EPA United States Environmental Protection Agency

Incorporating Metadata from US EPA's Inventories to Generate More Reliable Life Cycle Emissions Data

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Office of Research and Development
National Risk Management Research Laboratory

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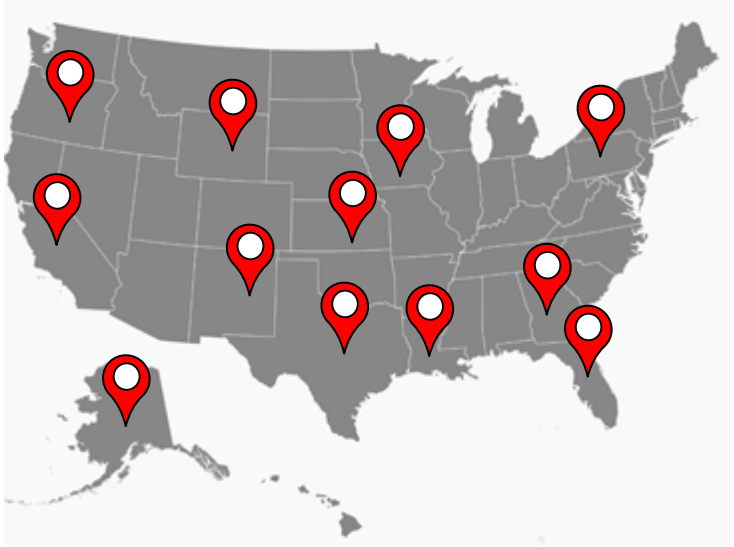
Inventories of Scale

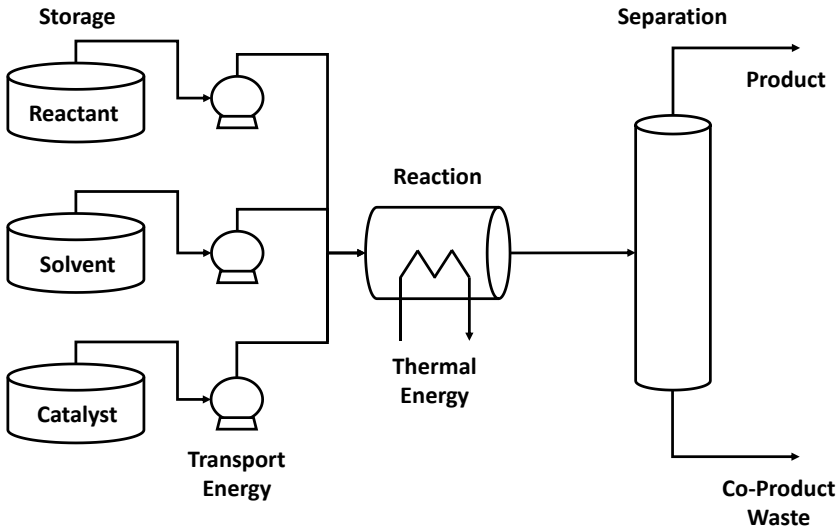
United States Environmental Protection Agency

Sector



Vs.

Process

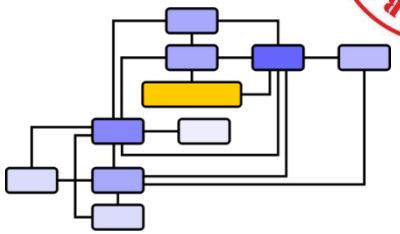


- Develop LCI by NAICS classification
- ***Uses:*** Input-Output LCA; Policy Analysis
- ***Challenges:*** millions of data points; multi-NAICS facilities; aggregate products and functional unit

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

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 publicly available



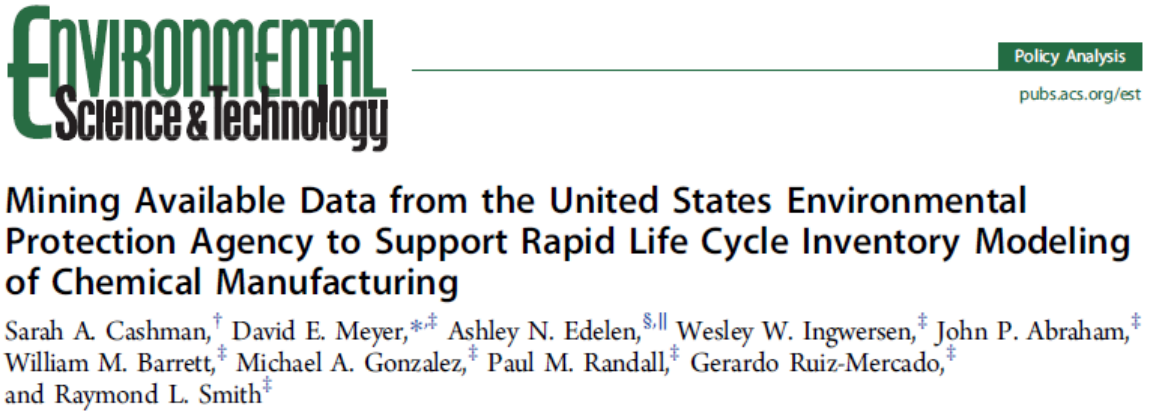
Emissions

Discharges

Waste

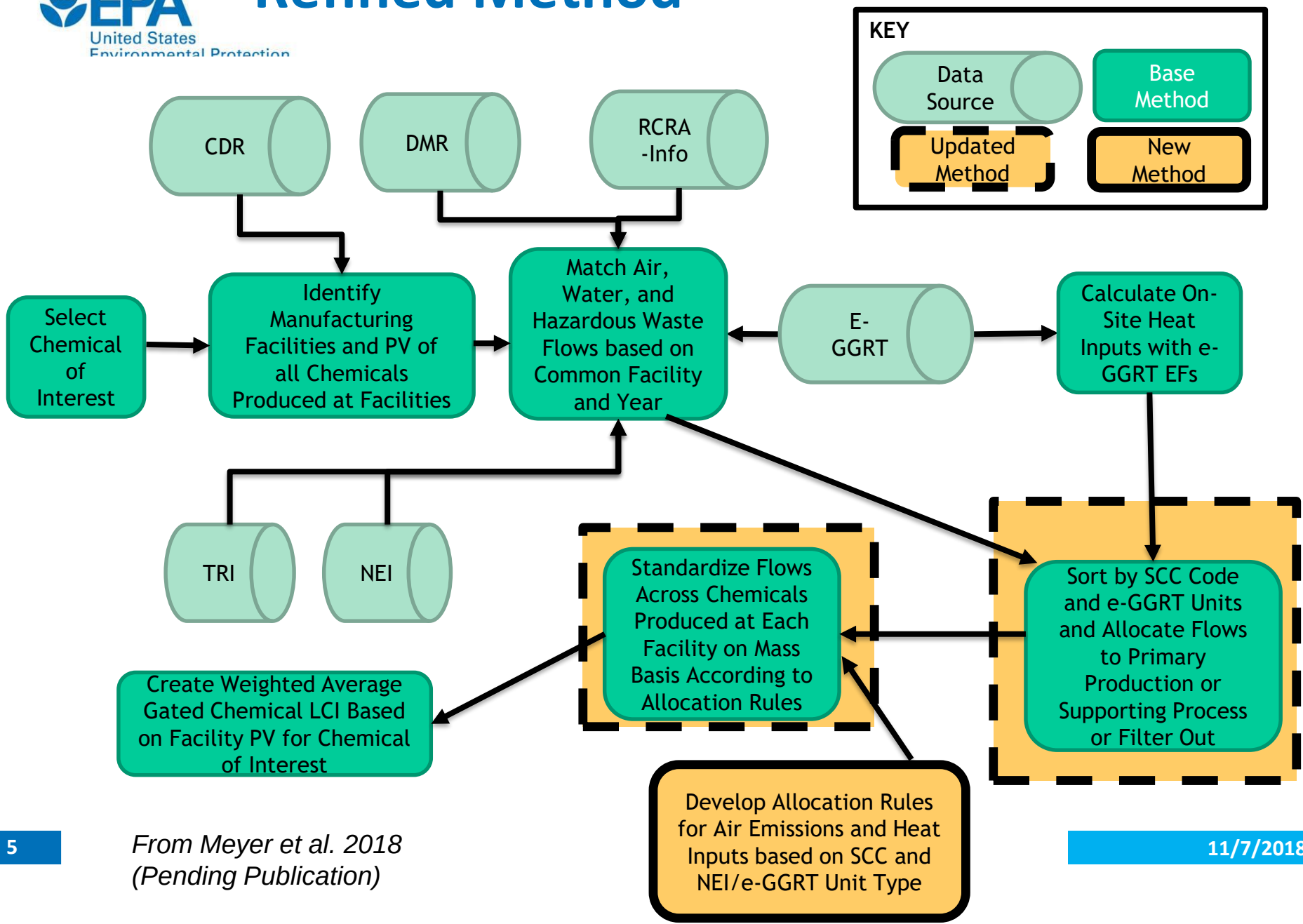
Data Mining EPA Data Sources: Original Method

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



- A method developed with automated data management in mind
  - 6 publicly available data sources
  - 12 discrete steps that can be translated into automated queries
  - repeatable
- Original method identified data quality issues
  - Facilities producing multiple chemicals
  - Overlap between data sources
  - Confidential production volumes

Refined Method



From Meyer et al. 2018 (Pending Publication)

Identify Key Process Metadata (NEI)

Source Classification Code Description	Emission Unit Description
External Combustion Boilers; Industrial; Natural Gas; 10-100 Million BTU/hr.	Boiler #2 (CMB2)
Industrial Processes; Chemical Manufacturing; Fuel Fired Equipment; Natural Gas: Process Heaters	Cumene unit process heater (CMB4)
Industrial Processes; Chemical Manufacturing; Plastics Production; Others Not Specified	Cumene process units
Industrial Processes; Chemical Manufacturing; Fugitive Emissions; Specify in Comments Field	Fugitive emissions
Industrial Processes; In-process Fuel Use; Liquified Petroleum Gas; General	Cumene unit process heater (CMB4)
Petroleum and Solvent Evaporation; Organic Chemical Transportation; Specific Liquid; Marine Vessels: Loading Rack	Barge loading rack (LR-B)
Industrial Processes; In-process Fuel Use; Liquified Petroleum Gas; General	Cumene unit process heater (CMB4)
Industrial Processes; Chemical Manufacturing; Phenol; General	Phenol unit
Industrial Processes; Chemical Manufacturing; Plastics Production; Others Not Specified	Cumene process units
Petroleum and Solvent Evaporation; Organic Chemical Transportation; Specific Liquid; Marine Vessels: Loading Rack	Phenol Loading rack (LR-1)
Industrial Processes; Chemical Manufacturing; Fugitive Emissions; Specify in Comments Field	Fugitive emissions
Industrial Processes; In-process Fuel Use; Liquified Petroleum Gas; General	Cumene unit process heater (CMB4)
Petroleum and Solvent Evaporation; Organic Chemical Storage; Fixed Roof Tanks - Aromatics; Benzene: Breathing Loss	Storage tanks #71 and 505
Petroleum and Solvent Evaporation; Petroleum Liquids Storage (non-Refinery); Bulk Plants; Loading Racks	Propane loading operation

Identify Key Process Metadata (e-GGRT)

Unit Name
Cumene Unit Process Heater
Cumene Unit Process Heater
Cumene Unit Process Heater
Boiler #1
Boiler #1
Boiler #1

Unit Typer
PRH (Process Heater)
PRH (Process Heater)
OB (Boiler, other)
OB (Boiler, other)
OB (Boiler, other)

Fuel Type
Natural Gas (Weighted U.S. Average)
Natural Gas (Weighted U.S. Average)
Natural Gas (Weighted U.S. Average)
Natural Gas (Weighted U.S. Average)
Natural Gas (Weighted U.S. Average)

Map combined unit type/fuel type/capacity to NEI's Source Classification Codes

Mine Metadata Text

Level-Unit Type-Chemical Type	Level	Unit Type	Chemical Type	SCC	SCC and NEI Unit Description (or e-GGRT and SCC Description)
combust-Heater-Cumene	combust	Heater	Cumene	30190003	Cumene unit process heater (CMB4) Unclassified Natural gas combustion Industrial Processes; Chemical Manufacturing; Fuel Fired Equipment; Natural Gas: Process Heaters
combust-Boiler-Distillate Oil	combust	Boiler	Distillate Oil	10200501	Boiler #2 (CMB2) Boiler distillate oil External Combustion Boilers; Industrial; Distillate Oil - Grades 1 and 2; Boiler
combust-Heater-Cumene	combust	Heater	Cumene	30190001	Cumene unit process heater (CMB4) Unclassified Oil fired Industrial Processes; Chemical Manufacturing; Fuel Fired Equipment; Distillate Oil (No. 2): Process Heaters
process-Fugitive Emissions-Unspecified	process	Fugitive Emissions	Unspecified	30188801	Fugitive emissions Process Equipment Fugitive Leaks Industrial Processes; Chemical Manufacturing; Fugitive Emissions; Specify in Comments Field

1. List if SCC related to combustion

2. Develop list of possible facility unit types

3. Develop list of possible chemical types

4. Mine text in full SCC/Unit descriptions to determine summary unit/chemical assignments

From Meyer et al. 2018 (Pending Publication)

Develop Process Allocation Rules

Level-Unit Type-Chemical Type	Allocation-Elementary Flow	Allocation-Intermediate Input
Combust-Boiler-Distillate Oil	Exclude-combust	Allocate over all chemicals
Combust-Boiler-Natural Gas	Exclude-combust	Allocate over all chemicals
Process-Chemical Production-caustic	Allocate 100% to sodium hydroxide	Exclude-process
Process-Chemical Production-chlorine	Allocate 100% to sodium hydroxide	Exclude-process
Process-Chemical Production-Ethylene Glycol	Exclude-unrelated chemical	Exclude-process
Process-Chemical Production-soda ash	Allocate 100% to sodium hydroxide	Exclude-process
Process-Chemical Production-Sulfur	Exclude-unrelated chemical	Exclude-process
Process-Chemical Production-Unspecified	Allocate over all chemicals	Exclude-process
Process-chloro-alkali-brine	Allocate 100% to sodium hydroxide	Exclude-process
Process-chloro-alkali-caustic	Allocate 100% to sodium hydroxide	Exclude-process
Process-chloro-alkali-chlorine	Allocate 100% to sodium hydroxide	Exclude-process
Process-chloro-alkali-hydrogen	Allocate 100% to sodium hydroxide	Exclude-process
Process-chloro-alkali-Sulfur	Allocate 100% to sodium hydroxide	Exclude-process
Process-chloro-alkali-Unspecified	Allocate 100% to sodium hydroxide	Exclude-process
Process-Tank-Benzene	Exclude-unrelated chemical	Exclude-process
Process-Terminal-Unspecified	Exclude-unrelated process	Exclude-process
Process-Cooling Tower-olefins	Exclude-unrelated chemical	Exclude-process

Green = all facility releases or intermediate heat inputs associated with this "Level-Unit Type-Chemical Type" to be allocated to focus chemical; orange = facility releases or intermediate heat inputs associated with this "Level-Unit Type-Chemical Type" to be filtered out of inventory; blue = facility releases or intermediate heat inputs associated with this "Level-Unit Type-Chemical Type" to be allocated over all chemicals produced at the facility

From Meyer et al. 2018 (Pending Publication)

Process-Allocated Inventory Example

Level-Unit Type-Chemical Type	Level	Unit Type	Chemical Type	SCC	SCC and NEI Unit Description (or e-GGRT and SCC Description)	Allocation-Elementary Flow	Allocation-Intermediate Input
combust-Heater-Cumene	combust	Heater	Cumene	30190003	Cumene unit process heater (CMB4) Unclassified Natural gas combustion Industrial Processes; Chemical Manufacturing; Fuel Fired Equipment; Natural Gas: Process Heaters	Exclude - combust	Allocate 100% cumene
combust-Boiler-Distillate Oil	combust	Boiler	Distillate Oil	10200501	Boiler #2 (CMB2) Boiler distillate oil External Combustion Boilers; Industrial; Distillate Oil - Grades 1 and 2; Boiler	Exclude - combust	Allocate across all chemicals
combust-Heater-Cumene	combust	Heater	Cumene	30190001	Cumene unit process heater (CMB4) Unclassified Oil fired Industrial Processes; Chemical Manufacturing; Fuel Fired Equipment; Distillate Oil (No. 2): Process Heaters	Exclude - combust	Allocate 100% cumene
process-Fugitive Emissions-Unspecified	process	Fugitive Emissions	Unspecified	30188801	Fugitive emissions Process Equipment Fugitive Leaks Industrial Processes; Chemical Manufacturing; Fugitive Emissions; Specify in Comments Field	Allocate across all chemicals	Exclude-process
combust-Heater-Cumene	combust	Heater	Cumene	39001099	Cumene unit process heater (CMB4) Unclassified Propane fired Industrial Processes; In-process Fuel Use; Liquified Petroleum Gas; General	Exclude - combust	Allocate 100% cumene
process-Tank-Organic Chemical	process	Tank	Organic Chemical	40714698	Chemical storage tanks (43 Tanks) Storage Tank Petroleum and Solvent Evaporation; Organic Chemical Storage; Fixed Roof Tanks - Miscellaneous; Specify In Comments: Working Loss	Allocate across all organic chemicals	Exclude-process
process-Tank-Cumene	process	Tank	Cumene	40703605	Storage tanks #72 and 506 Storage Tank Petroleum and Solvent Evaporation; Organic Chemical Storage; Fixed Roof Tanks - Aromatics; Cumene: Breathing Loss	Allocate 100% cumene	Exclude-process

From Meyer et al. 2018 (Pending Publication)

Process Allocation Inventory Effects

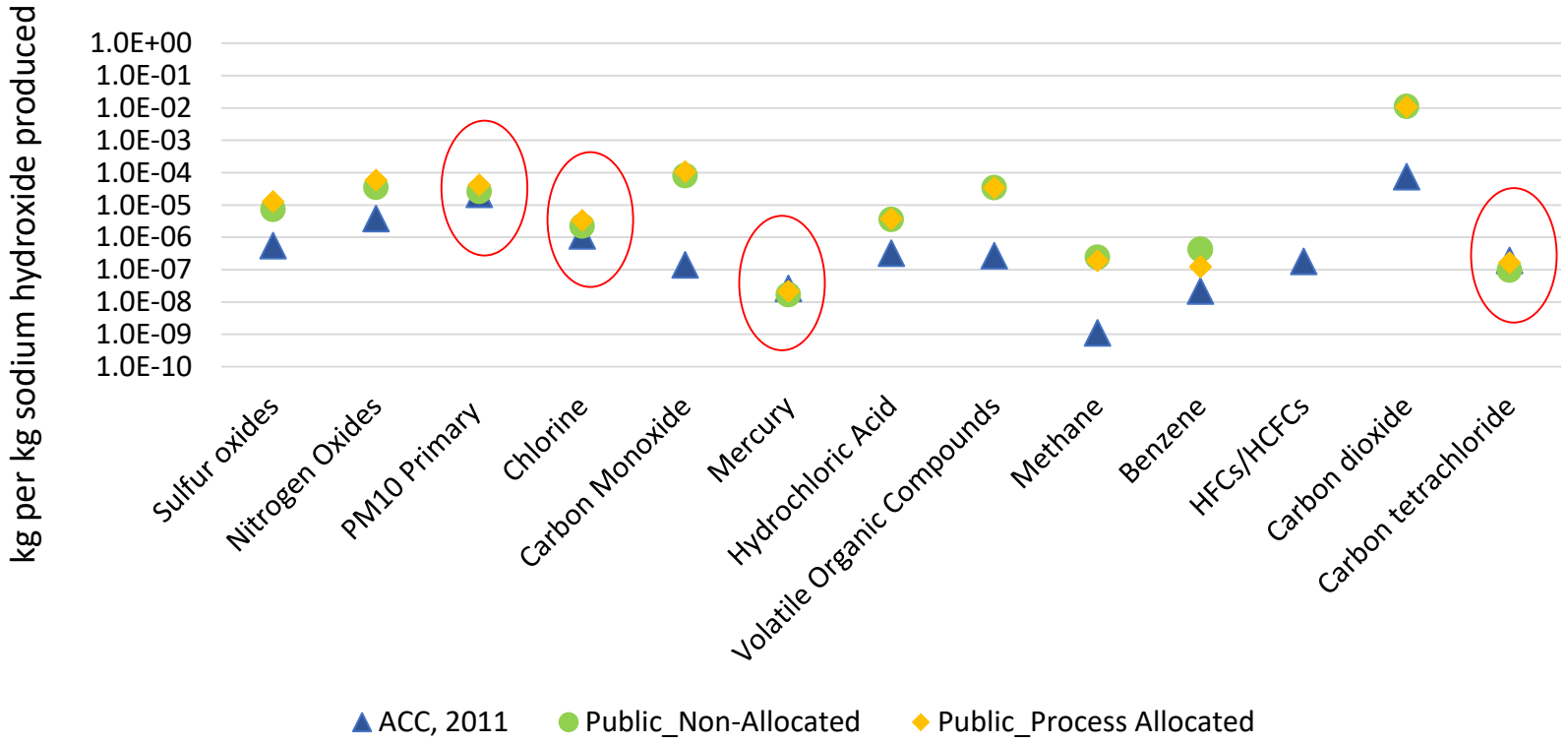
Air Releases reported by at least 7 of the 8 facilities

	kg per kg Cumene Produced					
Air Releases	**Non-Allocated**	**Process Allocated**	**% Change with Process Allocation**	**Facility Count**	**Flow Reliability Score**	**Data Source**
Toluene	6.3E-07	1.3E-06	110%	7.00	2.00	TRI NEI
Cumene	1.0E-05	1.9E-05	94%	7.00	2.20	TRI NEI
Benzene	4.3E-06	5.9E-06	37%	8.00	2.19	NEI
Propylene	5.9E-06	7.8E-06	33%	7.00	2.10	TRI
Volatile Organic Compounds	6.3E-05	6.2E-05	-2%	8.00	2.14	NEI
Ethyl Benzene	1.3E-07	1.0E-07	-21%	7.00	1.95	NEI
PM10 Primary	2.4E-06	1.8E-06	-27%	7.00	2.81	NEI
Nitrogen Oxides	3.9E-06	1.0E-06	-74%	7.00	1.94	NEI

Propylene, benzene, cumene, and carbon dioxide are commonly reported emissions from the manufacture of cumene in commercially available LCI databases

From Meyer et al. 2018 (Pending Publication)

Comparison to Existing Process-Level Inventory: Sodium Hydroxide



22 Air Emissions Completely Filtered from Sodium Hydroxide Inventory with Process Allocation

From Meyer et al. 2018 (Pending Publication)

Reporting Methods and Data Quality

- **Flow reliability** from data source bases of estimate

Source	Code	Description
NEI	1	Continuous monitoring system
NEI	2	Engineering Judgement
NEI	3	Material Balance
NEI	4	Stack Test
NEI	5	USEPA Speciation Profile
NEI	7	Manufacturer Specification
NEI	8	US EPA Emission Factor (no control efficiency used)
NEI	9	S/L/T Emission Factor (no control efficiency used)
NEI	10	Site-specific emission factor (no control efficiency used)
NEI	13	Other Emission Factor (no Control Efficiency used)

Source	Code	Description
TRI	O	other approaches
TRI	C	mass balance calculations
TRI	E1	published emission factors
TRI	E2	site-specific emission factors
TRI	M1	continuous monitoring data
TRI	M2	periodic or random data or measurements

- **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 e-GGRT metadata) and the coverage of total U.S. production
- **Sampling methods correlation** depends on the percentage of total U.S. production captured by CDR

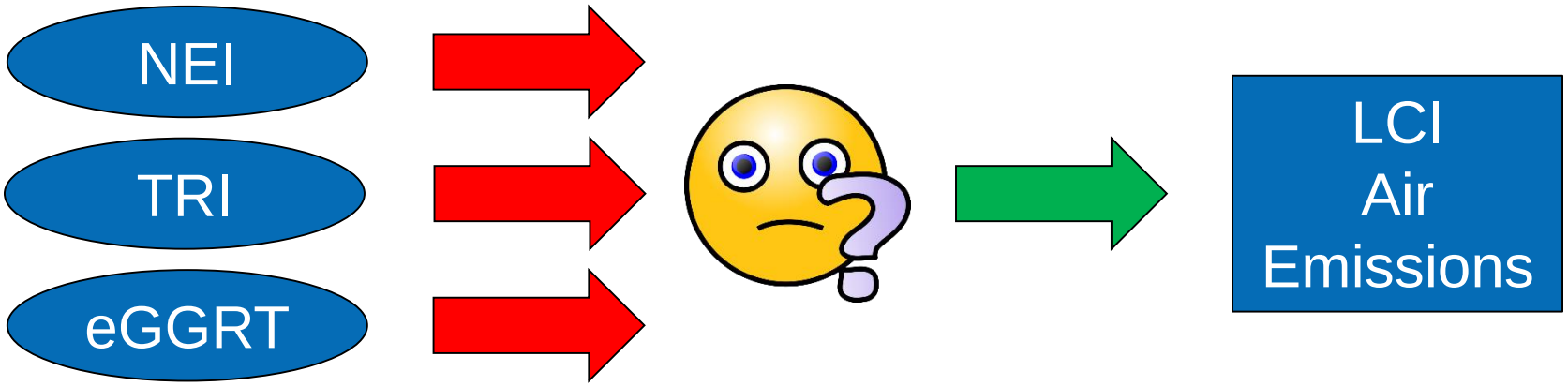
DQI Flow Reliability Scores

Using methods described in Edelen and Ingwersen (2016), assign flow reliability scores from data source bases of estimates:

Data Source	Basis of Estimate Code	Basis of Estimate Description	Basis of Estimate Type	DQI Flow Reliability Score
NEI	1	Continuous monitoring system	Verified measurement	1
NEI	2	Engineering Judgement	Undocumented estimate	5
TRI	E2	Site-specific emission factors	Verified calculation	2
TRI	M2	Periodic or random data or measurements	Verified measurement	1
e-GGRT	Tier 1 (Equation C-1)	CO_2 emission calculations from measured fuel use	Verified calculation	2
RCRAInfo	N.A.	N.A.	Verified measurement	1
DMR	N.A.	Chemical analysis and metered flow	Verified measurement	1

From Meyer et al. 2018 (Pending Publication)

Resolving Inventory Overlap



- ***NEI over TRI*** (greatest overlap between these databases)
  - Overlap related to HAPS
  - Facilities 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, 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

From Meyer et al. 2018 (Pending Publication)

CDR Production Volume Confidential Business Information

		Acetic Acid	Cumene	Sodium Hydroxide
Facility Count	At Least One Chemical PV Produced on Site Is CBI	6	5	5
	Focus Chemical PV is CBI	16	1	14
	No Chemical PV is CBI	2	3	19
	Facility Name/Location is CBI	1	1	8
	Total Facilities	25	10	46
	% Facilities with Focus Chemical CBI	64%	10%	30%
	% Facilities with CBI	92%	70%	59%
Production Coverage	Total Public Production (tonne)	45,142	2,609,310	3,878,022
	Total U.S. Production (tonne)	3,853,186	3,195,952	12,627,763
	% U.S. PV Coverage without CBI	**1.2%**	**82%**	**31%**

From Meyer et al. 2018 (Pending Publication)

Proposed CDR CBI Sanitization

Multiple types of CBI (focus chemical or other chemical produced at facility) and multiple aggregation steps

$$EF_{NOx,Site\ 1} = \frac{Z\ kg\ of\ NOx}{Y\ kg\ of\ total\ chemicals\ produced}$$

$$EF_{NOx,U.S.\ average} = \left[EF_{NOx,Site\ 1} \times \frac{X_{Site\ 1}}{X_{Site\ 1} + X_{Site\ 2} + X_{Site\ 3}}\right] + \left[EF_{NOx,Site\ 2} \times \frac{X_{Site\ 2}}{X_{Site\ 1} + X_{Site\ 2} + X_{Site\ 3}}\right] + \left[EF_{NOx,Site\ 3} \times \frac{X_{Site\ 3}}{X_{Site\ 1} + X_{Site\ 2} + X_{Site\ 3}}\right]$$

Where:

Z = Site 1 releases of NOx in kg

Y = Total chemicals produced at Site 1 or process allocated chemical production

X = Focus Chemical Production at Site

Summary of Recommendations

Indicator		Metadata Improvement
Flow Reliability		Source used for the same release types can be selected based on the best flow reliability score. Flow overlap between sources is removed.
Flow Representativeness	*Temporal Correlation*	Reporting year is known, sources are regularly updated.
	Geographical Correlation	Captures all large U.S. chemical manufacturers and full geospatial information is available.
	Technological Correlation	The process allocation approach improves the process design/operation representativeness.
	Data Collection Methods	Representation from >80% of chemical producers is achievable through the CDR CBI sanitization approach. All data collected on an annual basis.

From Meyer et al. 2018 (Pending Publication)

The Work Continues

- **CBI data modeling**
  - Working with EPA OPPT on production volume sanitization method
- **Metadata filtering**
  - RCRAinfo waste descriptions
- **Convert to automated modeling**

United States Environmental Protection Agency

Disclaimer

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