Expanding the Inventory of Emissions in the NETL Power Plant Flexible Model

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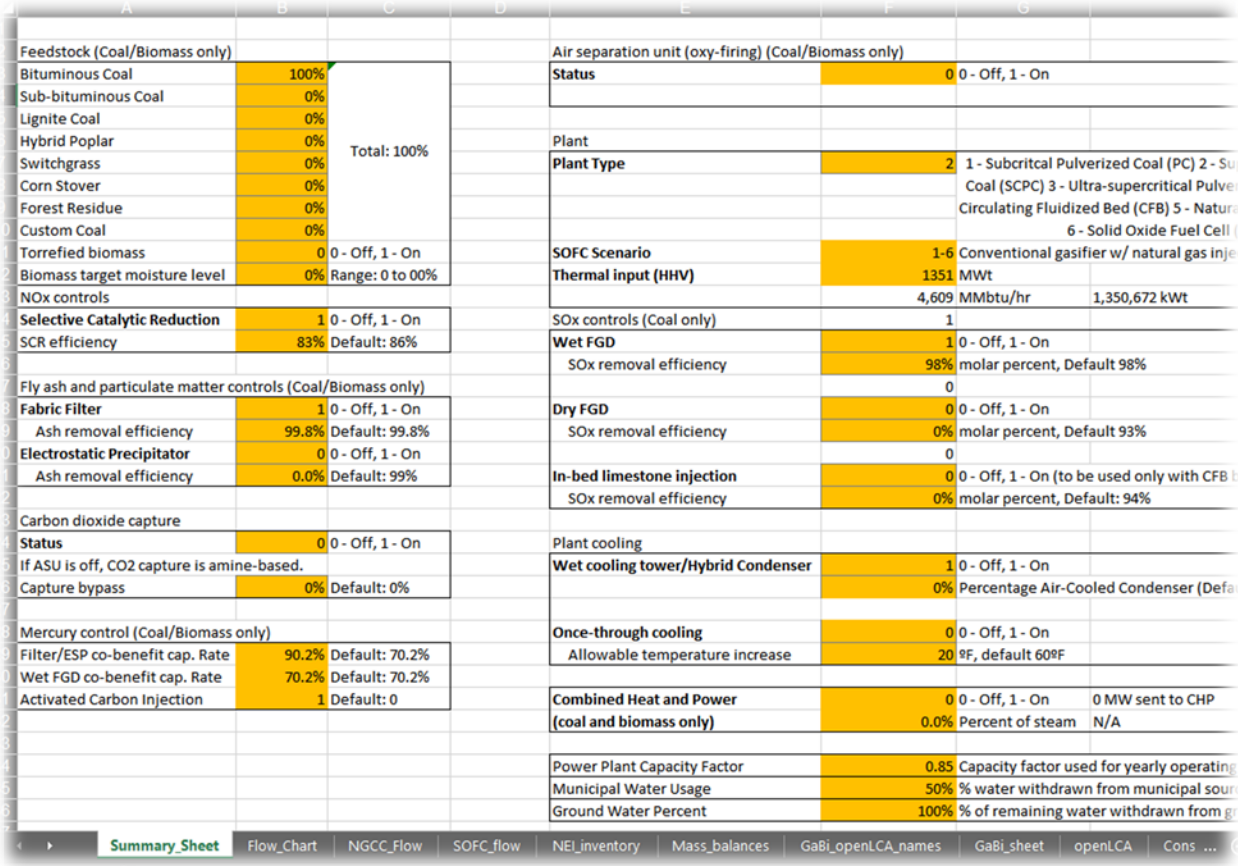
About the Power Plant Flexible Model

(PPFM)

- **Spreadsheet model for**
  - pulverized coal
  - circulating fluidized bed power plants
  - natural gas combined cycle
  - solid oxide fuel cell power plants
- **Reduced-order model allowing changing of coal characteristics and pollution control equipment configuration**
- **Emissions limited to those available in NETL techno-economic assessments**
  - CO_2, SO_2, Hg, NO_X, Particulate

https://netl.doe.gov/research/energy-analysis/search-publications/vuedetails?id=785



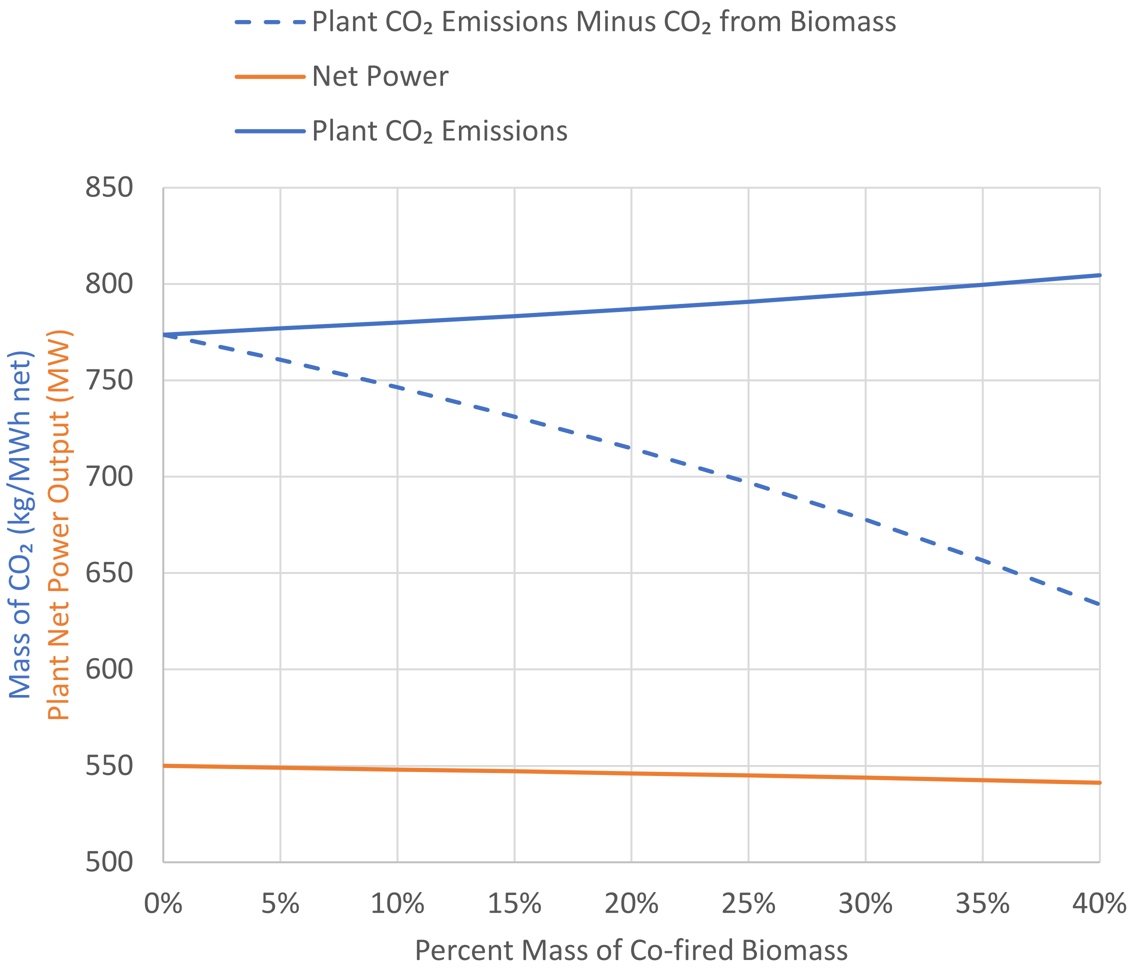
Feedstock (Coal/Biomass only)		
Bituminous Coal	100%	
Sub-bituminous Coal	0%	
Lignite Coal	0%	
Hybrid Poplar	0%	Total: 100%
Switchgrass	0%	
Corn Stover	0%	
Forest Residue	0%	
Custom Coal	0%	
Torrefied biomass	0	0 - Off, 1 - On
Biomass target moisture level	0%	Range: 0 to 00%
NOx controls		
Selective Catalytic Reduction	1	0 - Off, 1 - On
SCR efficiency	83%	Default: 86%
Fly ash and particulate matter controls (Coal/Biomass only)		
Fabric Filter	1	0 - Off, 1 - On
Ash removal efficiency	99.8%	Default: 99.8%
Electrostatic Precipitator	0	0 - Off, 1 - On
Ash removal efficiency	0.0%	Default: 99%
Carbon dioxide capture		
Status	0	0 - Off, 1 - On
If ASU is off, CO2 capture is amine-based.		
Capture bypass	0%	Default: 0%
Mercury control (Coal/Biomass only)		
Filter/ESP co-benefit cap. Rate	90.2%	Default: 70.2%
Wet FGD co-benefit cap. Rate	70.2%	Default: 70.2%
Activated Carbon Injection	1	Default: 0

Air separation unit (oxy-firing) (Coal/Biomass only)		
Status	0	0 - Off, 1 - On
Plant		
Plant Type	2	1 - Subcritcal Pulverized Coal (PC) 2 - Su Coal (SCPC) 3 - Ultra-supercritical Pulve Circulating Fluidized Bed (CFB) 5 - Natur 6 - Solid Oxide Fuel Cell
SOFC Scenario	1-6	Conventional gasifier w/ natural gas inje
Thermal input (HHV)	1351	MWt
	4,609	MMbtu/hr 1,350,672 kWt
SOx controls (Coal only)	1	
Wet FGD	1	0 - Off, 1 - On
SOx removal efficiency	98%	molar percent, Default 98%
	0	
Dry FGD	0	0 - Off, 1 - On
SOx removal efficiency	0%	molar percent, Default 93%
	0	
In-bed limestone injection	0	0 - Off, 1 - On (to be used only with CFB
SOx removal efficiency	0%	molar percent, Default: 94%
Plant cooling		
Wet cooling tower/Hybrid Condenser	1	0 - Off, 1 - On
	0%	Percentage Air-Cooled Condenser (Defa
Once-through cooling	0	0 - Off, 1 - On
Allowable temperature increase	20	ºF, default 60ºF
Combined Heat and Power	0	0 - Off, 1 - On 0 MW sent to CHP
(coal and biomass only)	0.0%	Percent of steam N/A
Power Plant Capacity Factor	0.85	Capacity factor used for yearly operating
Municipal Water Usage	50%	% water withdrawn from municipal sour
Ground Water Percent	100%	% of remaining water withdrawn from g

Power Plant Flexible Model Uses

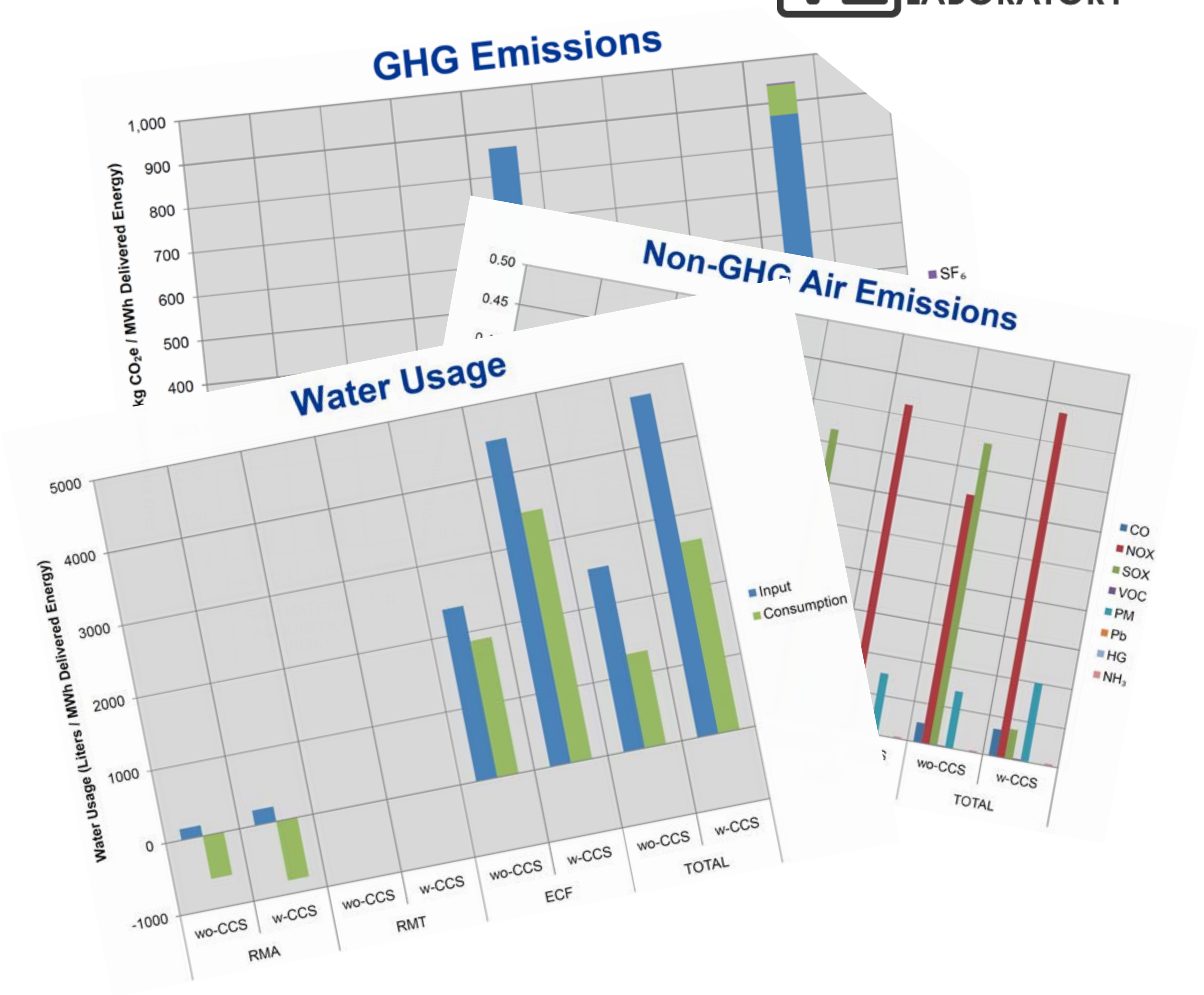
Co-fire biomass vs. CO_2 emissions and net plant power

- PPFM intended as a tool to quickly assess changes in equipment or feedstock
- Example: Can relatively quickly assess impacts of co-firing varying amounts of biomass while maintaining sulfur emissions
  - 98.0% to 97.6% removal rate for SO_2 (Wet FGD) at 0.327 kg SO_2/MWh net



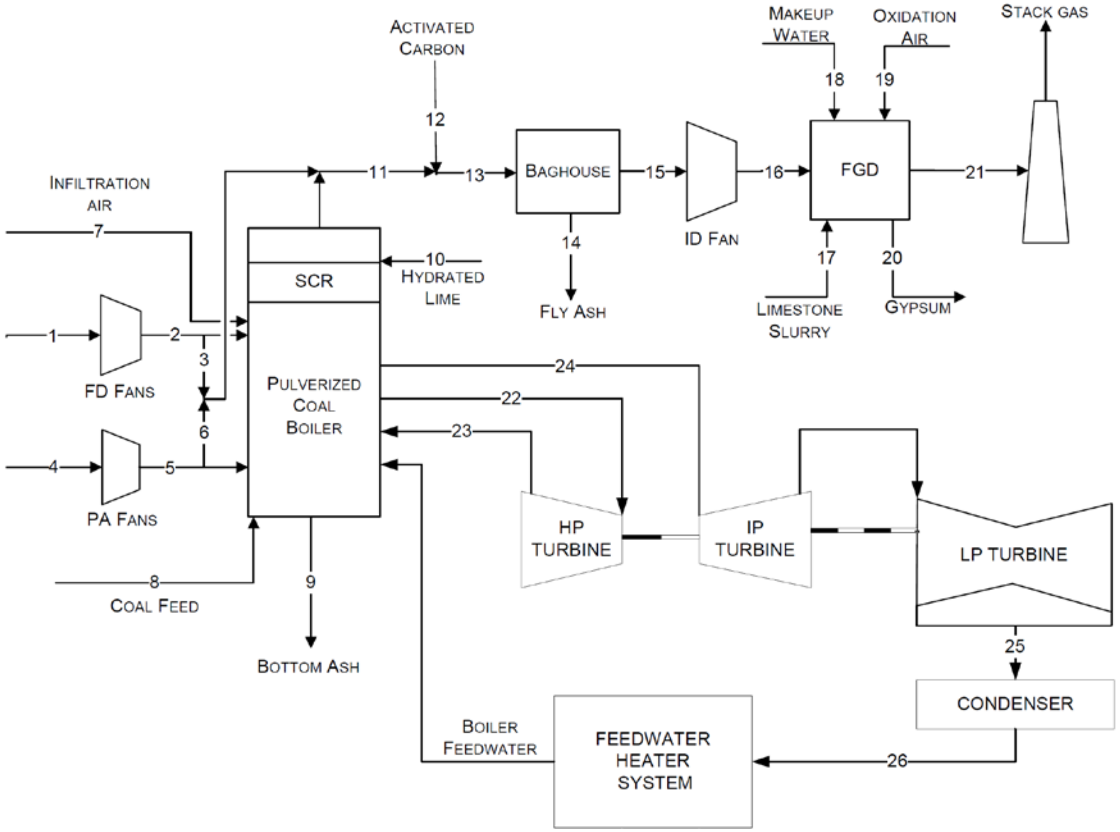
Moving Beyond GHGs, CAPs, and Water Use

- Past focus of LCAs have been on greenhouse gases (GHGs), criteria air pollutants (CAPs), and water use
- Expanding inventory across all NETL models to support broader analyses
  - Impact analysis via EPA TRACI 2.1
- As an input to other models (i.e., CO_2-enhanced oil recovery (CO_2-EOR), PPFM emissions inventory needed to be expanded

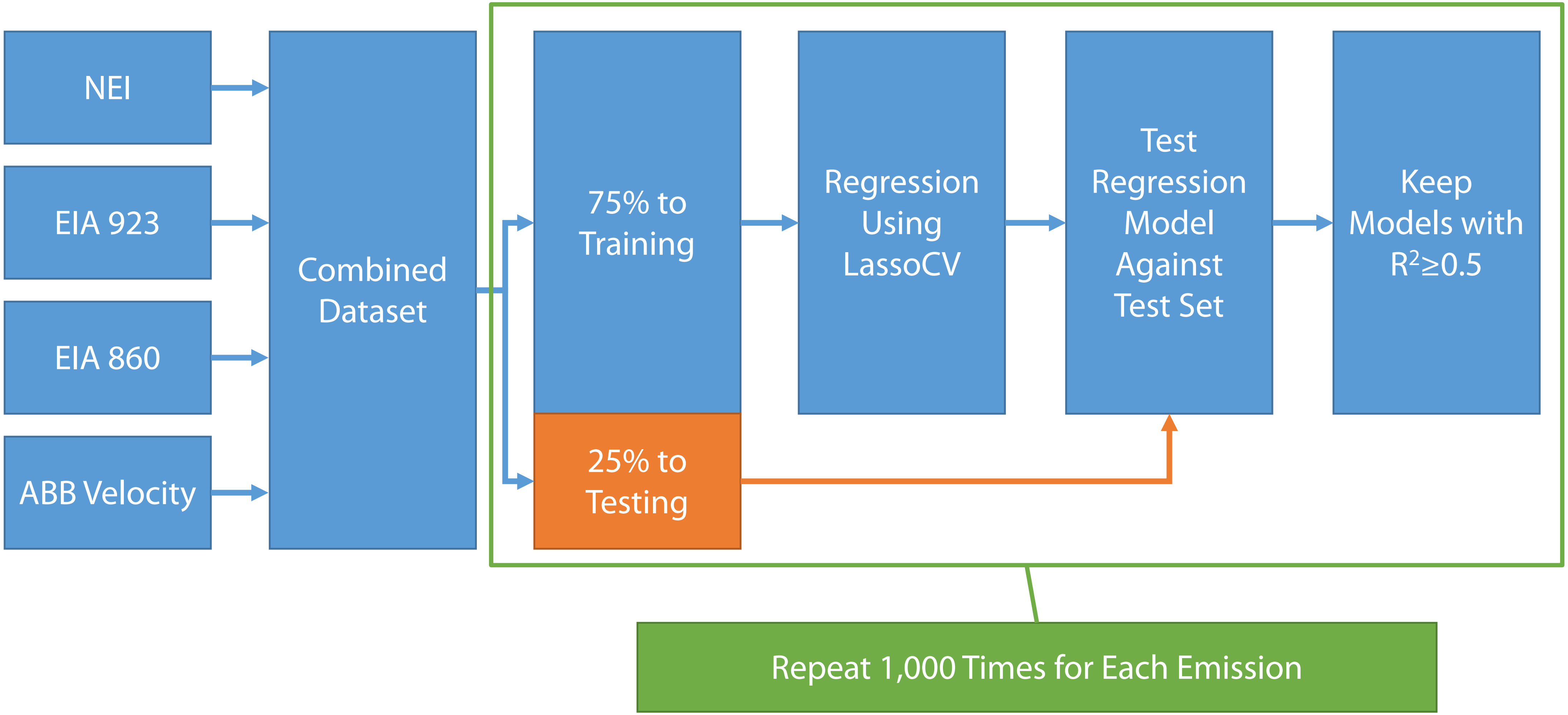


Goals for PPFM Inventory Expansion

- **Emissions that respond to changing plant configuration**
  - Boiler type (for coal): sub-critical vs. supercritical
  - Air pollution control: equipment type and operation
  - Coal type: bituminous vs. sub-bituminous vs. lignite
- **Use publicly available data**
  - National Emissions Inventory (NEI), Energy Information Administration (EIA) power plant data, etc.



Method Overview



Source Data

- 2011NEI: Annual emission rate for each plant
  - Combined with data below using crosswalk provided by Eastern Research Group (EPA Plant ID to NEI EIS Facility ID)

Coal Plants

Power Plant and Fuel Parameters	Data Source
Power Plant Unit Capacity (MW)	EIA 860
Power Plant Unit Generation (MWh)	EIA 923
Control Equipment (Boolean)	ABB Velocity
Supercritical (Boolean)	ABB Velocity
Fraction of Each Coal Type (BIT/SUB/LIG)	EIA 923
Coal Quality (heat/sulfur/ash content)	EIA 923
Heat Rate (BTU/kWh)	EIA 923 (calculated)

Natural Gas Plants

Power Plant Parameters	Data Source
Power Plant Capacity (MW)	EIA 923
Power Plant Generation (MWh)	EIA 923
Control Equipment (Boolean by type)*	ABB Velocity
Heat Rate (BTU/kWh)	EIA 923 (calculated)

*Water/Steam, Catalytic, Ammonia, Overfire, and Low NOx

Parameters for Regression Analysis

- The parameters were chosen based on configuration data available
- Some consideration given for options available within PPFM

Coal – 14 available parameters

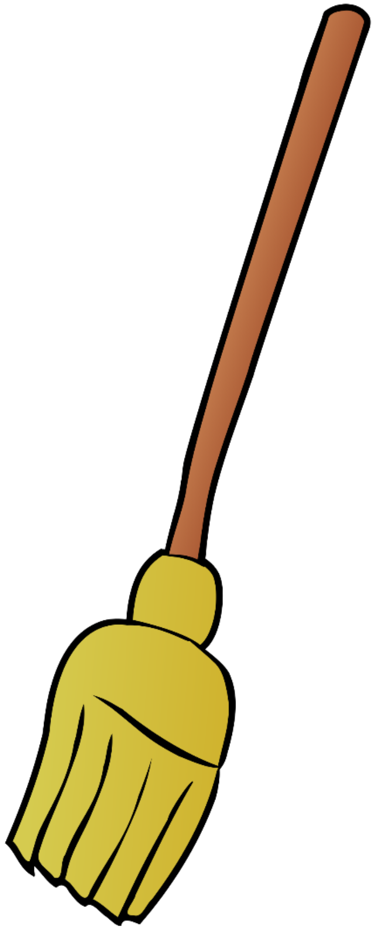
Nameplate Capacity	Bituminous Coal
Capacity Factor	Sub-bituminous Coal
Heat Rate	Lignite Coal
Heat Content of Coal	SO_2 Control (Boolean)
Sulfur Content of Coal	NO_X Control (Boolean)
Ash Content of Coal	PM Control (Boolean)
Supercritical Plant (Boolean)	Mercury Control (Boolean)

NGCC – 11 available parameters

Nameplate Capacity	**NO_X Control Types:**
Capacity Factor	Water
Heat Rate	Catalytic
Percent Gas	Ammonia
Percent NGCC	Overfire
NO_X Control (Boolean)	Low NO_X Burners

Data Cleanup

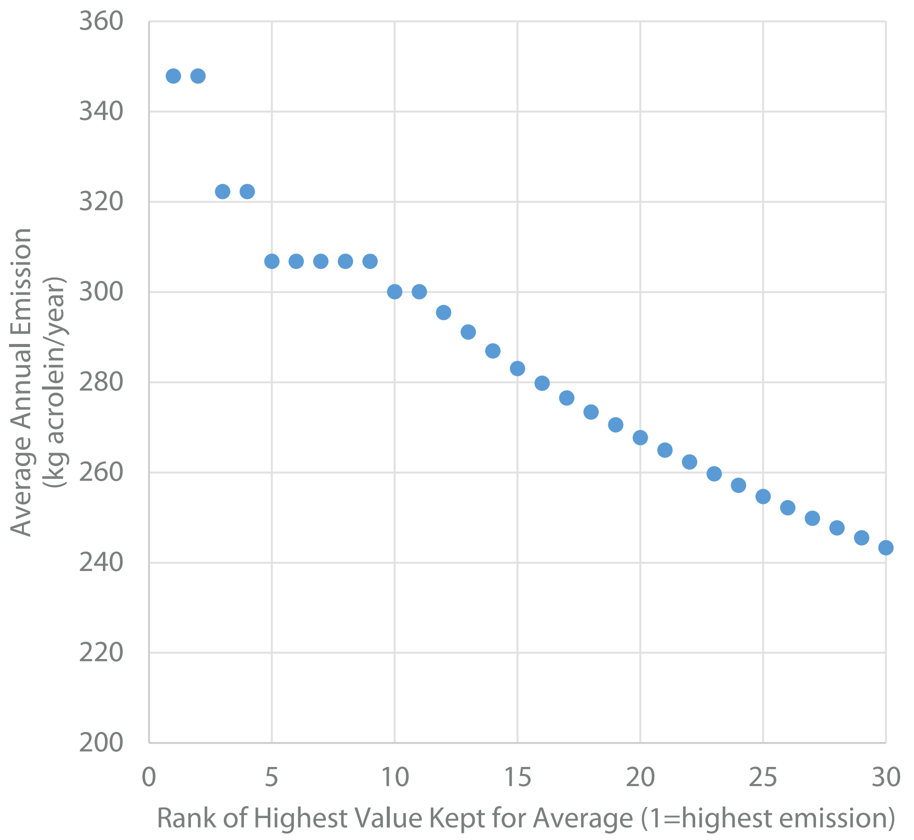
- **Plants removed based on heat rate – any plants outside of these heat rates were removed**
  - Coal: 7,500-12,000 BTU/kWh (28-45% efficiency)
  - Natural gas: 6,000-15,000 BTU/kWh (23-57% efficiency)
- **All negative values were removed**
- **Species filtering**
  - NEI has 151 emissions species for coal plants and 124 for NGCC plants
  - Species with less than 10 facilities reporting emissions were omitted
  - Remaining species count – coal: 90, NGCC: 38



https://commons.wikimedia.org/wiki/File:Broom_.svg

Outlier Filtering

- **Examined different ways to filter outliers – noticed trend to the right among most species**
  - The goal was to use as much of the data as possible to train and test the regression model
  - Graph shows the average as the highest values are incrementally removed
  - Only a handful of values need to be removed before the change in average stabilizes – in this case 4 values
- **This process was implemented in Python and used to filter outliers prior to creating testing and training datasets**
- **The remaining data was then split into training and test sets**



The Regression Method

Machine-learning algorithm LassoCV

2/3 Train

1/3 CV

1/3 CV

1/3 CV

3-fold Cross-Validation

Lasso Multiple Regression

Set of α to try

Measure MSE

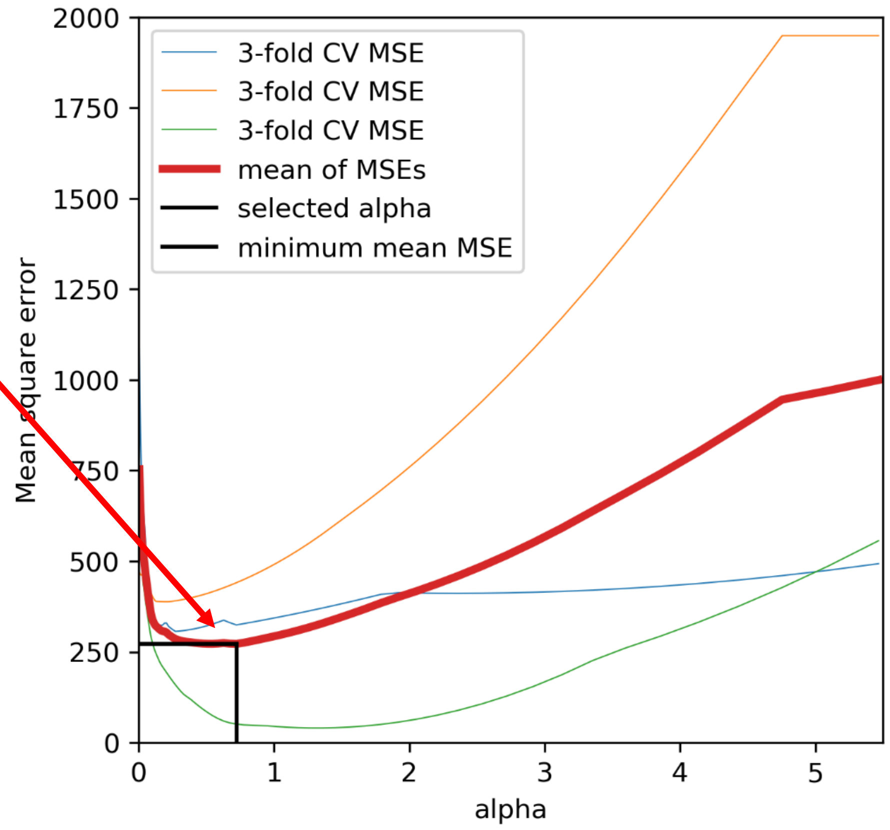
Repeat for 3 sets

Average MSE across 3 sets and use α at lowest MSE

Mean Square Error (MSE) =
$\frac{1}{n}\sum_{i=1}^{n}(Y_i - \sum_j x_{ij}\beta_j)^2$

Sum of regression coefficients (β_j)
$= \sum_{j=1}^{p}|\beta_j|$

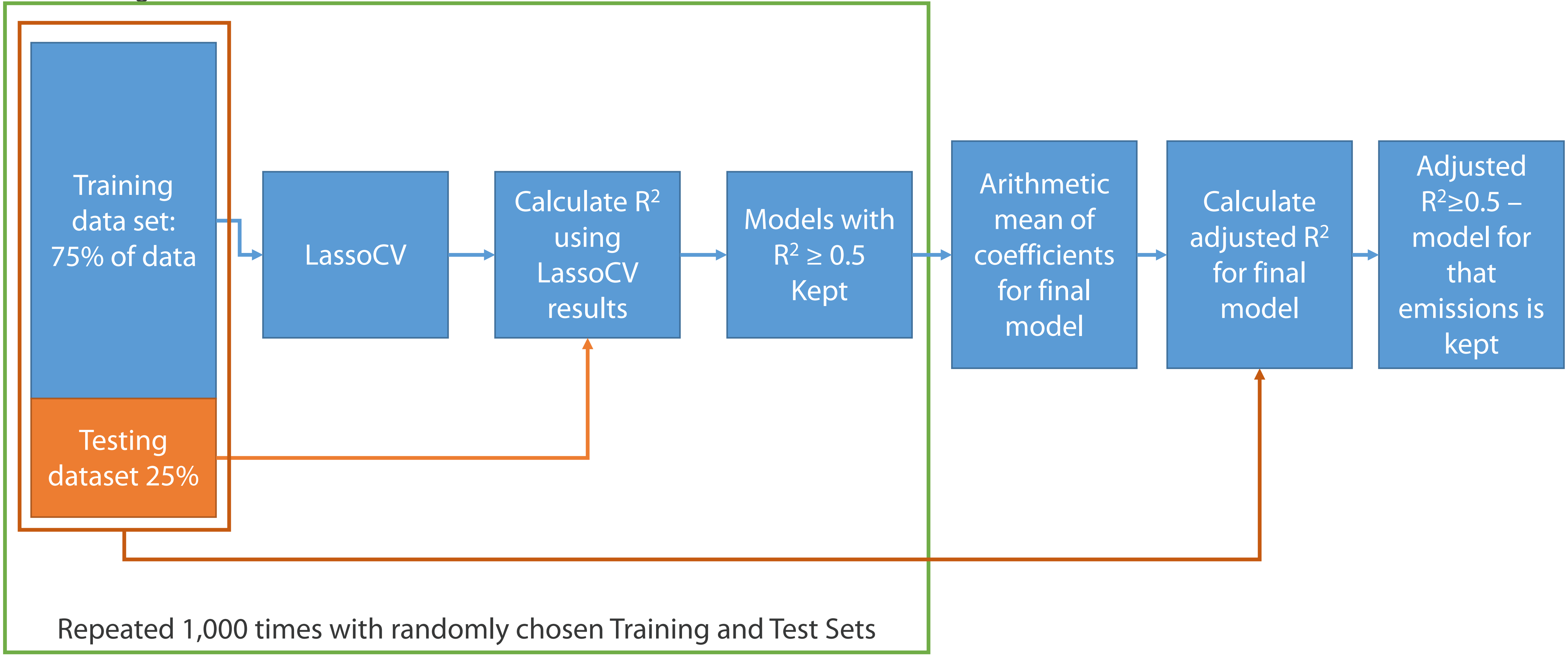
Lasso regression minimizes
$MSE + \alpha \cdot \sum_{j=1}^{p}|\beta_j|$



In minimizing, coefficients can be set to 0 (parameter selection)

Testing the Regression Model

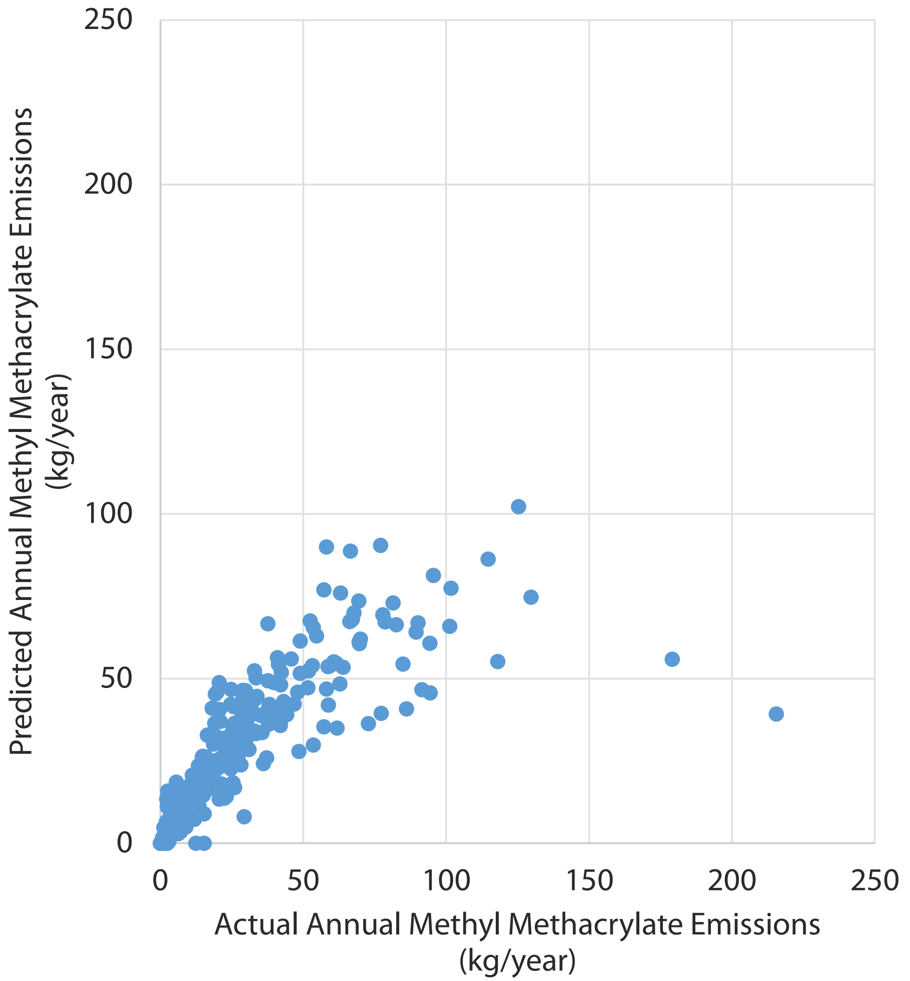
Getting to a final model



Regression Results

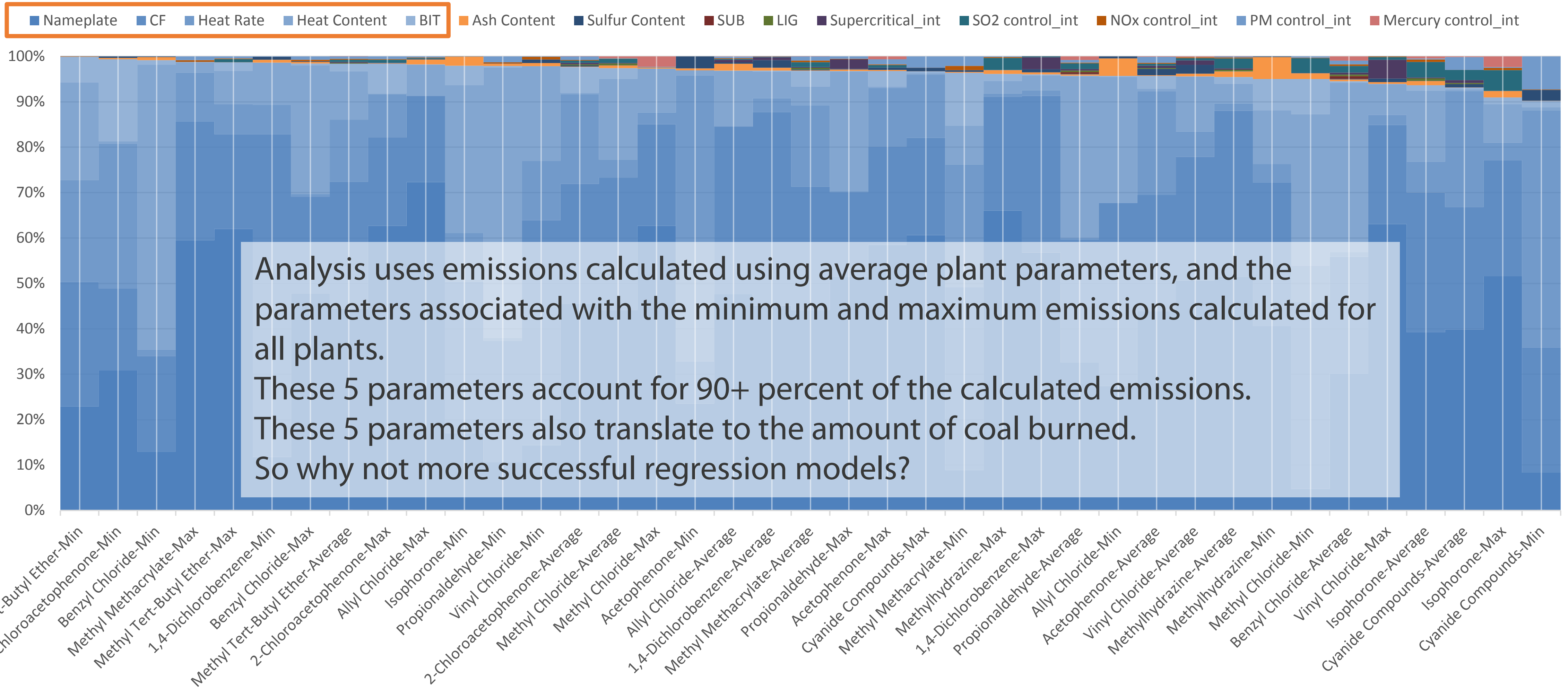
Sample results for methyl methalcrylate emissions

- **The number of successful models generated for each species ranged from 0 to 932 (of 1,000 possible)**
- **The final count of species with accepted emissions models (Adjusted $R^2 \geq 0.5$):**
  - Coal: 13 (of 32 species that had regression models generated)
  - NGCC: 0 (of 17 species that had regression models generated)



Contribution Analysis of Results

What are the most important parameters?



Analysis uses emissions calculated using average plant parameters, and the parameters associated with the minimum and maximum emissions calculated for all plants.

These 5 parameters account for 90+ percent of the calculated emissions.

These 5 parameters also translate to the amount of coal burned.

So why not more successful regression models?

Nameplate – Nameplate capacity (MW), **CF** – Capacity Factor, **Heat Rate** (btu/kWh), **Heat Content** [of coal] (MJ/kg), **BIT** – bituminous coal, **SUB** – sub-bituminous coal, **LIG** – lignite, **Supercritical_int** – Boolean for supercritical boiler, **SO2 control_int**, **Nox control_int**, **PM control_int**, **Mercury control_int** – Booleans for presence of pollution control equipment

Back to the Drawing Board

New Dataset!

- **Update the data to use 2014 NEI and power plant data**
  - Previous analysis used 2011 NEI and power plant data
- **NEI emissions are reported at the boiler level (Tennessee Valley Authority Kingston Plant has 9 boilers)**
- **EPA 860 data is available at the boiler level and includes**
  - Information on all pollution control equipment
    - 10 codes for FGD
    - 24 codes for NO_X control
    - 16 codes for PM control
    - 21 codes for Hg control
  - Boiler-level fuel consumption with sulfur and ash specs
    - Also includes combustion of DFO and natural gas for auxiliary operations

A Deeper Look at the NEI Data

What do the reported emissions actually represent?

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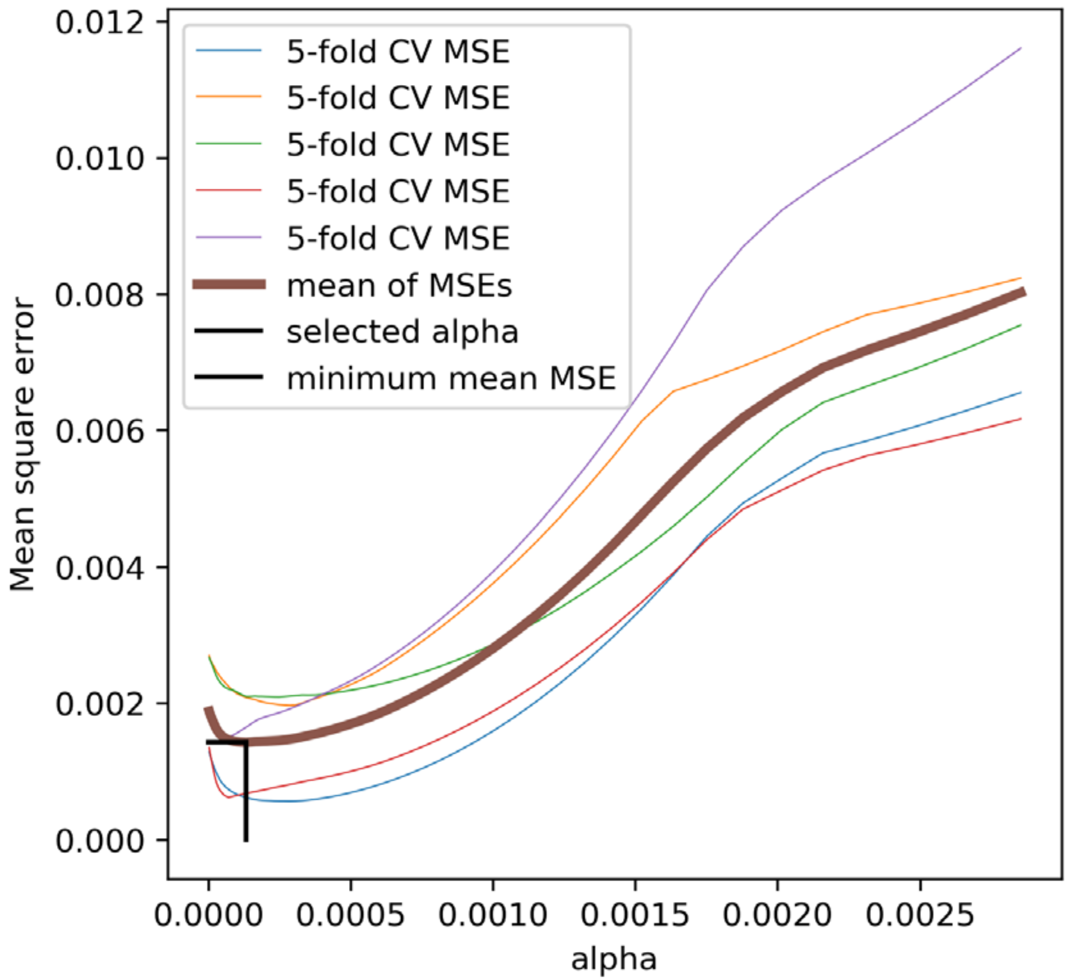
- **Working directly with the NEI database has revealed some more detail in the metadata:**
  - Of the 53,598 non-zero data points, over half use an EPA, no control emission factor – 119 of 119 species have an EPA emission factor
  - Most emission factors are based on coal throughput (skimming through comments for the calculations)
  - The majority of continuous emission monitoring system (CEMS) data is for NO_X, SO_2, VOCs, and PM

Continuous Emission Monitoring System	1,237	2.3%
Engineering Judgment	4,281	8.0%
Manufacturer Specification	66	0.1%
Material Balance	319	0.6%
Other Emission Factor (no Control Efficiency used)	833	1.6%
Other Emission Factor (pre-control) plus Control Efficiency	463	0.9%
S/L/T Emission Factor (no Control Efficiency used)	3,409	6.4%
S/L/T Emission Factor (pre-control) plus Control Efficiency	8	0.0%
S/L/T Speciation Profile	31	0.1%
Site-Specific Emission Factor (no Control Efficiency used)	906	1.7%
Site-Specific Emission Factor (pre-control) plus Control Efficiency	30	0.1%
Stack Test (no Control Efficiency used)	2,736	5.1%
Stack Test (pre-control) plus Control Efficiency	105	0.2%
Trade Group Emission Factor (no Control Efficiency used)	1,474	2.8%
Trade Group Emission Factor (pre-control) plus Control Efficiency	8	0.0%
USEPA Emission Factor (no Control Efficiency used)	29,135	54.4%
USEPA Emission Factor (pre-control) plus Control Efficiency	2,827	5.3%
USEPA Speciation Profile	5,719	10.7%
Vendor Emission Factor (no Control Efficiency used)	11	0.0%

Adjustment to Method

Changing LassoCV Parameter

- 5-fold cross-validation used for species with > 20 samples, 2-fold otherwise
- Example path for anthracene



Good News, Bad News

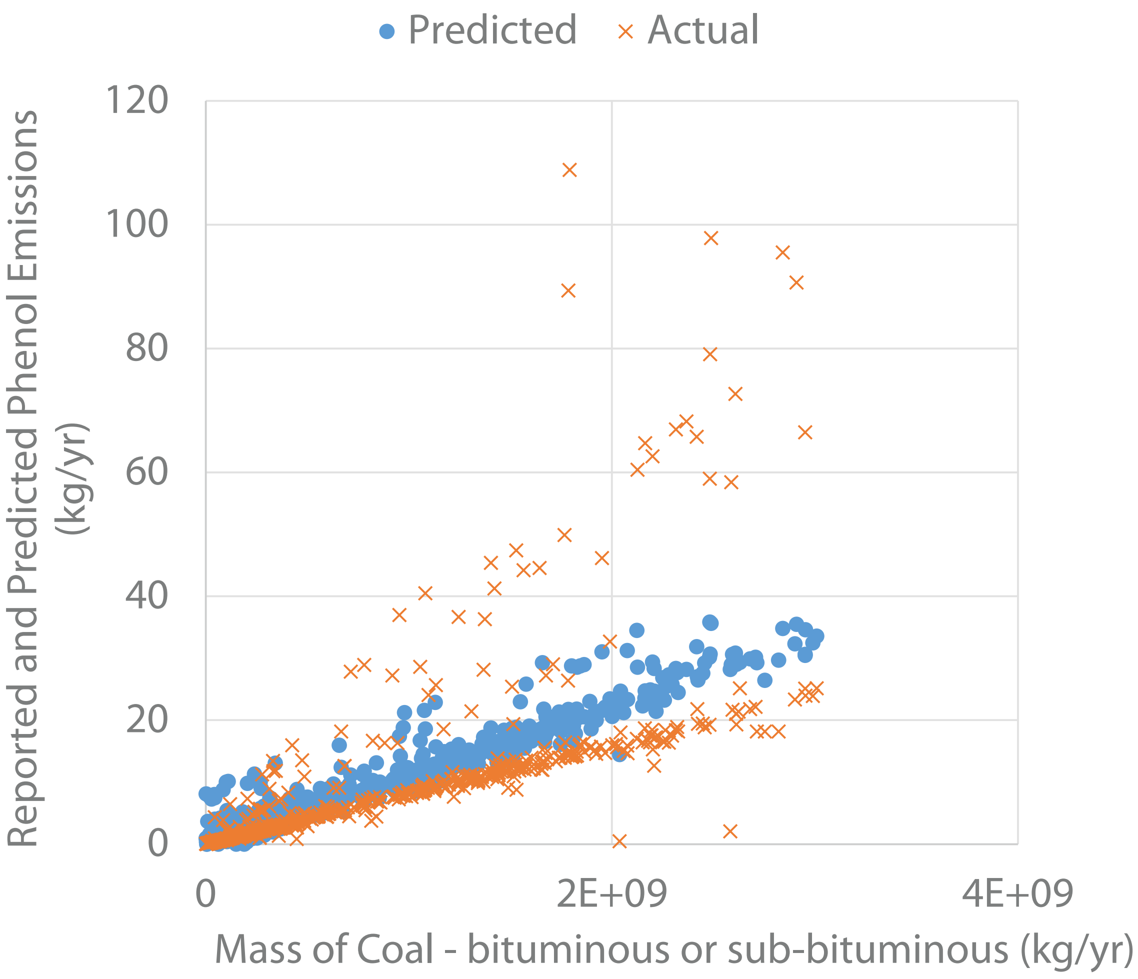
Example phenol results – species with the lowest passing final R^2 test

Good News

- **Species count for successful models and score of those models went up considerably**
  - 63 species now have "good" models from 13 previously
  - Notable omissions from the "good" model list due to bad final R^2 test (as opposed to too few emissions or no successful regressions):
    - SO_2, NO_X, ammonia, PM 10, PM 2.5
    - Suspect these score low because emissions are driven by regulation rather than any of the variables

Bad News

- **We're mostly regressing against emissions that are generated using emission factors rather than measured emissions**
  - There's still value in providing a weighted average without examining all of the metadata



Conclusions

- **A large number of NEI emissions are the result of emissions factors applied to coal throughput**
  - Depending on how you get NEI data this isn't readily apparent
  - Despite this, using this method to provide a weighted factor used by the fleet is still useful
- **The emissions that should be most responsive to plant configuration are not (SO_2, NO_X, CO, etc.)**
  - Suspect this is because permits drive these emissions more than the existence of particular control equipment
  - Would like to re-do the analysis for these emissions using locale as a parameter
- **More work to do**
  - Revisit the analysis for natural gas plants to see if boiler- or turbine-level data results in successful models
  - Include facility-level emissions: species count from original analysis was 158 vs. 119 in the new approach, presumably omitting facility-level emissions from TRI

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