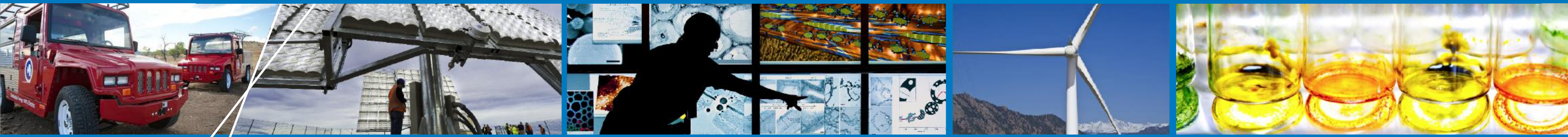
2013 DOE BETO Project Peer Review

NREL Sustainability Analysis: Life Cycle Inventory of Air Emissions



Date: May 22, 2013

Technology Area: Sustainability

PIs: Daniel Inman and Garvin Heath

Organization: National Renewable Energy Laboratory

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NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

NREL Sustainability Analysis Goals

This project provides analysis to assess the sustainability of renewable fuels in terms of **greenhouse gas emissions, water use, and air quality.**

The sustainability project is focused on addressing specific sustainability goals, as outlined in the 2012 multi-year programmatic plan (MYPP).

Specifically, this project will provide analysis that supports the following BETO sustainability goals:

- 2013: Identify metrics and target setting for air quality for agricultural residues, energy crops, and forestry resource (residues and short-rotation woody crops) pathways
- 2017: Implement best practices for all sustainability categories for a sustainable integrated biomass-to-biofuel process for agricultural residue
- 2022: Implement best practices for all sustainability categories for a sustainable integrated biomass-to-bioenergy process for energy crops (woody or herbaceous) and forest resources.

Quad Chart Overview: Sustainability Analysis

Timeline

- Start: 2009
- End: Sept 30th, 2017 (planned for AQ)
- 20% complete (AQ).

Barriers addressed

- *St-C. Sustainability Data across the Supply Chain*
- *St-D. Indicators and Methodology for Evaluating Sustainability*
- *St-E. Best Practices for Sustainable Bioenergy Production.*

Budget

- Funding for FY12: $690K
- Funding for FY13: $500K
- Two year funding avg = $595 K/yr.

Partners

- Closely coordinating with and receiving data inputs and technical advice from
  - DOE Labs: ORNL, INL, ANL, PNNL
  - Universities: MN (Marshall, Hill), TN (Hellwinckel), UW (Cooper)
  - Other agencies: EPA (NRMRL, NCEA, OAQPS)
  - Industry: NCGA
  - Consultants: ERG.

Task Overview: Part I

- Project started in 2008 under BETO’s Analysis Platform. Expanded in 2010 and in 2011 became managed under BETO’s Sustainability Analysis Task
- Initial work focused on ethanol produced from corn grain, stover, straw, switchgrass, and forest residues in the year 2022 (“LCA of EISA”)
  - Life cycle environmental impacts of multiple feedstock-to-ethanol pathways as compared to conventionally-produced gasoline
  - Phase II significantly expands the model’s capabilities by including additional feedstocks, conversion technologies, fuels, and life cycle metrics
- We have expanded the project to include additional metrics and modeling platforms in response to BETO’s sustainability goals.

Task Overview: Part II

- Overall, the sustainability task supports the following analysis efforts:
  - **Lifecycle Inventory and Assessment** of NREL process designs (e.g., cellulosic ethanol, biological conversion of sugars to hydrocarbon).
  - **Sustainability metrics** for the conversion facility:
    - Greenhouse gas emissions, water use- baseline and target setting for BETO as well as supply data for the technology SOT reports.
  - **Air Quality** modeling across the biofuel supply chain.

Project Overview: Air Quality

Long-term goal: Compare air quality and human health impacts from scenarios of large scale deployment of cellulosic biofuels to incumbent fuels (first-generation biofuels, gasoline) on a life cycle basis.

Objectives support BETO MYPP:

1. Establish spatially, temporally, and chemically explicit **baseline emissions inventory** of air pollutants relevant to ozone and secondary particulate matter (PM) formation for all life cycle processes of selected cellulosic feedstocks and biofuels
2. Evaluate **tradeoffs** and set **targets** for potential improvements across cellulosic biofuels' life cycle
3. Quantify **air quality and human health impacts** of ozone and PM resulting from emissions from large scale use of cellulosic biofuels, and compare them to alternative energy systems.

Approach

For each life cycle stage, based on inventory

For life cycle impact evaluation, considering all stages and net effects

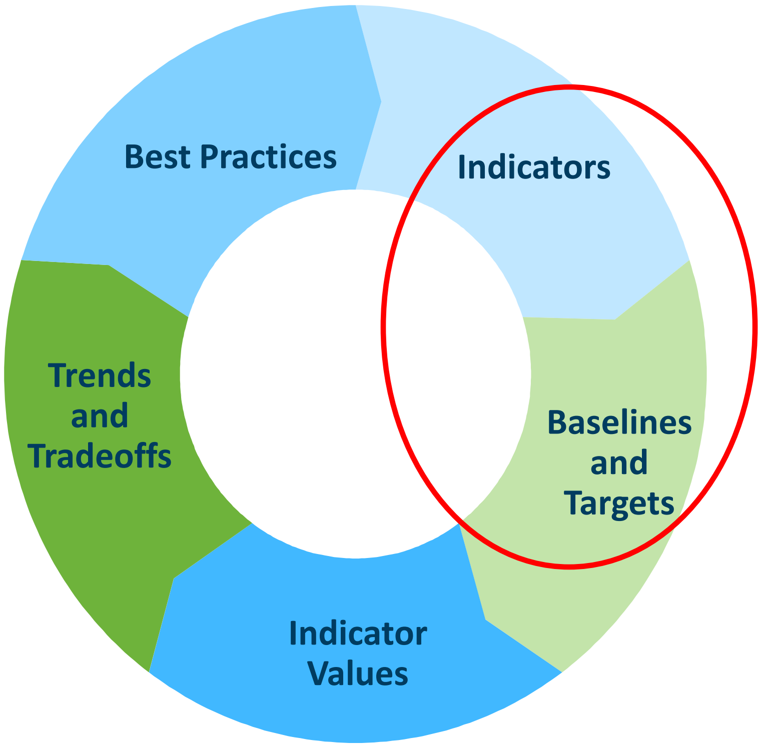
- Spatially, temporally, and chemically explicit inventory
- Air quality modeling
- Exposure assessment
- Health impact assessment and externalities estimation

Management

- Work plan, milestones, schedule, and deliverables described in project management plan (PMP) managed by DOE Golden Office and Headquarters
- Interface with other BETO sustainability activities via program teleconferences, meetings, inter-laboratory conference calls and visits, and collaborative projects.

Progress

For each life cycle stage, based on inventory



For life cycle impact evaluation, considering all stages and net effects

- Spatially, temporally, and chemically explicit inventory
- Air quality modeling
- Exposure assessment
- Health impact assessment and externalities estimation

Feedstock Production → Logistics → Conversion → Distribution → End Use

FY12-13

FY12 (biochemical EtOH)
FY13 (fast pyrolysis)

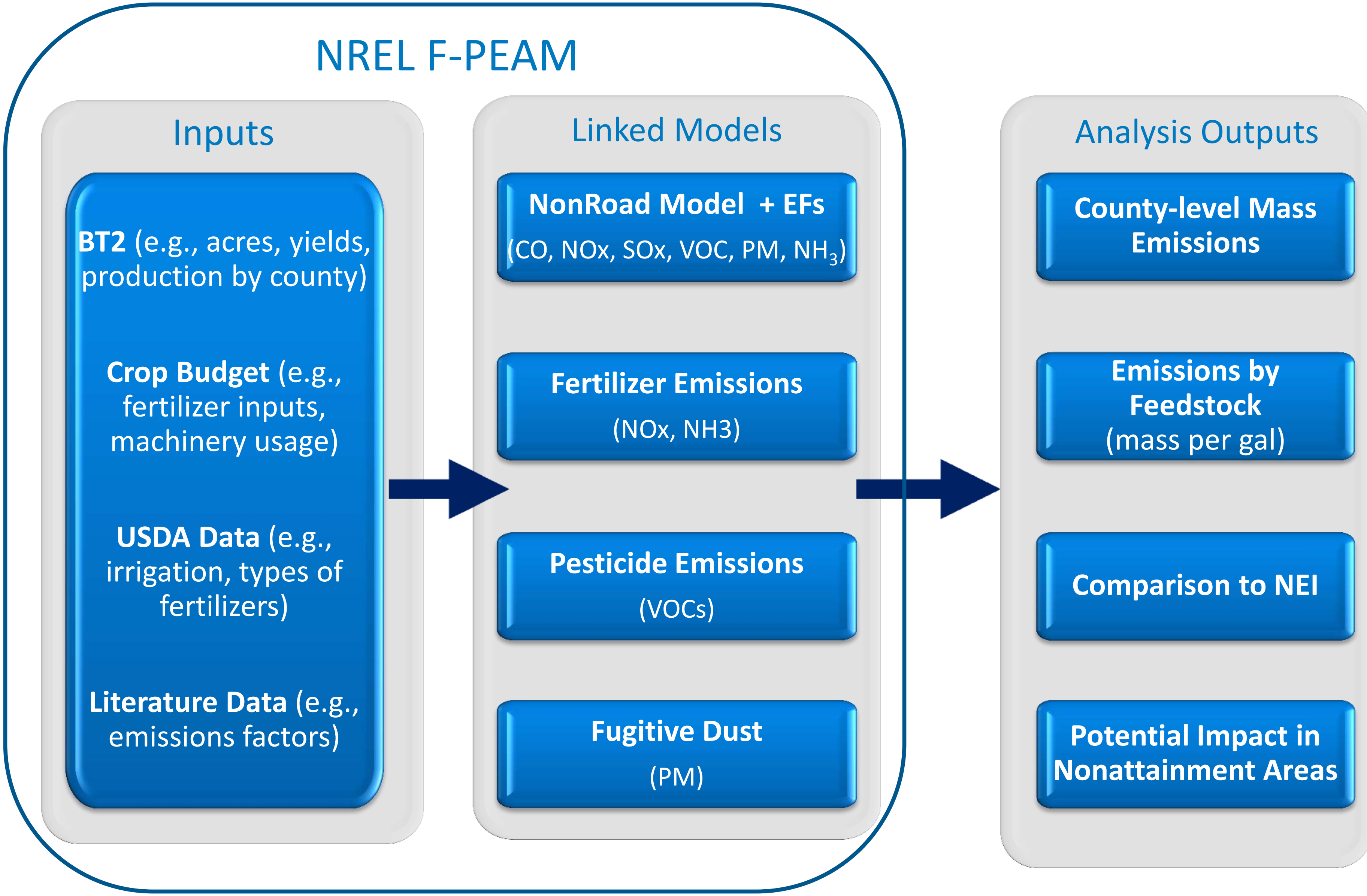
Unique Contributions

- **Integrate latest research on DOE-supported designs and other state-of-the-art models and data sources (e.g., EPA's NONROAD) across supply chain to consider air emission implications**
  - Already helping ORNL and INL understand implications of their designs
  - Valuable as updates to GREET and to gain insight by comparison
- **Examine multiple biomass feedstocks and biofuels**
  - This is distinct from Jason Hill's most recent work, which evaluated ethanol from corn and corn stover
- **Consider regional variability in practices, climate at high spatial resolution**
- **Improve estimates of pollutant emissions from cellulosic biofuel conversion processes, including complex species such as NOx, VOCs and PM which aren't accurately predicted by current mass balance-based process models**
- **Develop high-resolution insights into source-level emission reduction opportunities, tradeoffs, targets for improvements, and R&D prioritization at the point of greatest control—emissions**
- **Provide valuable information for air quality planners to compare to current baselines, anticipate potential outcomes of future scenarios and consider control strategies.**

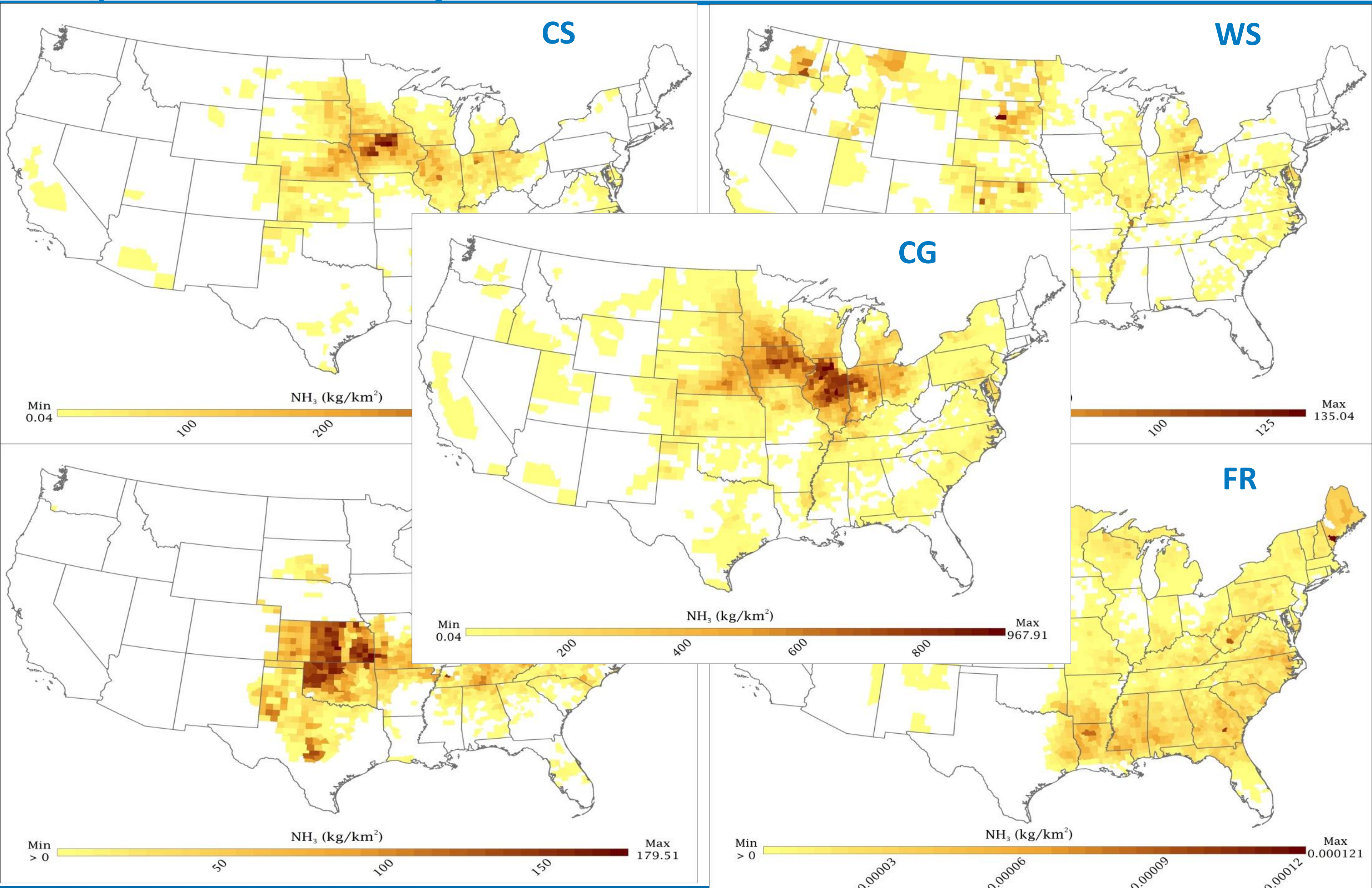
Technical Accomplishments/Progress/Results

- Completed all prior milestone progress reports on time
  - Q1 FY12: Progress report on feedstock production
  - Q3 FY12: Progress report on biochemical EtOH air emissions
  - Q2 FY13: Progress report on fast pyrolysis air emissions
- Q2 FY13: Journal manuscript prepared on feedstock production air emissions
  - Responding to feedback
- Q3 milestone on schedule: Baseline and targets for feedstock production air emissions
  - Developed a model capable of rapid assessment of alternative scenarios
- Results of feedstock production shared with ANL, ORNL, INL
  - Ensuring quality and accuracy of our modeling
  - Informing their designs
- Results of fast pyrolysis biorefinery analysis to be shared with PNNL, and biochemical EtOH with NREL's NBC
  - Parallel assessment of sustainability to cost and technical performance targets
- Results will be made available to other agencies and databases (e.g., EPA, US LCI, etc.).

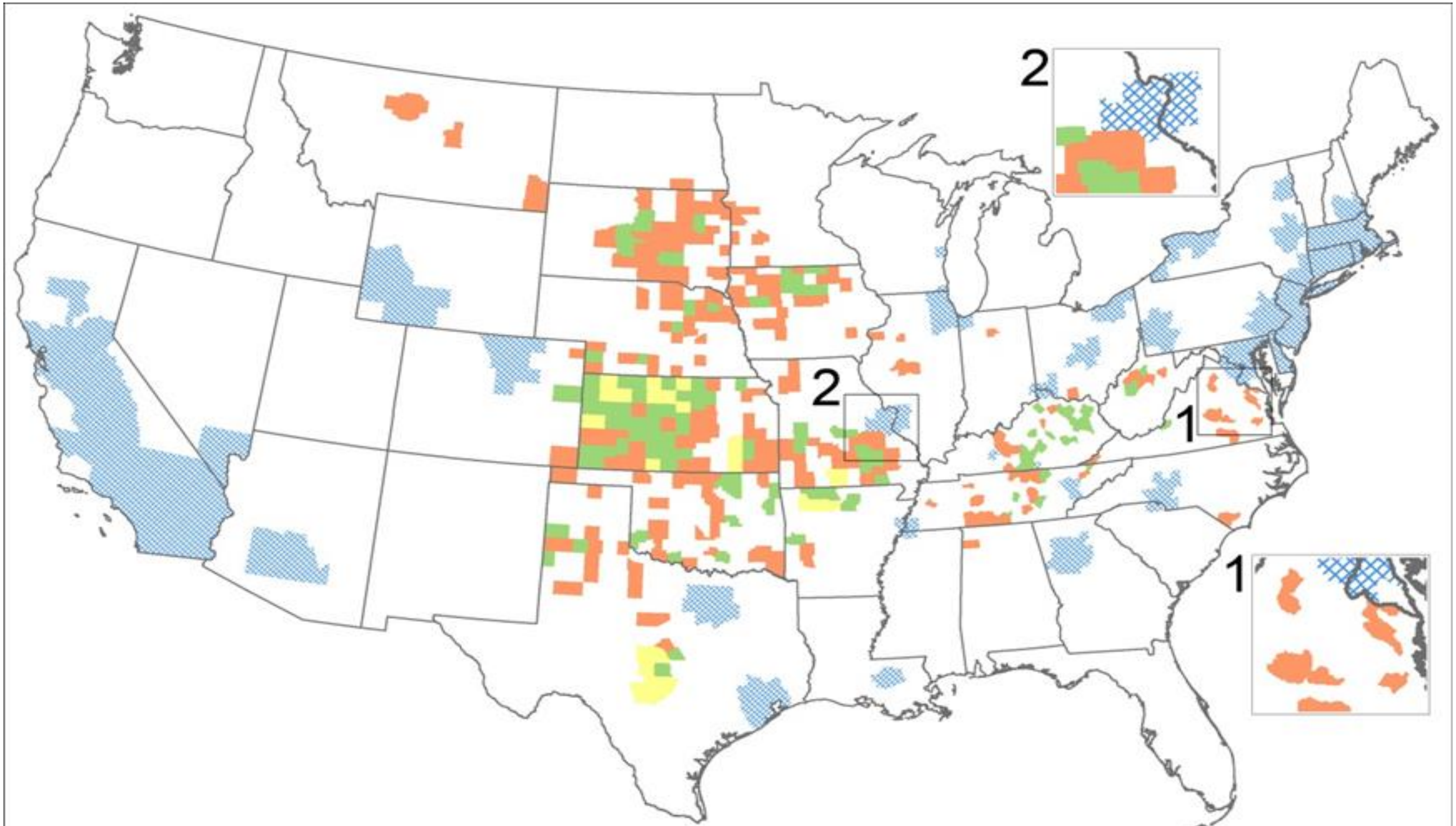
NREL Feedstock Production Emissions to Air Model (F-PEAM)



Emissions Density for Feedstocks:
NH_3 emissions density for each cellulosic feedstock



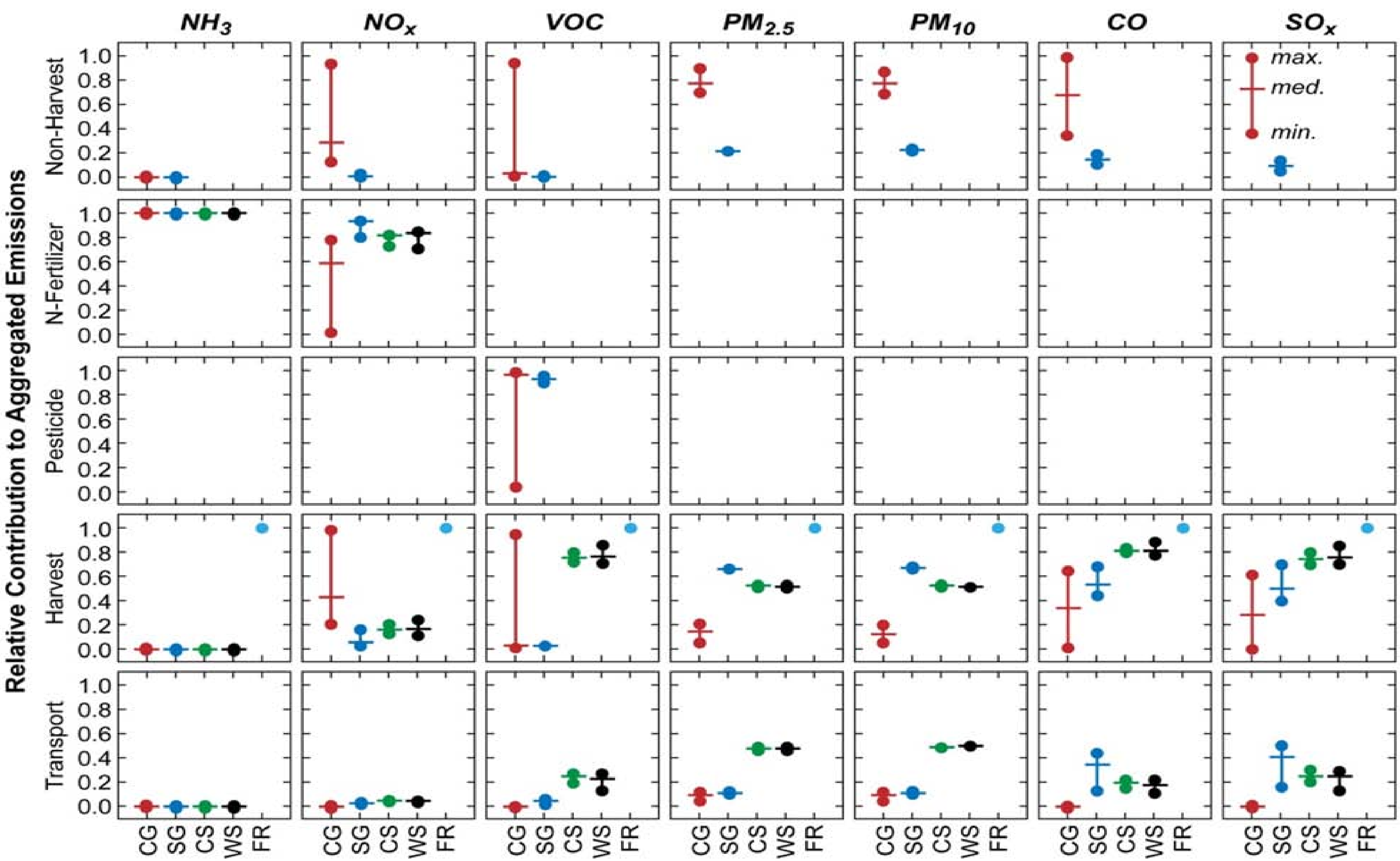
Counties with Cellulosic Feedstock O_3 Precursor Emissions Exceeding 3 NEI Thresholds, Alongside Current O_3 Nonattainment Areas



Ozone	No. Counties in Nonattainment
R > 0.2	0
R > 0.1	0
R > 0.05	0

Contribution by Activity Category to County Emissions:

First step to target setting



Blanks represent no emissions of that pollutant for that feedstock.

CHEMKIN: Detailed Kinetic Modeling
for improved emission estimation from conversion processes

- CO_2 and SO_2 emissions estimated through process models (ASPEN, CHEMCAD) based on mass balance (complete oxidation)
- The levels of NOx, VOCs, and PM emissions from combustion depend on
  - Incomplete combustion of a small fraction of the fuel
  - Complicated chemical and physical processes during the combustion.

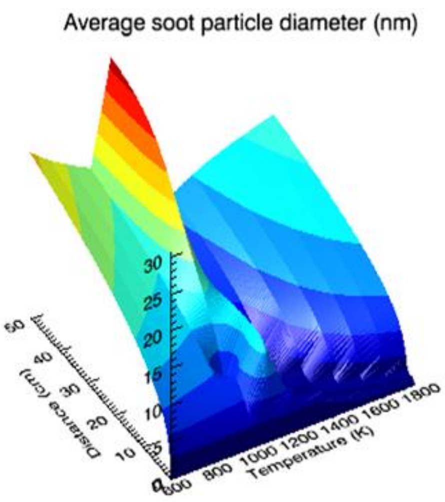
Goal: Develop accurate estimates of NOx, VOCs, and PM emissions for prioritized conversion platforms

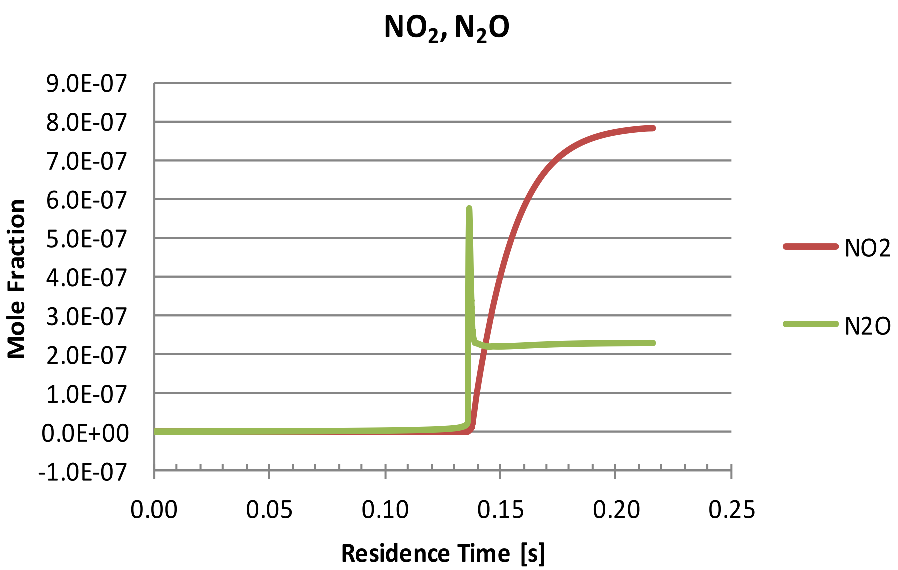
Approach: Develop an air emissions prediction tool for each conversion platform that leverages published kinetic mechanisms utilizing a commercial modeling platform (CHEMKIN).

CHEMKIN Progress

- Progress
  - Preliminary model developed for establishing baselines for lignin combustion in biochemical EtOH conversion and char combustor for fast pyrolysis
    - Chemical mechanisms: NOx formation chemistry, lignin devolitilization, oxidation, PM formation
  - Models are deterministic and allow for scenario analysis and parametric studies
    - e.g., operating conditions, different input compositions
    - e.g., sensitivity of results to residence time, air/fuel ratio and temperature.

……
O2+CH3OH=HO2+CH2OH
O2+CH3OH=HO2+CH3O
O2+C2H4=HO2+C2H3
O2+CH3CHO=HO2+CH3CO
O2+C3H8=HO2+NC3H7
HNO+OH<=>NO+H2O
HNO+O2<=>HO2+NO
CN+O<=>CO+N
CN+OH<=>NCO+H
CN+O2<=>NCO+O
CN+H2<=>HCN+H
NCO+O<=>NO+CO
NCO+H<=>NH+CO
NCO+OH<=>NO+H+CO
………





Relevance

- **Results from this project directly inform BETO sustainability MYPP goals**
  - 2013 Mission Critical Goal: *Identify metrics [establish baseline] and set targets for air quality and soil quality for agricultural residues, energy crops, and forest resources and at least one conversion pathway*
  - NREL Feedstock Production Emissions to Air Model (F-PEAM) provides capability to be used
    - in conjunction with ORNL/POLYSYS to develop sustainable resource assessment considering air emissions.
    - to assess alternative feedstock production scenarios, enabling efficient analysis in support of target setting, consideration of trade-offs, state of technology assessment, etc.
  - CHEMKIN models can quantify emissions of pollutants not predicted through ASPEN/CHEMCAD.
- **Results from this project inform other efforts within NREL, as well as activities at other national labs and government agencies**
  - PNNL and NREL (NBC): Inform conversion platform design and sustainability analyses
  - ORNL: Evaluate air emissions from the Billion Ton Update (BT2) cases
  - INL: Evaluate air emissions from advanced logistics designs
  - ANL: Update GREET
  - EPA: Inform ORD research.
- **Results can inform air quality planning activities by states and regions**
  - Given ever-tightening standards and requirements that states demonstrate compliance with air quality regulations, information on potential changes to air emissions can aid planning efforts and meeting air quality objectives.

Critical Success Factors

- ***Providing detailed analyses of life cycle costs and benefits and environmental impact from air emissions***
- ***Supplying sustainability data across the supply chain***
- ***Defining indicators and a methodology for evaluating sustainability in terms of air quality***
- ***Increasing coordination across labs with regard to alignment of assumptions and knowledge of potential effects of designs to this additional sustainability factor***
- ***Establishing extensive documentation and transparent publication strategy (journals, KDF) improves quality and provides public access.***

Future Work

- Ultimate goal: Estimate air emissions-related health effects and costs (externalities) from advanced biofuels compared to incumbent fuels
- Upcoming milestones
  - Q3: Baseline and analytical targets for six air pollutants from biomass production and harvest
  - Q4: Baseline emissions from biological conversion of sugars to hydrocarbons pathway
- Future plans
  - FY14: Logistics and siting, including biorefineries; biofuel distribution; additional conversion pathway(s)
  - FY15: Update inventory across supply chain; air quality modeling and health effects estimation
  - FY16: Establish best practices for air emissions from BETO prioritized feedstocks and pathways
- Challenges
  - Developing spatially explicit emission inventory of petroleum life cycle
    → plan to leverage previous work of our collaborator, Jason Hill
  - Modeling net effects of land converted from prior use, displaced gasoline emissions
    → continue collaboration with ORNL/U TN, Biomass Scenario Model, NREL's Biomass Energy Atlas (spatial analysis of feedstock for different markets)
  - PM mass estimation and VOC speciation for conversion tool
    → work with CHEMKIN designers to extract required information
  - Empirical validation of theoretical CHEMKIN predictions
    → opportunities : experiments at NREL/PNNL, work with vendors or demonstration projects.

Summary

- **Assisting BETO in meeting *2013 mission critical goal* for sustainability**
- **Significant collaboration and integration across labs, as well as other agencies and experts**
- **Responding to previous peer review comments that life cycle models should be spatially disaggregated to account for regional variability**
    - Required for assessment of air quality impacts
- **Development of models that can rapidly evaluate alternative designs and scenarios to aid target setting, changes in design, maintenance of state of technology, etc.**
- **Milestones are consistently met and wider public release is in process.**

Acknowledgments

Thank you BETO for supporting our research!

Thank you to our team:

- **Yimin Zhang**
- **Eric Tan**
- **Alberta (Birdie) Carpenter**
- **Noah Fisher**

Thank you to our Collaborators!

Additional Slides

Responses to Previous Reviewers' Comments

If this [LCA] tool is developed, it will be a key means of comparing different fuel alternatives and will likely be more comprehensive than GREET. I hope the PIs can achieve what they have set out to do.

Response: We envisage the data from our work to be provided to GREET. Also, our work plan is aggressive, but our milestones are designed to keep us on track and moving forward at an acceptable pace.

The project seems solid and comprehensive and it appears to be done according to LCA principles? One concern is that the project deals with multiple biomass feedstocks, but only NREL conversion designs. There are more and more cellulosic biofuel processes that are being developed outside NREL and the most promising of these need to be included in comprehensive modeling efforts.

Response: We are working with PNNL to develop and incorporate other conversion processes.

The LCA principles, boundary conditions, allocations, and sensitivity analysis seem transparent in this project. It is important to continue with the LCA methodology.

Response: We intend to adhere to LCA methodology and remain transparent.

Publications and Presentations: LCA and metrics work

- Publications
  - Argo, A. M., Tan, E. C., Inman, D., Langholtz, M. H., Eaton, L. M., Jacobson, J. J., Wright, C. T., Muth, D. J., Wu, M. M., Chiu, Y.-W. and Graham, R. L. 2013. Investigation of biochemical biorefinery sizing and environmental sustainability impacts for conventional bale system and advanced uniform biomass logistics designs. *Biofuels, Bioprod. Bioref*.. doi: 10.1002/bbb.1391
  - Miner, G.L, N. C. Hansen, D. Inman, L.A. Sherrod, and G.A. Peterson. 2013. Constraints and Capabilities of No-Till Dryland Agroecosystems as Bioenergy Production Systems. *Agron. J.* doi: 10.2134/agronj2012.0243.
  - Adler, P. S.J. Del Grosso, D. Inman, R.E. Jenkins, S. Spatari, and Y. Zhang. 2011. Life Cycle Assessment of Bioenergy Feedstock Production: Uncertainty, Landscape Heterogeneity, and Mitigation Opportunities. In: *Managing Agricultural Greenhouse Gases.* Eds. M. Liebig, A.J. Franzluebbers, R.F. Follett. Elsevier, Amsterdam, The Netherlands.
  - Hsu D. 2012. Life cycle assessment of gasoline and diesel produced via fast pyrolysis and hydroprocessing. *Biomass and Bioenergy*, Vol. 45 (October 2012), pp. 41-47, doi:10.1016/j.biombioe.2012.05.019
  - Hsu, DD; Inman, D; Heath, GA; Wolfrum, EJ; Mann, MK; Aden, A. 2010. Life Cycle Environmental Impacts of Selected US Ethanol Production and Use Pathways in 2022. *Environmental Science & Technology* 44 (13):5289-5297.
  - Williams, PRD; Inman, D; Aden, A; Heath, GA. 2009. Environmental and Sustainability Factors Associated With Next-Generation Biofuels in the US: What Do We Really Know? *Environmental Science & Technology* 43 (13):4763-4775.

Publications and Presentations: AQ work

- Publications
  - “Air pollutant emissions inventory of large-scale production of selected biofuels feedstocks in 2022” (journal article, under revision)
  - “Air pollutant emissions from bioenergy feedstock production in 2022 in relation to National Emissions Inventory” (accepted paper for *A&WMA Conference*, June 2013)
  - “Comparative air pollutant emissions of selected biofuels feedstocks in 2022” (Paper submitted to *International Congress on Sustainability Science and Engineering*, August 2013).

- Presentations
  - Seminar to EPA National Risk Management Research Laboratory (Dec 2010)
  - Mini-symposium with LBNL and EBI (April 2011)
  - Seminar to U Minn (Dec 2011)
  - International LCA Conference (Oct 2012)
  - Air & Waste Management Association (June 2013)
  - International Congress on Sustainability Science and Engineering (August 2013).

Technical Accomplishments LCA and metrics work

Milestone Completion Reports

FY	Quarter	Title	WBS	Status
2012	Q2	Joint milestone with PNNL, sustainability SOTs for thermochemical, biochemical, and fast pyrolysis process models.	11.1.1.3	Completed on-schedule
2012	Q4	Joint milestone with ORNL to identify metrics and set targets for climate, water, and land management for agricultural residues and energy crops pathways.	11.1.1.3	Completed on-schedule
2013	Q4	Lifecycle Inventory (LCI) and preliminary report on the greenhouse gas and energy return on investment (EROI) for the fermentation of sugars to hydrocarbons pathway.	11.1.1.3	On-schedule

Technical Supplemental Slides

- Slides 28-36 on results of using NREL's Feedstock Production Emissions to Air Model (F-PEAM)
- Slide 37-38 on CHEMKIN modeling of biorefinery emissions.

Feedstock Production Scenario

- **Scenario examined**
  - Large scale deployment of cellulosic biofuels based on RFS2 mandates in 2022 (i.e., 16 billion gallons of cellulosic biofuels)
- **Biomass production - BT2 baseline**
  - 1% per annum average yield increases for corn and 1% for all energy crops
- **Harvest practices utilize advanced uniform design (INL)**
  - e.g., Single-pass harvest of agricultural residues
- **System boundary (area of focus in FY13):** feedstock production through harvest and on-farm transport (to farm gate)

Methods for Metrics Evaluated

- **Emission per gallon of ethanol**

$$= \frac{\sum Emissions\ from\ all\ activities}{Feedstock\ production * EtOH_{yield}}$$

- **Contribution analysis**

$$Contribution_{activity} = \frac{\sum pollutant\ by\ activity}{\sum across\ all\ activities}$$

- **Comparison of emissions from cellulosic feedstocks to NEI (R)**

$$= \frac{Emissions\ from\ production\ of\ cellulosic\ biofuel\ feedstock}{Nonroad{+}Nonpoint\ emissions\ from\ 2008\ NEI}$$

- **NEI ratio thresholds compared to Attainment Status for National Ambient Air Quality Standards (NAAQS).**

NAAQS and Precursor Pollutants

NAAQS Pollutant	***Ozone***	***$PM_{2.5}$***	***SO_2***
Precursor	NO_x, VOC	NO_x, VOC, SO_2, $PM_{2.5}$, NH_3	SO_2

Feedstock Allocation

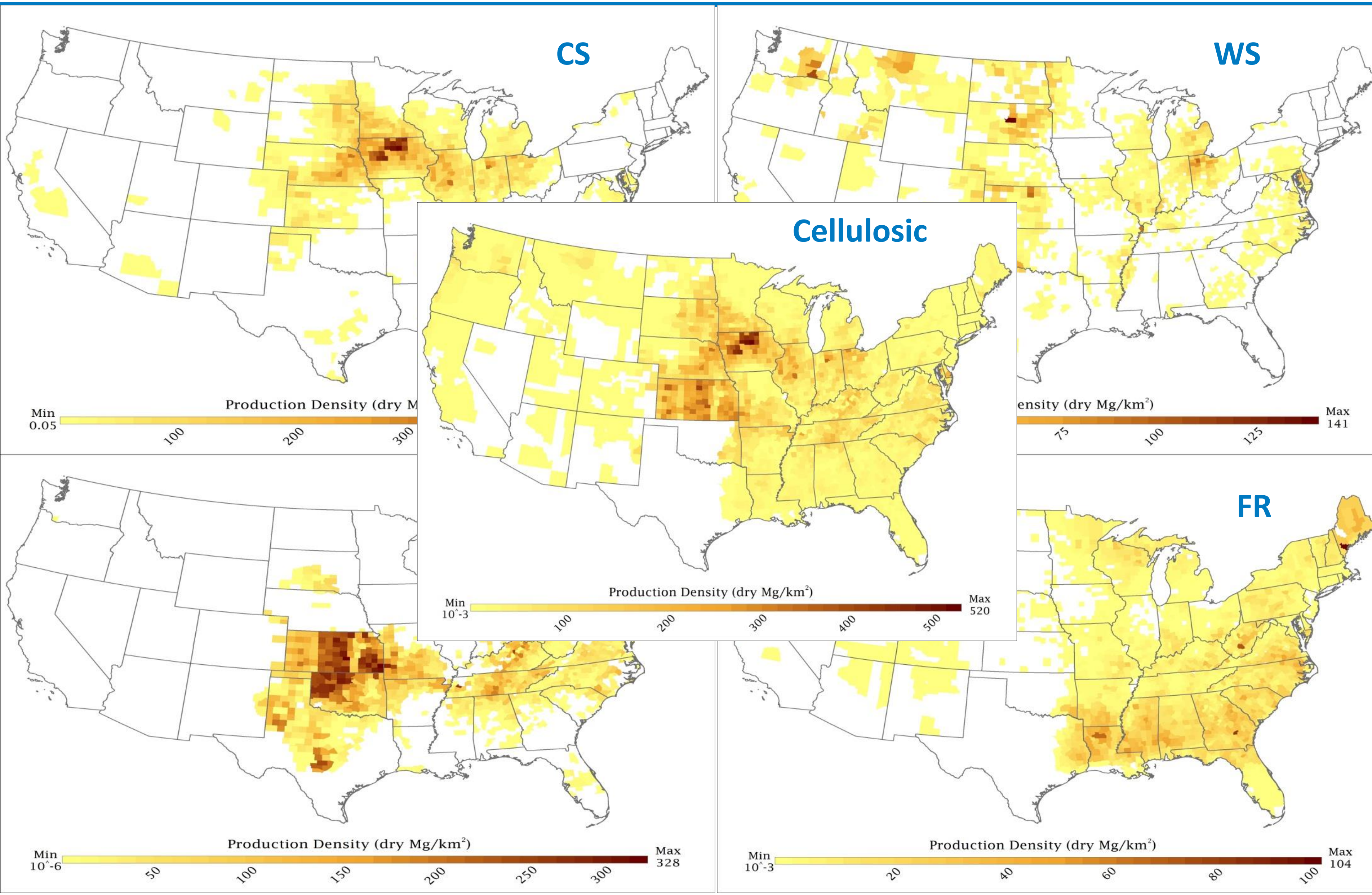
Feedstock production: BT2 estimates biomass feedstock production for multiple bioenergy and bioproducts industries

- Assume national average allocation to these markets applies to each county (52%) and to each feedstock

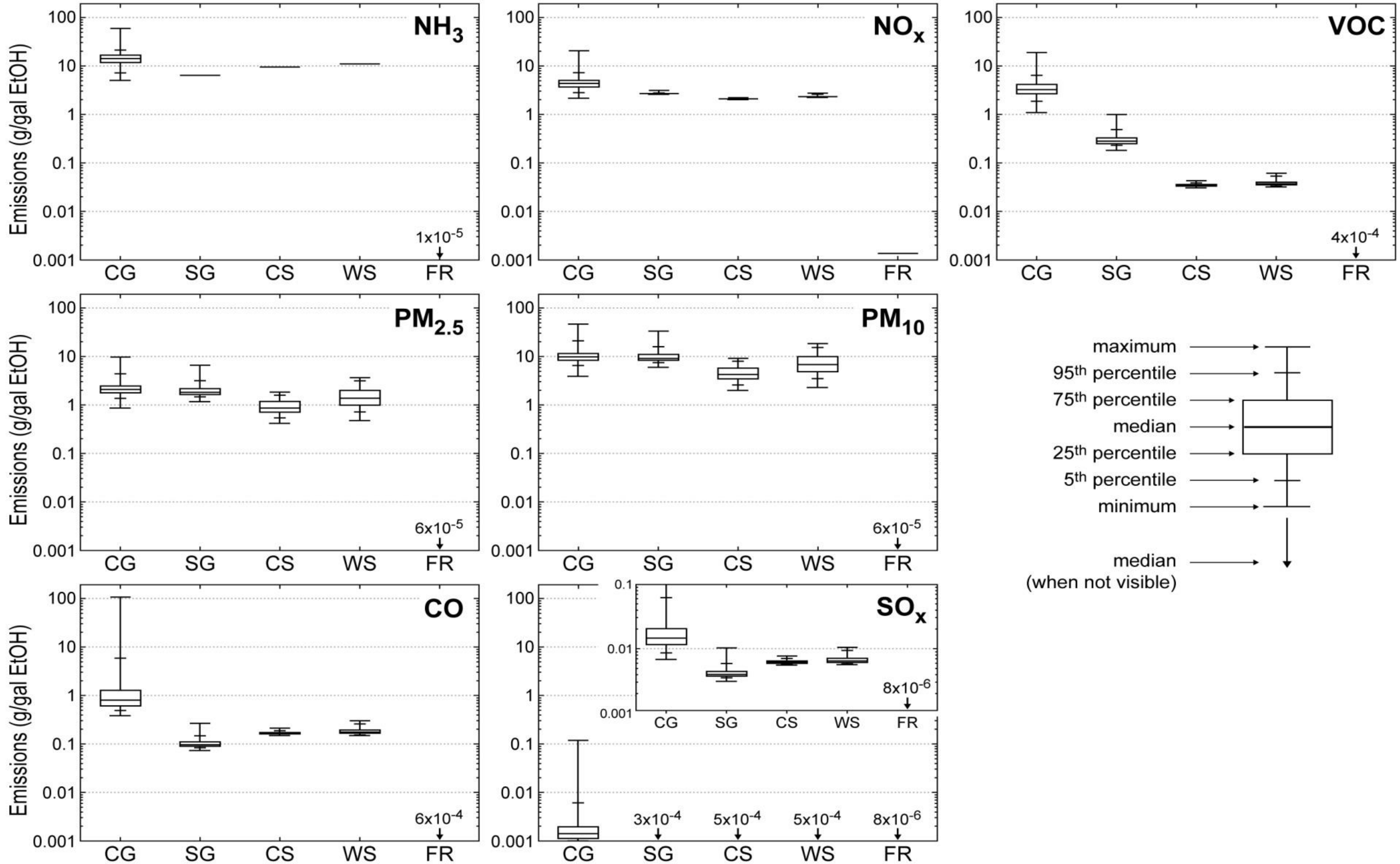
Multi-product systems: Use product-purpose allocation (Wang et al. 2007)

Multi-year systems: Switchgrass assumed 10-year cycle, with 10% of emissions allocated to each year.

Results: Cellulosic Feedstock Production Density

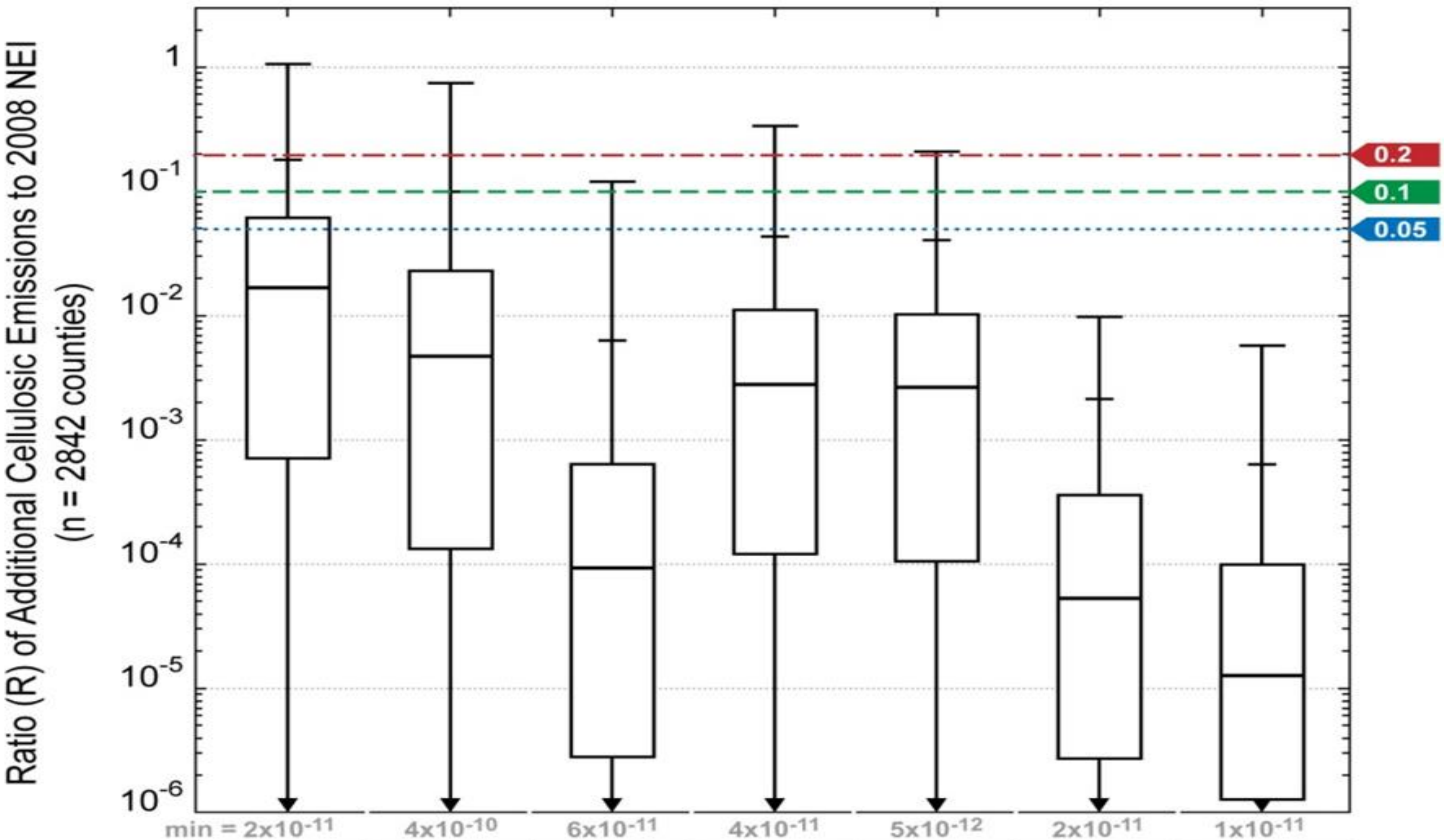


Results: Baseline Distribution of County-level Emissions by Feedstock



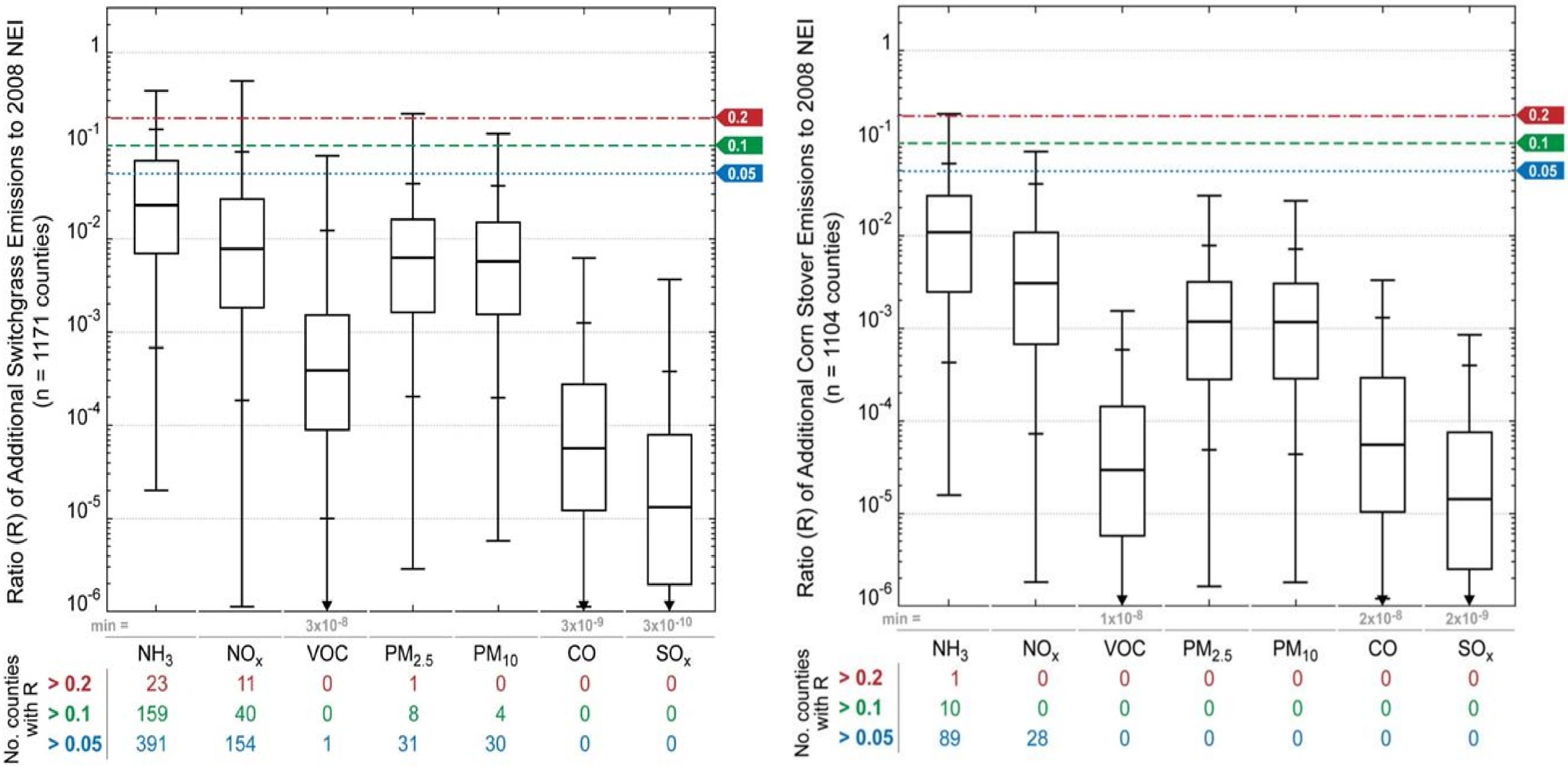
CG = corn grain; SG = switchgrass; CS = corn stover; WS = wheat straw; FR = forest residues; EtOH = ethanol.

Results: County-level Ratio of Sum of Cellulosic Biofuel Emissions to 2008 National Emissions Inventory (NEI) (Non-road + Non-point)



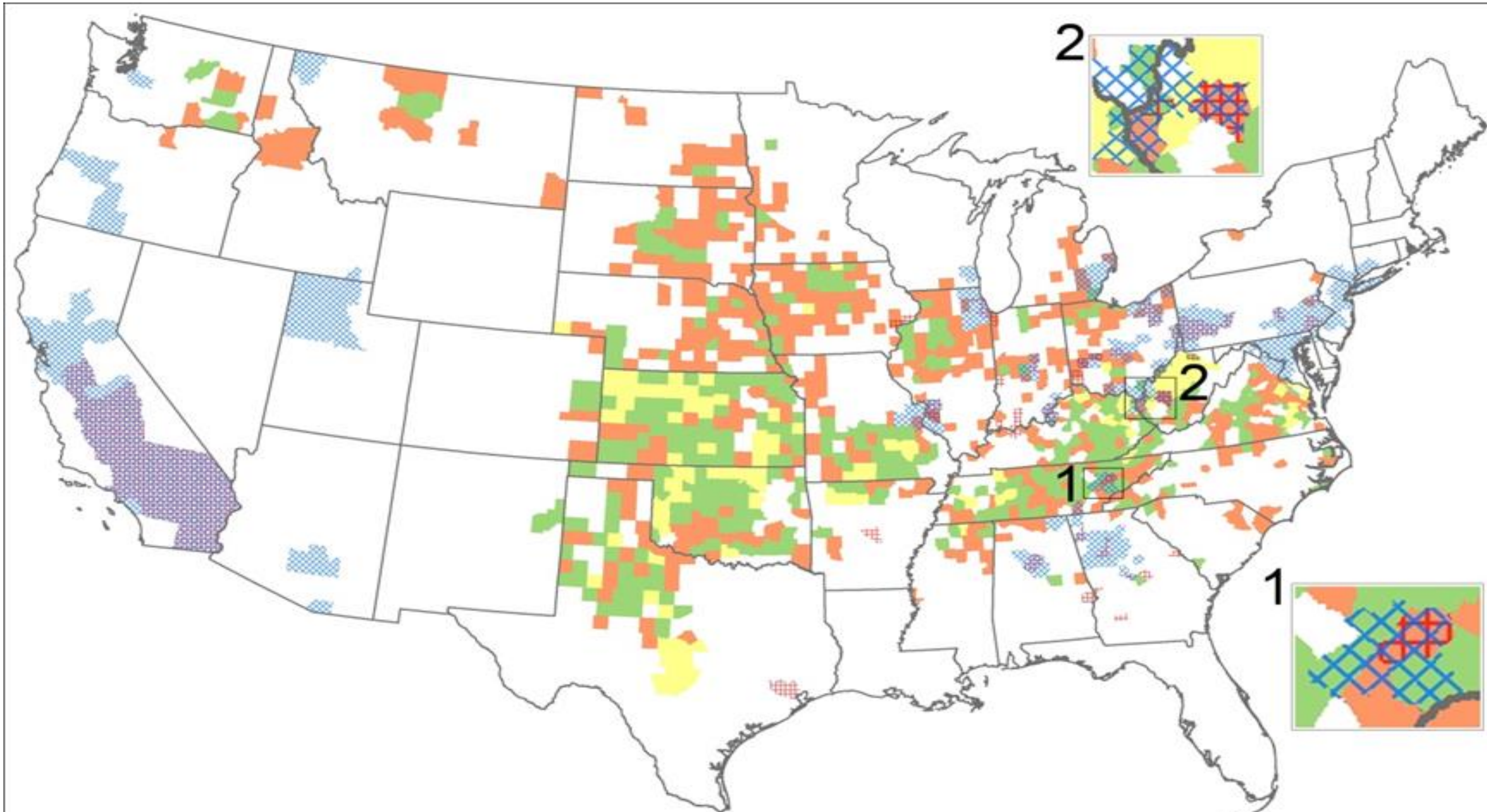
No. counties with R	NH_3	NO_x	VOC	$PM_{2.5}$	PM_{10}	CO	SO_x
> 0.2	108	27	0	3	1	0	0
> 0.1	407	147	1	20	14	0	0
> 0.05	841	372	6	106	93	0	0

Results: Distribution of SG and CS Emissions to 2008 NEI



Emissions for wheat straw similar to CS and for forest residues, far lower.

Results: Counties Exceeding NEI Thresholds and Current NAAs for 1997 and/or 2006 $PM_{2.5}$ NAAQS or Having $PM_{2.5}$ Concentration Currently Exceeding the 2012 NAAQS



$PM_{2.5}$	Number of Counties	
	1997/2006	2012
R > 0.2	3	0
R > 0.1	13	4
R > 0.05	34	12

Counties in nonattainment for 1997 or 2006 $PM_{2.5}$ NAAQS

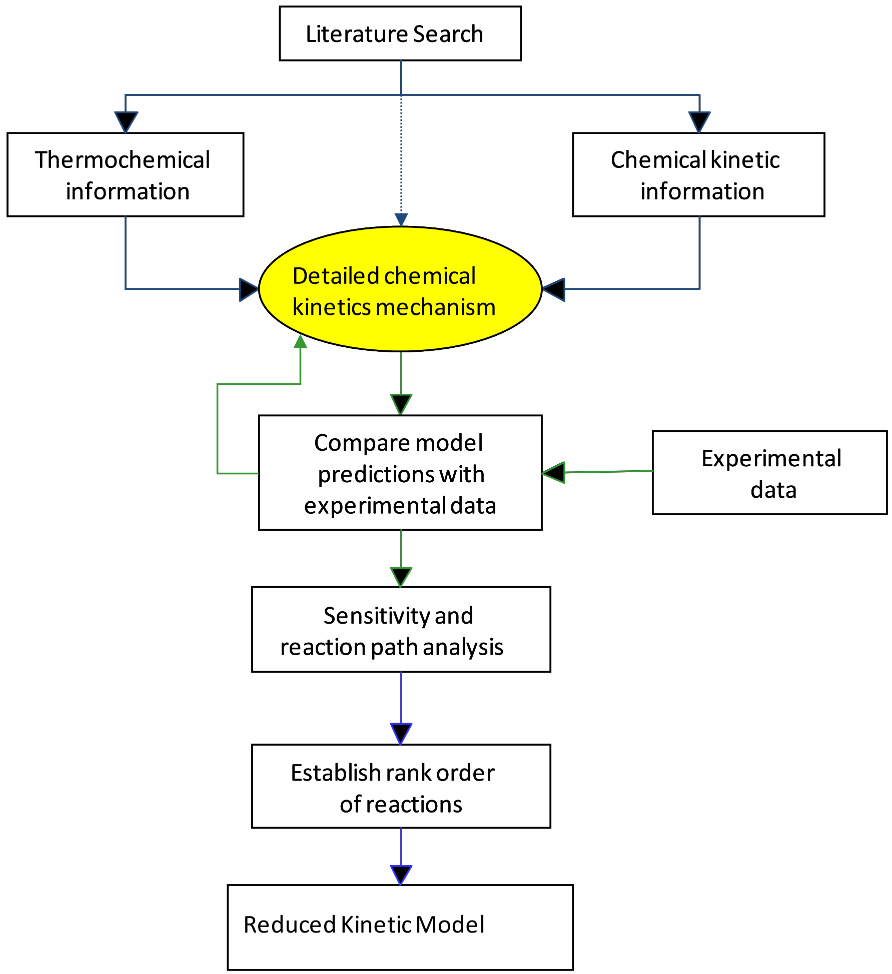
Counties with concentration greater than 2012 $PM_{2.5}$ NAAQS

Comparisons to GREET and Tessum (2012) for Current Corn Grain

g/gal EtOH	GREET (for 2011)	Our estimates (for 2011)			Tessum et al. (2012)
	Mean	Max	Mean	Min	Mean
VOC	0.18	19.5	3.71	1.11	0.152
CO	0.98	108	1.66	0.388	0.841
NO_x	4.37	20.4	4.62	2.15	3.61
PM_{10}	0.112	47.6	11.1	4.03	0.097
$PM_{2.5}$	0.101	9.74	2.35	0.875	0.088
SO_x	0.01	0.124	0.0023	0.0006	0.011
NH_3	N.A.	59.9	14.3	5.03	5.48

Tessum, C.W., Marshall, J.D. and Hill, J.D. 2012. A Spatially and Temporally Explicit Life Cycle Inventory of Air Pollutants from Gasoline and Ethanol in the United States. Environmental Science & Technology, 46(20): 11408–17.

Algorithm for the development of a detailed reaction mechanism



Reference: Key, R. J. C., M. E.; Glarborg, P. (2003). Chemically Reacting Flow : Theory and Practice, John Wiley & Sons, Inc., Hoboken, New Jersey.

CHEMKIN Modeling Key Assumptions

Biochemical conversion – lignin combustion (FY12 Q4 milestone report)

•A chemical kinetic model is constructed by assembling various related reaction mechanisms provided in published literature.

•The reference species guibourtinidol ($C_{15}H_{14}O_4$) is chosen to represent lignin.

•The feeds to the combustor are lignin and methane, a key component of biogas from anaerobic digestion. Unconverted cellulose and hemicellulose from the feedstock and biomass sludge from WWT are not considered in this study and are substituted with inert gas (N2).

Fast pyrolysis – char combustion (FY13 Q2 milestone report)

•The char combustion mechanism is developed based on the global kinetics of wood char devolatilization and combustion reported in literatures.

•The impact of ash on char combustion kinetics is not investigated in this study.

•The chemical entity of the char after the devolatilization is assumed to be elemental carbon; this is the same as the bulk carbon.

•A fraction of the char is assumed be condensed-phase particles. It is further assumed that disproportionation of carbon monoxide into carbon dioxide and carbon occurs.

•CHEMKIN Particle Tracking only considers particles generated via homogeneous nucleation (or self-nucleation); that is, no foreign nucleus is involved in the nucleation process.