.

Method: The Nuts and Bolts

- Create a weighted-average chemical manufacturing unit process

$$\overline{EF}^{PD}_{Pollutant\ X} = \frac{\sum_i^N \left(EF_{Pollutant\ X, Facility\ i} \times PV_{PD, Facility\ i}\right)}{\sum_i^N PV_{PD, Facility\ i}}$$

Where:

- $\overline{EF}^{PD}_{Pollutant\ X}$ is the weighted average emission factor, specific to pollutant X and, in this example, the production of the chemical product (kg/kg)
- $EF_{Pollutant\ X,\ Facility\ i}$ is an emission factor for pollutant X at a specific facility (a pollutant emission normalized by total chemical production, kg/kg)
- $PV_{PD,\ Facility\ i}$ is the production volume of the chemical product at a specific facility (kg)
- Subscript *Pollutant X* refers to a unique pollutant-media combination (e.g., CO_2 emissions to air, ammonia emissions to water)
- Subscript *Facility i* refers to a specific facility (e.g., Facility A)
- *N* is the total number of all facilities
- *PD* refers to the chemical product of interest

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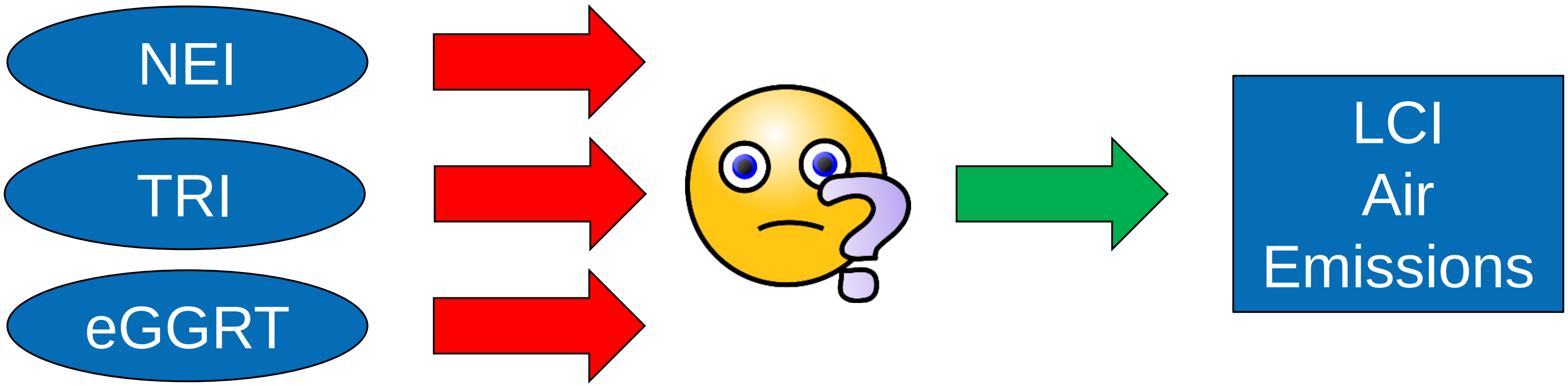
Resolving Overlap



- ***NEI over TRI*** (greatest overlap between these databases)
  - Overlap related to HAPS
  - Facilities more accountable for toxics under TRI, but reporting lacks process specificity
  - Need to use NEI over TRI to employ process-level allocation
  - If not conducting process-level allocation, could select database based on flow reliability score
- ***eGGRT over NEI*** for GHG overlap

Intra-Database Speciation in NEI

Note: For impact characterization, speciated emissions are always preferred because they are more compatible with characterization factors.

- **VOCs**: Deduct speciated HAP VOCs from aggregated VOCs at the facility-level to avoid double-counting.
- **PM**: Deduct PM2.5-primary flow from PM10-primary at the facility-level. Report both PM2.5-primary and adjusted PM10-primary flows.
- **Metal HAPs**: Technically these will overlap some with PM. However, there is not overlap in LCIA methods for these flows. Reporting both metal HAP and PM is fine for LCA purposes.
- **Other groupings**: glycol ethers, PAH/POMs, dioxins/furans, xylenes, cresols, fine mineral fibers, PCBs, and radionuclides
  - Speciated or non-speciated flows can be reported, but not both
  - Include both speciated and non-speciated pollutants

Reporting Methods and Data Quality

- **Flow reliability** based on reporting method

Code	Description	Type	Reliability
1	Continuous monitoring system	Verified measurement	1
2	Engineering Judgement	Undocumented estimate	5
3	Material Balance	Undocumented estimate	5
4	Stack Test	Verified measurement	1
5	USEPA Speciation Profile	Verified calculation	2
7	Manufacturer Specification	Undocumented estimate	5
8	US EPA Emission Factor (no control efficiency used)	Verified calculation	2
9	S/L/T Emission Factor (no control efficiency used)	Verified calculation	2
10	Site-specific emission factor (no control efficiency used)	Verified calculation	2
28	USEPA Emission Factor (pre-control) plus Control Efficiency	Verified calculation	2

- **Temporal correlation** based on reporting year
- **Geographical correlation** = 1 as method only covers U.S. facilities (assuming level of resolution is national)
- **Technological correlation** depends on the ability to determine the technology used by a facility (based on NEI and GHGRP metadata) and the coverage of total U.S. production
- **Sampling methods correlation** depends on the percentage of total U.S. production captured by CDR

Chemical Case Studies

- **Objective:** Develop U.S. national-average LCI for the production of Acetic Acid and Cumene ((Propan-2-yl)benzene)

	Acetic Acid	Cumene
Total # of Faclities	25	10
CBI Facilities	17	2
Public Facilities	8	8
% of Total Production Volume	1.17%	80.75%

Low coverage without CBI facilities

# of Reporting Facilities (Public CDR Only) for 2011 Databases

	NEI	TRI	eGGRT	DMR	RCRAinfo
Acetic Acid	7	8	3	4	3
Cumene	8	8	8	7	8

- Working with multiple EPA databases can be challenging because of variations in reporting thresholds and requirements.

Example: Facility Raw Inventory

NEI

Substance	Value	Unit	DQ Score
1,3-Butadiene	0	kg	2
2,2,4-Trimethylpentane	0	kg	2
Ammonia	1.27E-08	kg	5
Benzene	3.35E-07	kg	2
Biphenyl	2.22E-10	kg	5
Carbon Disulfide	7.04E-09	kg	5
Carbon Monoxide	9.76E-06	kg	2
Cobalt	3.71E-11	kg	5
Cumene	1.17E-07	kg	2
Ethyl Benzene	0	kg	2
Ethylene Dichloride	5.14E-11	kg	2
Hexane	0	kg	2
Hydrochloric Acid	3.87E-07	kg	5
Hydrogen Fluoride	5.63E-10	kg	5
Hydrogen Sulfide	0	kg	2
Lead	1.96E-11	kg	2
Mercury	3.28E-10	kg	5
Methanol	4.09E-09	kg	5
Methyl Tert-Butyl Ether	0	kg	2
Naphthalene	0	kg	2
Nickel	9.86E-10	kg	5
Nitrogen Oxides	3.49E-06	kg	2
PAH, total	1.44E-10	kg	5
PM10 Primary (Filt + Cond)	1.74E-06	kg	2
PM2.5 Primary (Filt + Cond)	1.70E-06	kg	2
Styrene	0	kg	2
Sulfur Dioxide	2.81E-06	kg	2
Toluene	5.07E-08	kg	2
Volatile Organic Compounds	1.60E-05	kg	2
Xylenes (Mixed Isomers)	0	kg	2

TRI

Substance	Value	Unit	DQ Score
1,2,4-TRIMETHYLBENZENE	1.67E-07	kg	5
BENZO(G,H,I)PERYLENE	4.45E-12	kg	5
CARBONYL SULFIDE	0	kg	5
COPPER COMPOUNDS	3.93E-10	kg	5
CYCLOHEXANE	7.98E-09	kg	5
DIOXIN AND DIOXIN-LIKE COMPOUNDS	1.73E-14	kg	5
ETHYLENE	1.04E-07	kg	5
MOLYBDENUM TRIOXIDE	5.19E-10	kg	5
NITRATE COMPOUNDS	0	kg	#DIV/0!
PROPYLENE	3.17E-07	kg	5
TERT-BUTYL ALCOHOL	0	kg	5
ZINC COMPOUNDS	1.31E-08	kg	5

eGGRT

Substance	Value	Unit	DQ Score
carbon dioxide	1.40E-02	kg	3.43
dinitrogen monoxide	8.01218E-08	kg	3
methane	7.28416E-06	kg	3.89

<u>Process</u> emissions for a refinery producing cumene. Emissions for combustion have been filtered out by SCC code.

Learning from the Metadata

Filter using additional information about an emission:

- SCC codes
- process and unit descriptions

NEI Unit Description	NEI Unit Type Description	NEI Unit Type Group	NEI Process Description	Action
T007, 1-7-TK-7 Cumene Storage Tank	Storage Tank	Evaporative Sources	CUMENE BL TANK 7	Allocate 100% to cumene
CT07, 2-603-CT-05 New North area cooling tower	Unclassified	Unclassified	2-603-CT-5, NNA	Allocate across all chemicals
T855, 2-606-TK-855 Gas Oil / Distillate Tank	Storage Tank	Evaporative Sources	DISTILLATE TANK 855 WL	Exclude - unrelated
H042, 1-35-B-03 Cumene Column Reboiler	Process Heater	Fuel Comb. Equipment	1-35-B-3 1 CUMENE COL REB	Exclude - energy process

Source	Substance	Value Raw	Value Filtered	Unit	Change %	DQ Score
eGGRT	carbon dioxide	1.40E-02	2.14E-03	kg	-85%	3.43
eGGRT	dinitrogen monoxide	8.01E-08	1.32E-08	kg	-83%	3
eGGRT	methane	7.28E-06	6.95E-06	kg	-5%	3.89
NEI	1,3-Butadiene	0	0	kg	-	2
NEI	2,2,4-Trimethylpentane	0	0	kg	-	2
NEI	Ammonia	1.266E-08	0	kg	-100%	5
NEI	Benzene	3.354E-07	2.34E-05	kg	6889%	2
NEI	Biphenyl	2.223E-10	0	kg	-100%	5
NEI	Carbon Disulfide	7.04E-09	0	kg	-100%	5
NEI	Carbon Monoxide	9.756E-06	0	kg	-100%	2
NEI	Cobalt	3.705E-11	0	kg	-100%	5
NEI	Cumene	1.169E-07	2.50E-05	kg	21319%	2
NEI	Ethyl Benzene	0	0	kg	-	2
NEI	Ethylene Dichloride	5.138E-11	0	kg	-100%	2
NEI	Hexane	0	0	kg	-	2
NEI	Hydrochloric Acid	3.869E-07	0	kg	-100%	5
NEI	Hydrogen Fluoride	5.632E-10	0	kg	-100%	5
NEI	Hydrogen Sulfide	0	0	kg	-	2
NEI	Lead	1.96E-11	0	kg	-100%	2
NEI	Mercury	3.283E-10	0	kg	-100%	5
NEI	Methanol	4.091E-09	0	kg	-100%	5
NEI	Methyl Tert-Butyl Ether	0	0	kg	-	2
NEI	Naphthalene	0	0	kg	-	2
NEI	Nickel	9.856E-10	0	kg	-100%	5
NEI	Nitrogen Oxides	3.489E-06	0	kg	-100%	2
NEI	PAH, total	1.438E-10	0	kg	-100%	5
NEI	PM10 Primary (Filt + Cond)	1.738E-06	1.46E-06	kg	-16%	2
NEI	PM2.5 Primary (Filt + Cond)	1.701E-06	1.44E-06	kg	-16%	2
NEI	Styrene	0	0	kg	-	2
NEI	Sulfur Dioxide	2.81E-06	0	kg	-100%	2
NEI	Toluene	5.072E-08	0	kg	-100%	2
NEI	Volatile Organic Compounds	1.599E-05	3.88E-05	kg	143%	2
NEI	Xylenes (Mixed Isomers)	0	0	kg	-	2

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Cumene U.S.-Average Emission Profile

Substance	Value	Unit	Flow Count	DQI Score	Database
1,2,4-TRIMETHYLBENZENE	4.4E-08	kg	5	2.15	TRI
1,3-Butadiene	1.9E-08	kg	5	1.62	NEI
2,2,4-Trimethylpentane	3.9E-08	kg	4	2	NEI
2-Methylnaphthalene	3.5E-13	kg	1	2	NEI
4,4'-ISOPROPYLIDENEDIPHENOL	1.6E-08	kg	2	3.03	TRI
7,12-Dimethylbenz[a]Anthracene	2.3E-13	kg	1	2	NEI
Acenaphthene	1.2E-13	kg	1	2	NEI
Acetaldehyde	1.1E-07	kg	2	2	NEI
Acetamide	2.2E-11	kg	1	2	NEI
Acetonitrile	1.8E-08	kg	1	2	NEI
Acetophenone	1.2E-06	kg	3	2.25	NEI
ALLYL ALCOHOL	2.0E-09	kg	1	1.91	TRI
Ammonia	3.1E-07	kg	6	2.33	TRI NEI
Antimony	1.5E-11	kg	1	2	NEI
ANTIMONY COMPOUNDS	1.5E-11	kg	1	2	TRI
Arsenic	1.0E-11	kg	1	2	NEI
Benzene	5.6E-06	kg	8	2.19	NEI
Benzo[a]Pyrene	0	kg	1	2	NEI
Benzo[g,h,i,]Perylene	5.6E-13	kg	4	3.39	TRI NEI
Beryllium	2.3E-13	kg	1	2	NEI
Biphenyl	0	kg	1	5	NEI
Cadmium	3.6E-11	kg	1	2	NEI
Carbon dioxide	2.3E-03	kg	5	2.10	eGGRT
Carbon Disulfide	0	kg	2	2.64	NEI
Carbon Monoxide	1.2E-07	kg	7	1.83	NEI
CARBONYL SULFIDE	0	kg	2	2.64	TRI NEI
Catechol	4.7E-10	kg	1	2	NEI
Chlorine	1.4E-10	kg	3	4.52	NEI TRI
Chloroform	6.1E-10	kg	1	2	NEI
CHLOROMETHANE	7.0E-09	kg	1	5	TRI
Chromium (VI)	5.8E-13	kg	1	2	NEI
Coal Tar	0	kg	1	2	NEI
Cobalt	0	kg	2	5	NEI
COPPER COMPOUNDS	4.3E-11	kg	1	5	TRI

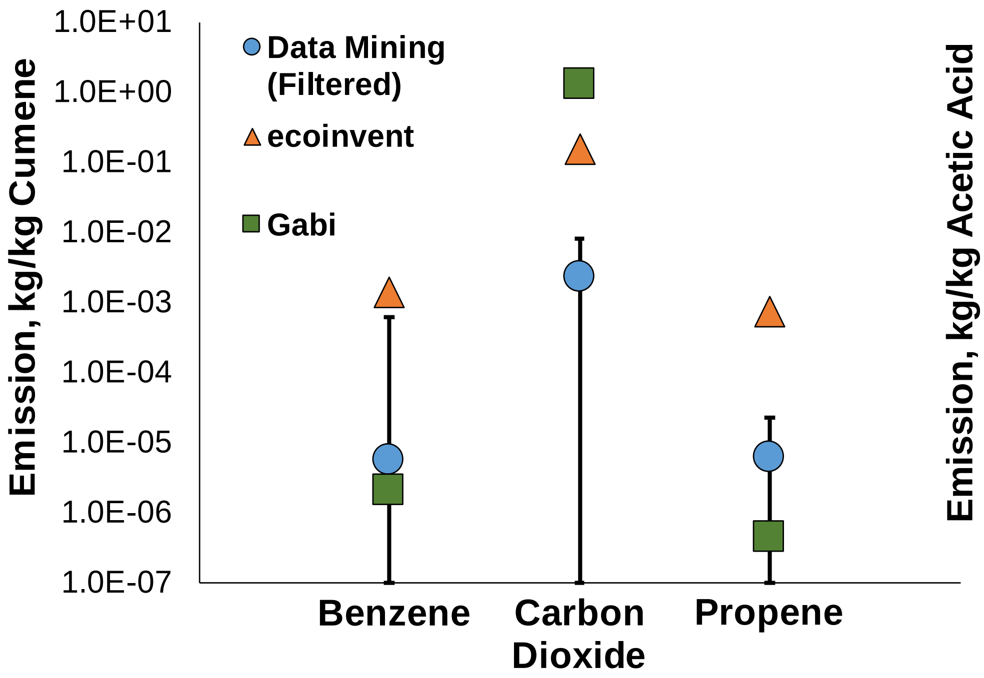
Substance	Value	Unit	Flow Count	DQI Score	Database
CUMENE	1.9E-05	kg	7	2.21	NEI TRI
CUMENE HYDROPEROXIDE	1.3E-08	kg	3	1.31	TRI
Cyanide	0	kg	1	5	NEI
CYCLOHEXANE	6.5E-08	kg	6	1.99	TRI
DICYCLOPENTADIENE	2.4E-09	kg	1	2	TRI
DIETHANOLAMINE	1.8E-08	kg	3	2.00	TRI NEI
Dinitrogen monoxide	8.7E-09	kg	5	1.99	eGGRT
DIOXIN AND DIOXIN-LIKE COMPOUNDS	4.2E-15	kg	3	2.98	TRI
Epichlorohydrin	9.6E-09	kg	1	1.96	NEI
Ethyl Benzene	4.8E-08	kg	7	1.95	NEI
ETHYLENE	3.1E-07	kg	5	2.12	TRI
Ethylene Dichloride	3.1E-12	kg	2	2	NEI
Ethylene Glycol	1.9E-10	kg	2	3.14	NEI TRI
Fluoranthene	1.2E-13	kg	1	2.00	NEI
Formaldehyde	1.3E-09	kg	2	2	NEI
FORMIC ACID	4.1E-11	kg	1	4.958	TRI
GLYCIDOL	0	kg	1	3.50	TRI
Glycol Ethers	9.4E-10	kg	1	2	NEI
Hexane	8.5E-08	kg	6	2.009	NEI
Hydrochloric Acid	4.2E-09	kg	4	3.744	NEI TRI
Hydrogen Cyanide	6.5E-08	kg	2	1.303	NEI
HYDROGEN FLUORIDE	4.7E-12	kg	3	4.084	NEI
Hydrogen Sulfide	0	kg	1	2.00	NEI
ISOPRENE	1.4E-08	kg	1	3.89	TRI
Lead	2.9E-11	kg	4	4.32	TRI NEI
Manganese	3.1E-10	kg	1	2	NEI
Mercury	1.6E-10	kg	5	2.305	NEI TRI
Methane	2.4E-06	kg	5	2.151	eGGRT
METHANOL	2.3E-08	kg	5	2.51	NEI TRI
Methyl Isobutyl Ketone	4.0E-09	kg	1	2.162	NEI
Methyl Tert-Butyl Ether	7.3E-10	kg	3	2.00	NEI
Methylene Chloride	1.2E-12	kg	1	2	NEI
MOLYBDENUM TRIOXIDE	5.7E-11	kg	2	5	TRI
M-XYLENE	6.9E-10	kg	1	5	TRI

Substance	Value	Unit	Flow Count	DQI Score	Database
Naphthalene	1.2E-08	kg	5	2.00	NEI
Nickel	2.5E-10	kg	3	4.08	NEI
Nitrogen Oxides	6.8E-07	kg	7	1.91	NEI
O-XYLENE	2.8E-10	kg	1	1.75	TRI
Phenanthrene	3.5E-13	kg	1	2	NEI
Phenol	2.4E-07	kg	5	2.66	NEI TRI
Phosphorus	2.1E-11	kg	1	2	NEI
PM10 Primary (Filt + Cond)	1.7E-06	kg	8	2.7887	NEI
PM2.5 Primary (Filt + Cond)	1.4E-06	kg	8	2.5435	NEI
POLYCYCLIC AROMATIC COMPOUNDS	1.7E-09	kg	5	3.2116	TRI NEI
Propionaldehyde	0	kg	1	2	NEI
PROPYLENE	6.2E-06	kg	7	2.1027	TRI
Pyrene	1.2E-13	kg	1	2.00	NEI
Selenium	1.2E-11	kg	1	2.00	NEI
Styrene	9.4E-10	kg	3	2	NEI
Sulfur Dioxide	2.7E-07	kg	7	2.25	NEI
SULFURIC ACID	1.9E-07	kg	2	1.3347	TRI
TERT-BUTYL ALCOHOL	0	kg	1	5.00	TRI
TETRACHLOROETHYLENE	0	kg	3	5.00	TRI NEI
Toluene	1.1E-06	kg	7	2.00	TRI NEI
Vinyl Acetate	1.2E-12	kg	1	2	NEI
Volatile Organic Compounds	5.3E-05	kg	8	2.14	NEI
Xylenes (Mixed Isomers)	8.3E-08	kg	7	2.00	NEI
ZINC COMPOUNDS	1.4E-09	kg	1	5	TRI

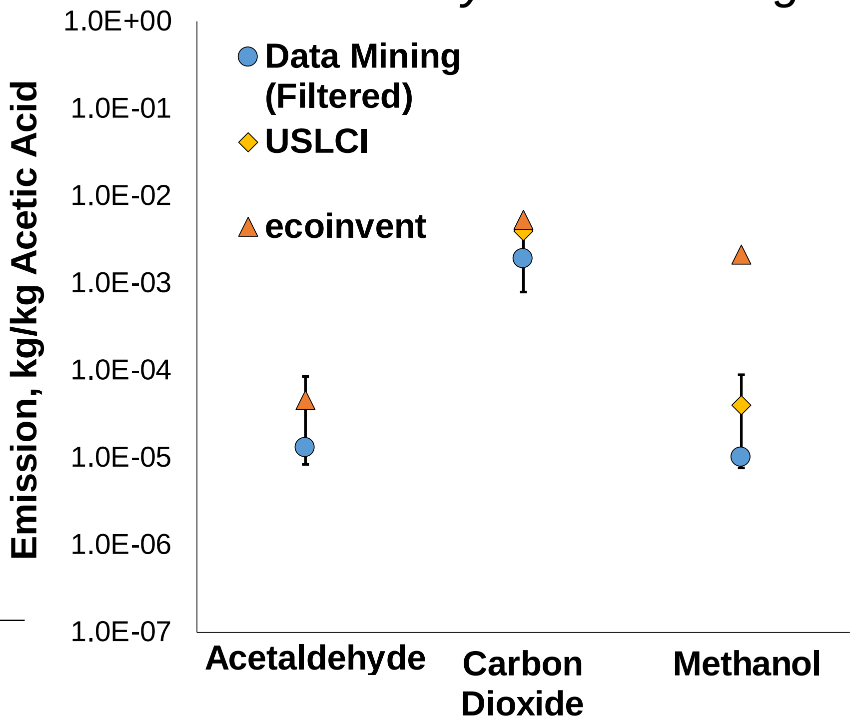
92 substances reported for the 8 facilities.
26 substances reported by >4 facilities.

Comparing Data Mining with Other LCI Datasets

Metadata-based filtering



Chemistry-based filtering



Data mining provides emission data that are lower than the theoretical ecoinvent data and within range of inventories based on more reliable sampling methods such as field studies (GaBi, USLCI).

The Work Continues

- **CBI data modeling**
  - Working with OPPT on PV sanitization method
  - Modeling all facilities for acetic acid, cumene, and sodium hydroxide
- **Metadata filtering**
  - Refine NEI procedures
  - TRI chemical use descriptions
  - RCRAinfo waste descriptions
- **Chemistry filtering**
  - Predict reaction side products using semantic data models
- **Convert NEI to Linked Open Data for automated modeling**

Disclaimer

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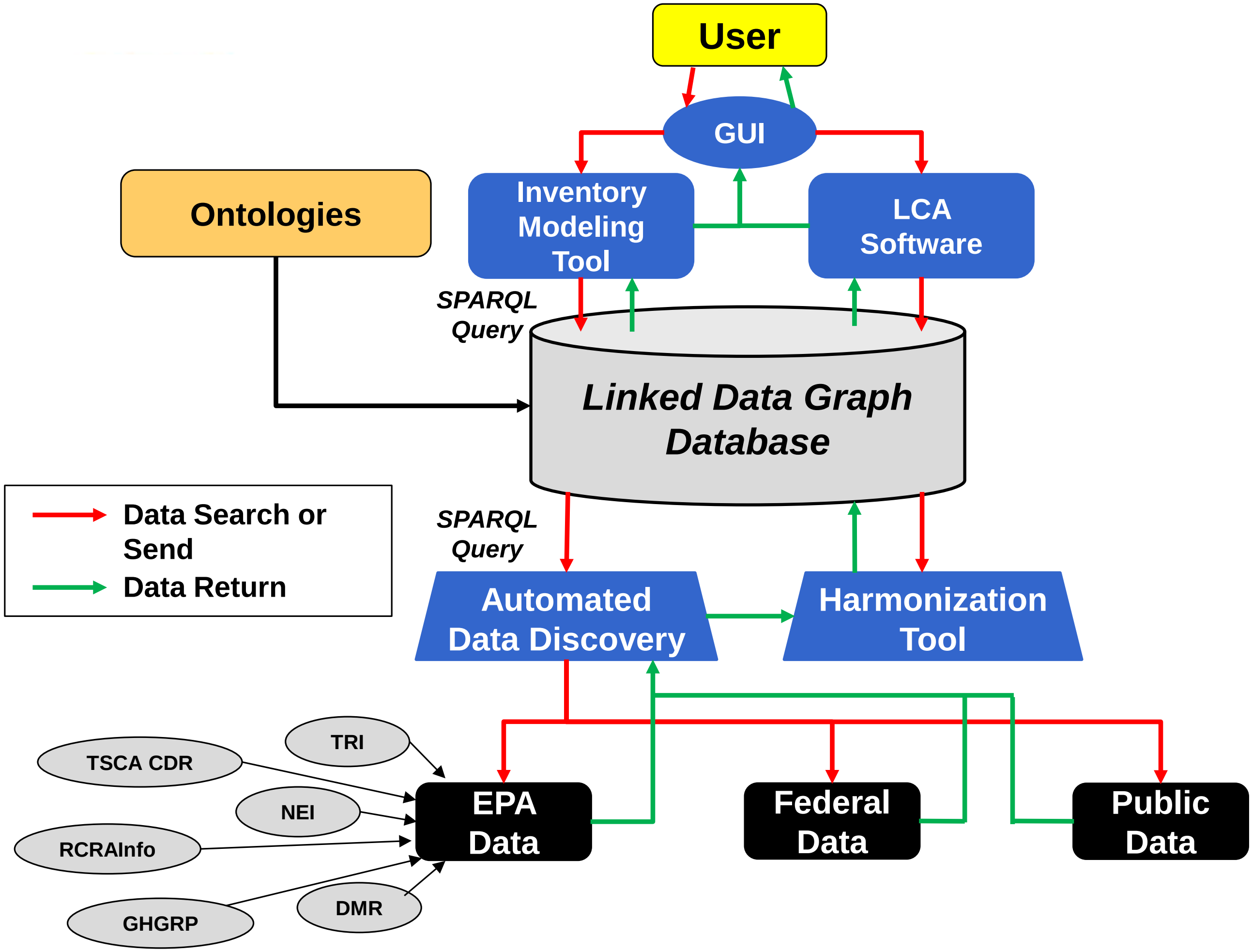
  - Chemical Safety and Sustainability National Research Program

"Ambient informatics is a state in which information is freely available at the point in space and time someone requires it, generally to support a specific decision."

- Adam Greenfield - Everyware

Thank you!

Future Vision: Life Cycle Inventory Modeling System



Note: Block coloring is used to identify similar system elements.