

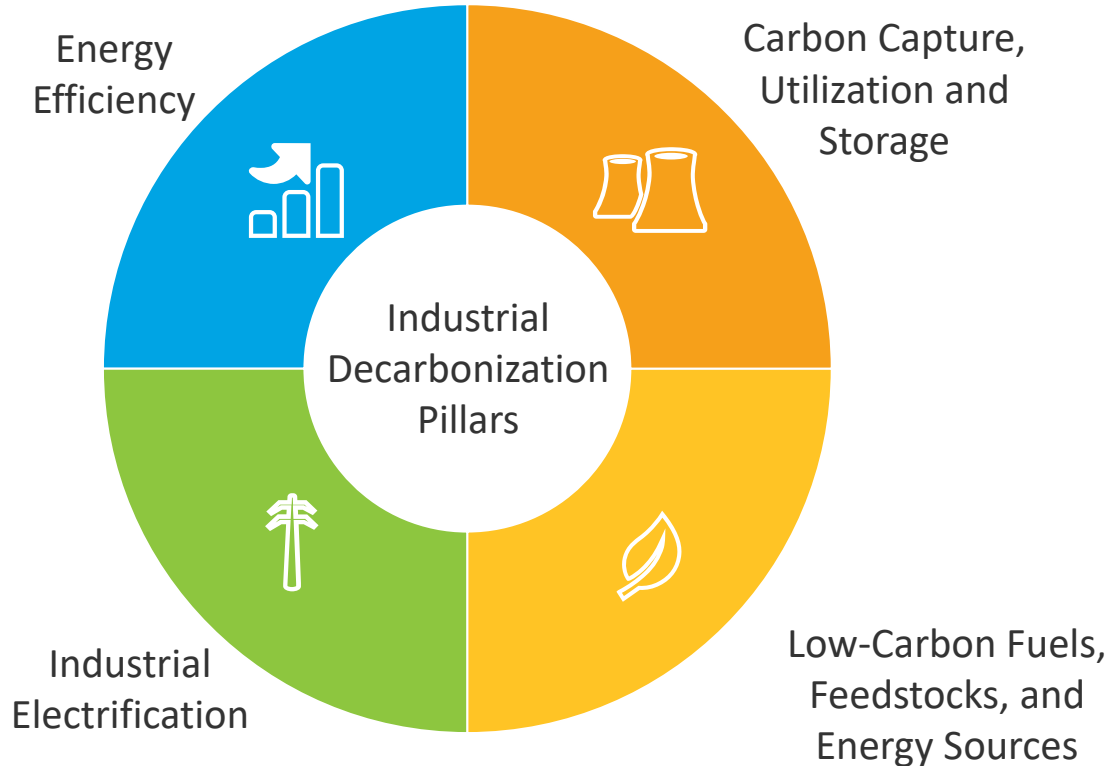
Generating Emissions Inventory for Carbon Capture and Storage Analysis for Carbon-Intensive Industrial Sectors

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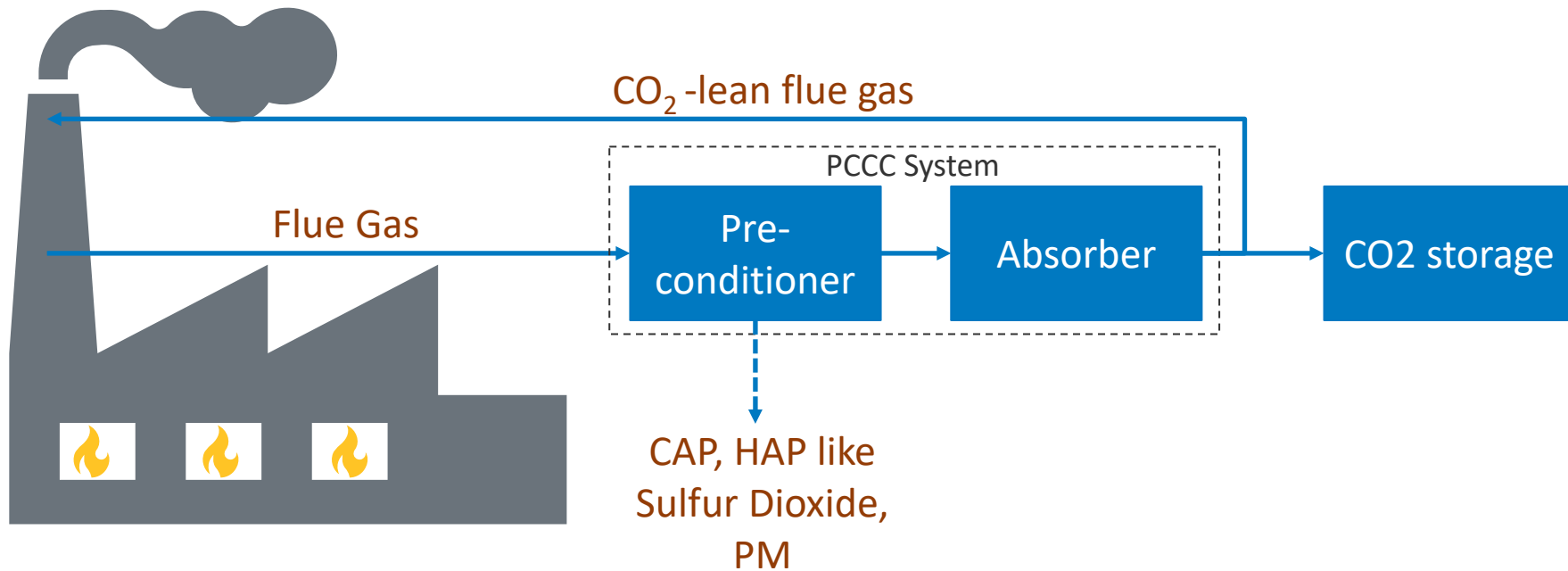
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Carbon Capture, Storage and Utilization (CCUS) is crucial to reaching net-zero emissions by 2050



Post Combustion Carbon Capture (PCCC) can result in capture of pollutants other than CO₂



The type and amount of CAP/HAP which can be captured is not well understood

Co-benefits of carbon capture depend on the characteristics of the industrial process:

- Concentration and type of pollutants
- Physical properties of the flue gas

However, there is a lack of data about flue gas pollutant concentrations at the national level



Air Emissions Grouped by Industrial Sectors (AEGIS)



SIGNIFICANCE: Facilitate the estimation of co-benefits of post-combustion carbon capture in industrial facilities for emissions reductions of regulated pollutants.



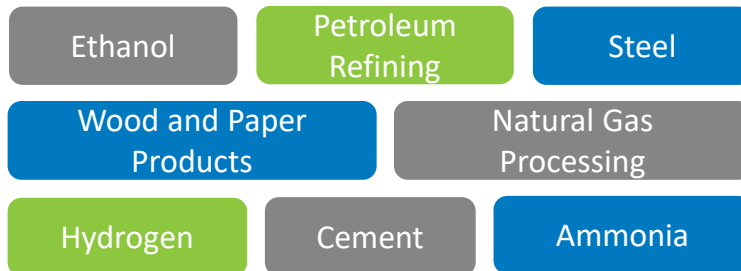
OBJECTIVE: Develop a high-resolution inventory of air pollutant flows from carbon-intensive industrial point emissions sources in 8 industrial sectors.



CALCULATED PARAMETERS:

- Types and amounts of pollutants in flue streams
- Concentration of pollutants
- Temperature of the flue gas
- Height of the flue stack

Sectors Covered



Methods: The inventory was developed in 3 steps

Compile AEGIS database of industrial facilities and pollutant flows from EPA databases

Calculate total amount and concentration of pollutants in the flue gas

Statistical analysis

Methods: Data Sources

Compile AEGIS database of industrial facilities and pollutant flows from EPA databases

Calculate total amount and concentration of pollutants in the flue gas

Statistical analysis

GHGRP

The Greenhouse Gas Reporting Program (GHGRP) estimates the **total greenhouse gas emissions** across all sectors using national-level data. Approximately 8,000 facilities are required to report their emissions annually. (U.S. Environmental Protection Agency [a])

NEI

The National Emissions Inventory (NEI) provides detailed estimates of **air emissions of criteria pollutants, criteria precursors, and hazardous air pollutants from air emissions sources** reported every 3 years. NEI point sources include emissions estimates for larger sources that are located at a fixed location. (U.S. Environmental Protection Agency [b])

TRI

The Toxics Release Inventory (TRI) is a resource for learning about **toxic chemical releases** and pollution prevention activities reported by industrial and federal facilities. (U.S. Environmental Protection Agency [c])

Methods: Facility Level AEGIS Compilation

Databases and STEWI

EPA Databases

GHGRP

NEI

TRI

NEI Stack Information

Standardized Emissions and Waste Inventories (StEWI)
[Ingwersen et al. (2021)]

Sectoral Grouping

NAICS Codes

Facility Level Information on GreenHouse gases Tool (FLIGHT)
OR
User-Defined

Combined Flow Inventory

Sectoral Inventory

FRS IDs

GHGRP

NEI

TRI

Combined Flow Inventory

Final Sectoral Inventory

GHGRP FRS IDs

Issues and Debugger

Solvable

- NAICS code partly wrong
- FRS ID mismatch with at least one correct FRS ID
- Multiple NAICS code for same sector

Unsolvable

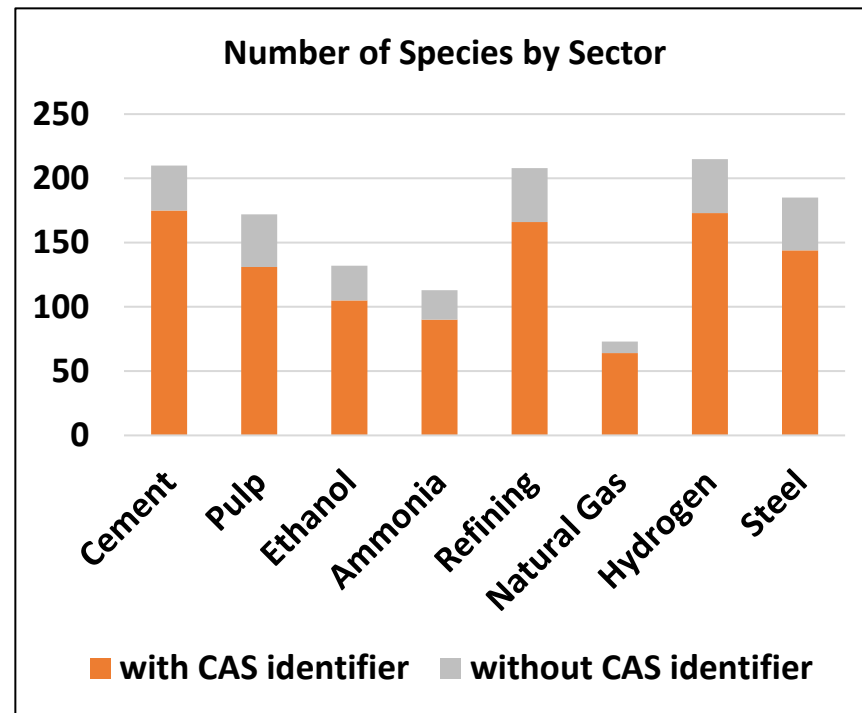
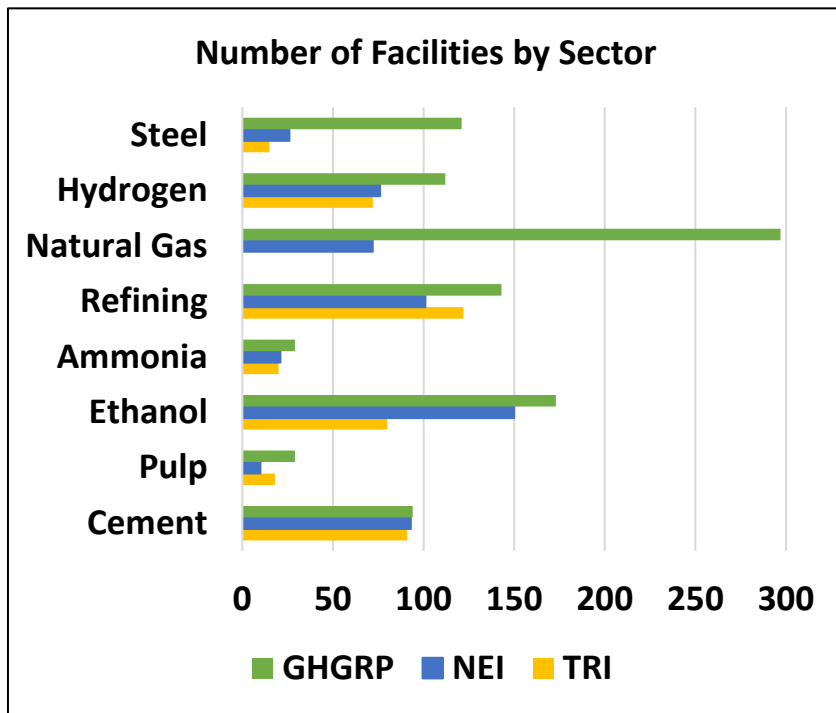
- Facility completed missing from STEWI
- All NAICS code wrong
- All FRS IDs are wrong
- Facility IDs within the same database wrong

Debugger

Issue Files

AEGIS 1.0

Results – Industrial Sectors Overview

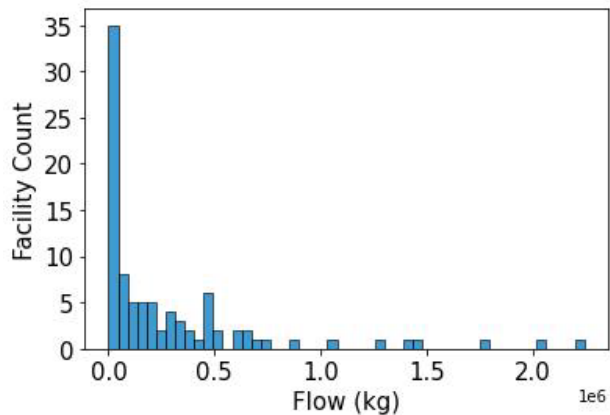


CAS = Chemical Abstract Services: Enables connections to other databases

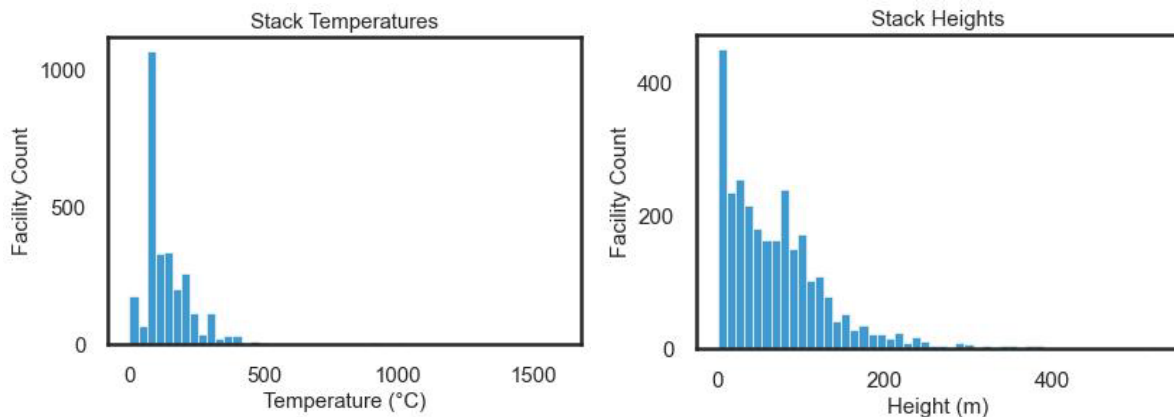
Cement Sector Exploration

Emissions	Total (million metric ton)	% of US emissions
CO ₂	67	1.3
SO ₂	0.027	1.13
VOC	0.005	
PM _{2.5-10}	0.008	

Distribution of SO₂ flow from cement facility stacks



Distribution of stack parameters across 93 facilities with 2960 stacks



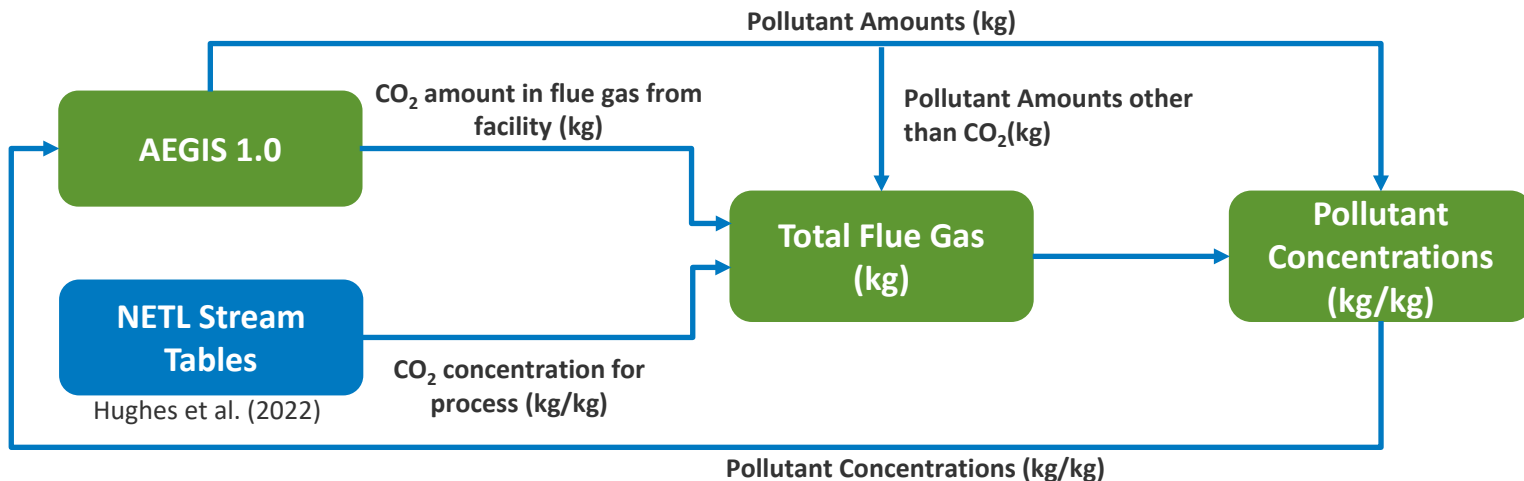
Stack Data	Temp Range	Height Range
68% of all fac	60-200 C	1 – 100m

Methods: Concentration

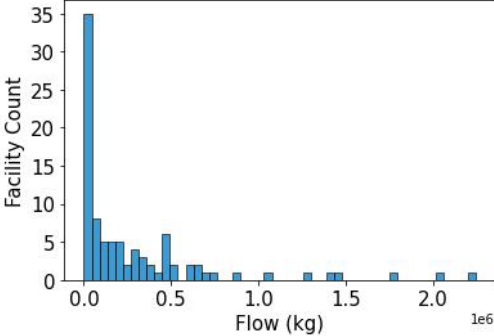
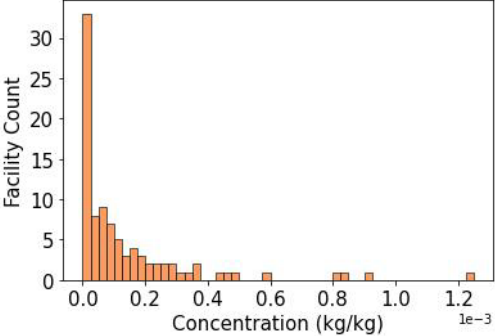
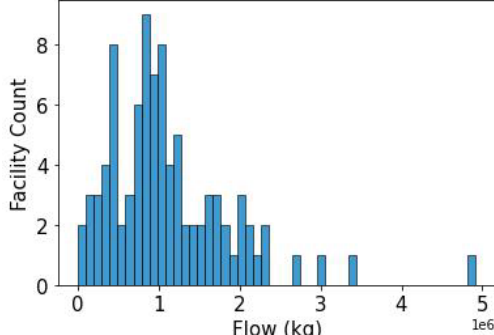
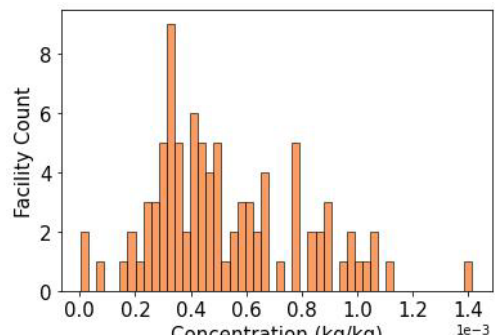
Compile AEGIS database of industrial facilities and pollutant flows from EPA databases

Calculate total amount and concentration of pollutants in the flue gas

Statistical analysis



Cement Sector: Emissions Distribution

Distribution of Pollutants in Cement Facility Stacks		
	Total Flow Amount	Concentration
Sulfur Dioxide (SO ₂)	 <p>A histogram showing the distribution of Sulfur Dioxide total flow amounts across various cement facilities. The x-axis is labeled 'Flow (kg)' with a multiplier of 1e6, ranging from 0.0 to 2.0. The y-axis is labeled 'Facility Count', ranging from 0 to 35. The distribution is highly skewed to the right, with a peak facility count of approximately 35 for flow amounts between 0.0 and 0.1 million kg.</p>	 <p>A histogram showing the distribution of Sulfur Dioxide concentrations across various cement facilities. The x-axis is labeled 'Concentration (kg/kg)' with a multiplier of 1e-3, ranging from 0.0 to 1.2. The y-axis is labeled 'Facility Count', ranging from 0 to 30. The distribution is highly skewed to the right, with a peak facility count of approximately 32 for concentrations between 0.0 and 0.05 kg/kg.</p>
Nitrogen Oxide (NOx)	 <p>A histogram showing the distribution of Nitrogen Oxide total flow amounts across various cement facilities. The x-axis is labeled 'Flow (kg)' with a multiplier of 1e6, ranging from 0 to 5. The y-axis is labeled 'Facility Count', ranging from 0 to 8. The distribution is roughly bell-shaped, peaking at a facility count of 9 for flow amounts between 0.8 and 1.0 million kg.</p>	 <p>A histogram showing the distribution of Nitrogen Oxide concentrations across various cement facilities. The x-axis is labeled 'Concentration (kg/kg)' with a multiplier of 1e-3, ranging from 0.0 to 1.4. The y-axis is labeled 'Facility Count', ranging from 0 to 8. The distribution is roughly bell-shaped, peaking at a facility count of 9 for concentrations between 0.3 and 0.4 kg/kg.</p>

Methods: Removing Outliers

Compile AEGIS database of industrial facilities and pollutant flows from EPA databases

Calculate total amount and concentration of pollutants in the flue gas

Statistical analysis

AEGIS 1.0

(per sector)

Emission A
Concentration
List

Emission B
Concentration
List

Emission C
Concentration
List

(per compound)

**Isolation
Forest Model
[Liu et al.
(2008)] outlier
detection**

Removing
outlier
facilities

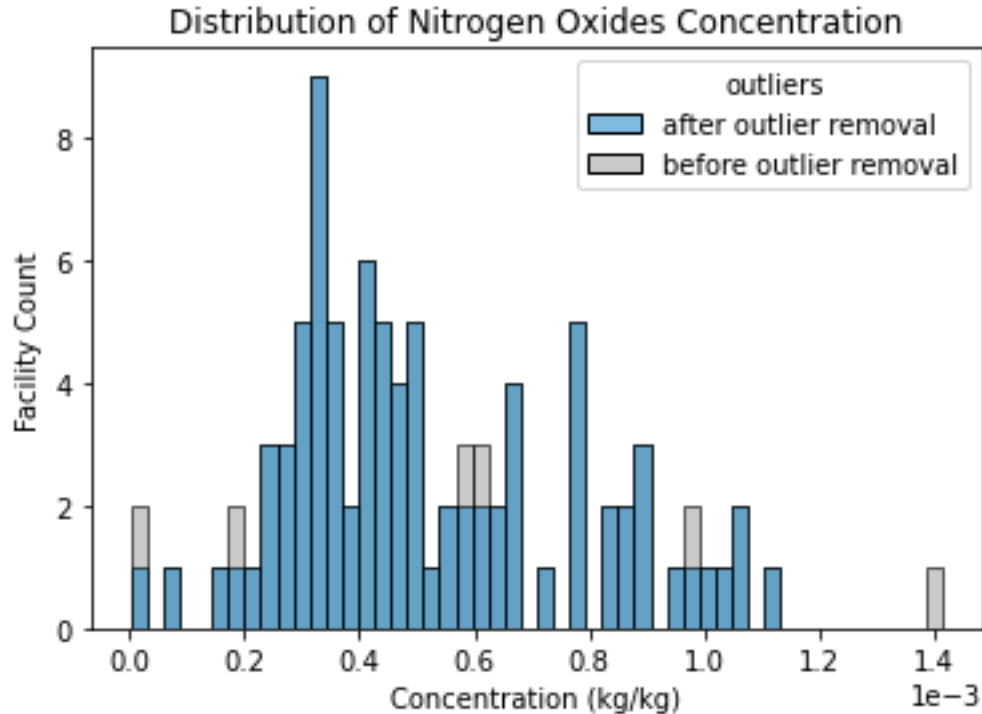
Cleaned List A

Cleaned List B

Cleaned List C

AEGIS 2.0

Cement Sector Exploration



Outlier Removal Status	1 st -2 nd -3 rd Quartile Values
Before	0.33-0.46-0.67
After	0.33-0.45-0.66

Methods: Process Level

Databases and StEWI

EPA Databases

GHGRP

Fuel

Unit

NEI

StEWI [Ingwersen
et al (2021)]

Source
Classification
Code

Sectoral Grouping

NAICS Codes

Facility Level Information on GreenHouse gases
Tool (FLIGHT)
OR
User-Defined

Improving the NAICS Code Grouping
(Future)

GHGRP
Process
inventory

NEI
process
inventory

GHGRP process
sectoral

NEI process
sectoral

Current results

GHGRP

Methane
CO₂
Nitrogen Oxide
Biogenic CO₂

Unit models
Unit types

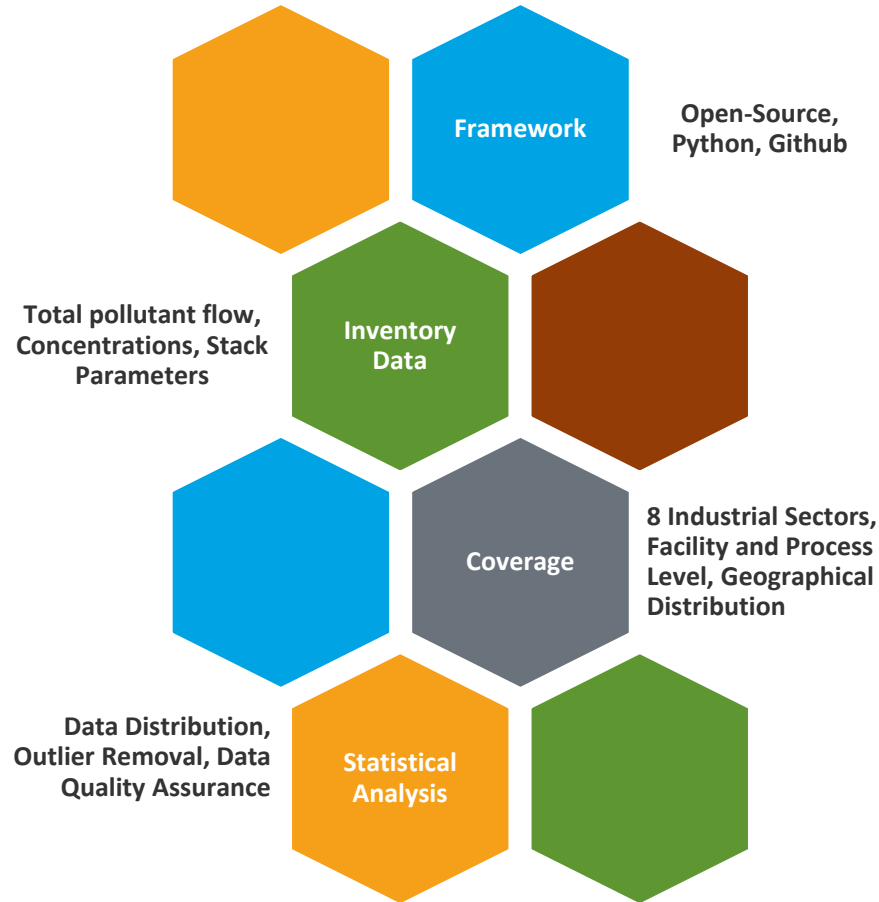
Fuel used

NEI

139 pollutants

Unit types
Unit description

Conclusion



Future plans for AEGIS

EPA

Providing feedback to the StEWI development group regarding the issues concerning the harmonization of databases, errors in the original data sources etc.

Process Level Resolution

Detailed inventory development at the process level within each facility to explore flue gas concentration within individual unit operations of the facility.

Life Cycle Inventory Development

Creating a robust life cycle inventory from collected emissions data, informing the U.S. Life Cycle Inventory (National Renewable Energy Laboratory, 2012) repository development etc.

AEGIS - Air Emissions Grouped By Industrial Sectors



OBJECTIVE: Develop a high-resolution inventory of pollutant flows from carbon-intensive industrial point emissions sources.

Compile database of industrial facilities and pollutant flows from EPA databases

Calculate concentration of pollutants in the flue gas

Statistical analysis



SIGNIFICANCE: Facilitate the estimation of co-benefits of post-combustion carbon capture (PCCC) in industrial facilities for emissions reductions of regulated pollutants.

Sectors Covered

Ethanol

Petroleum Refining

Steel

Wood and Paper Products

Natural Gas Processing

Hydrogen

Cement

Ammonia



TEAM:





Thank you! Questions?

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NREL/PR-6A20-86511

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Complete Automated Python Framework

