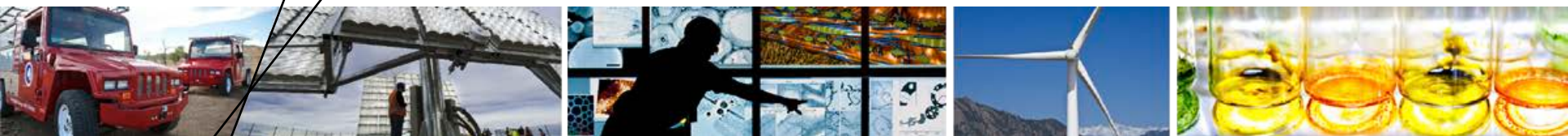


# Selected Highlights of LCA Activities at NREL



**LCA XIII Special Session:  
LCA at DOE**

**October 2, 2013**

**NREL/PR-6A20-60059**

TEAM:

Alberta Carpenter

Garvin Heath

Daniel Inman

Margaret Mann

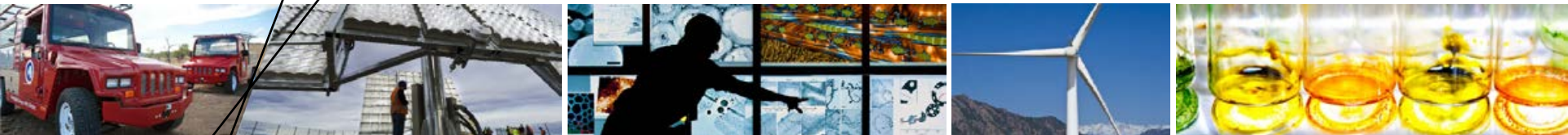
Ethan Warner

Yimin Zhang

# Highlighted projects

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- 1. Life cycle air pollutant emissions inventory for biofuels; spatially, temporally, and chemically explicit life cycle inventories**
- 2. Materials Flows through Industry (MFI) tool for energy impacts**
- 3. Land use change modeling methodology.**



# Comparative air pollutant emissions of selected biofuels feedstocks in 2022

Yimin Zhang, Garvin Heath, Alberta Carpenter, Noah Fisher

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

## NREL F-PEAM

### Inputs

**BTS** (e.g., acres, yields, production by county)

**Crop Budget** (e.g., fertilizer inputs, machinery usage)

**USDA Data** (e.g., irrigation, types of fertilizers)

**Literature Data** (e.g., emissions factors)

### Linked Models

**NonRoad Model + EFs**  
(CO, NO<sub>x</sub>, SO<sub>x</sub>, VOC, PM, NH<sub>3</sub>)

**Fertilizer Emissions**  
(NO<sub>x</sub>, NH<sub>3</sub>)

**Pesticide Emissions**  
(VOCs)

**Fugitive Dust**  
(PM)

### Analysis Outputs

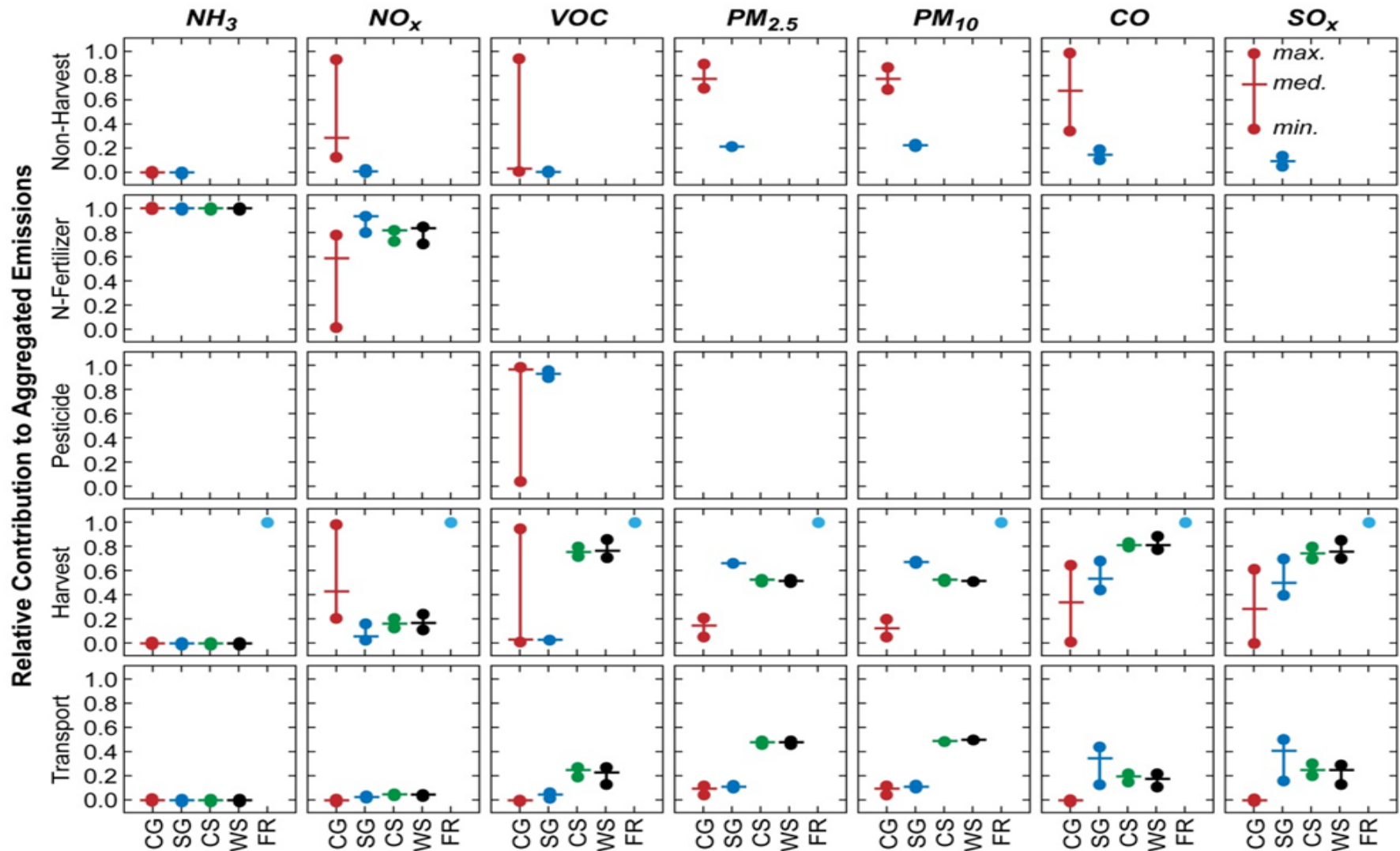
**County-level Mass Emissions**

**Emissions by Feedstock**  
(mass per gal)

**Comparison to NEI**

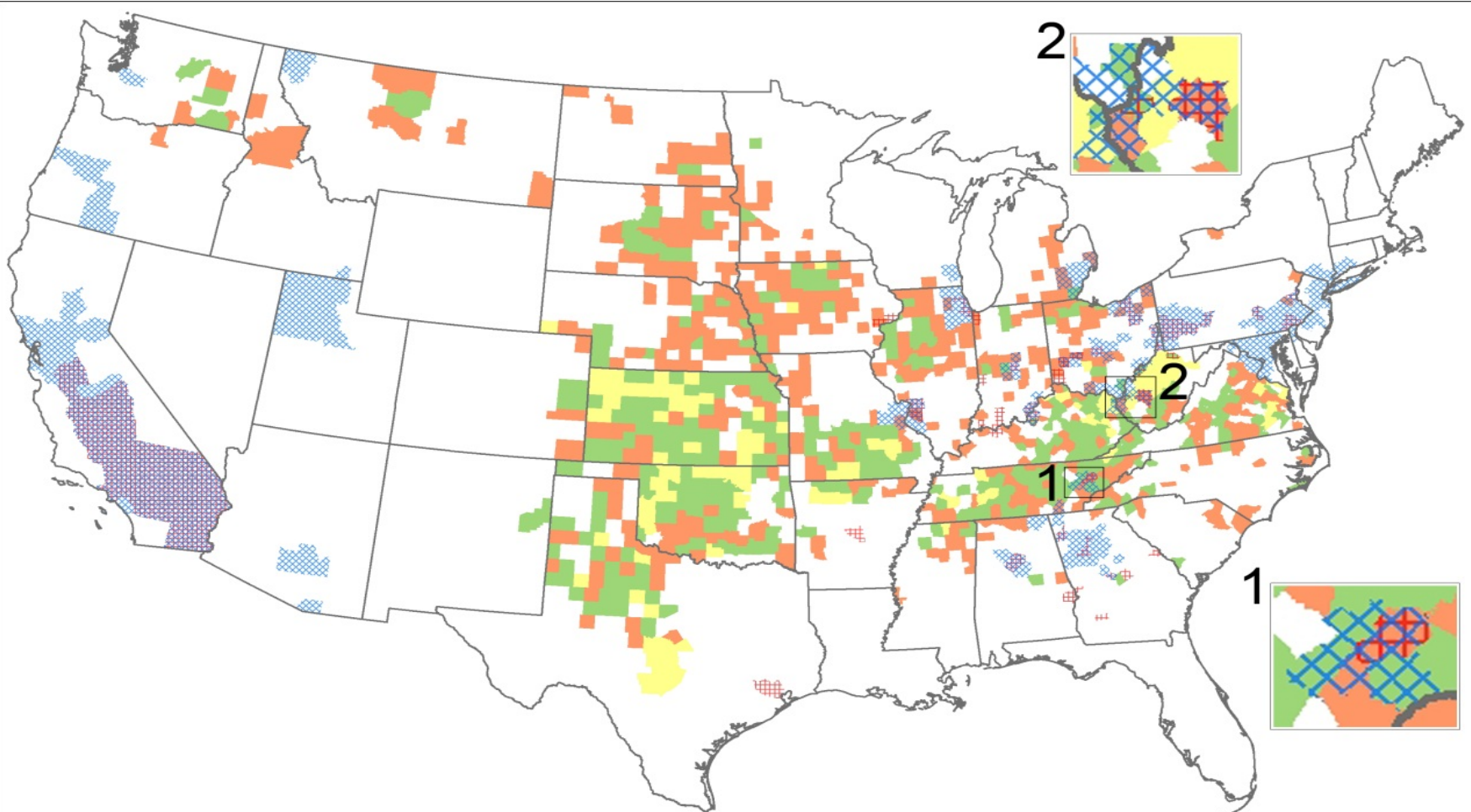
**Potential Impact in Nonattainment Areas**

# Contribution by Activity Category to County Emissions: First Step to Target Setting





Blanks represent no emissions of that pollutant for that feedstock.

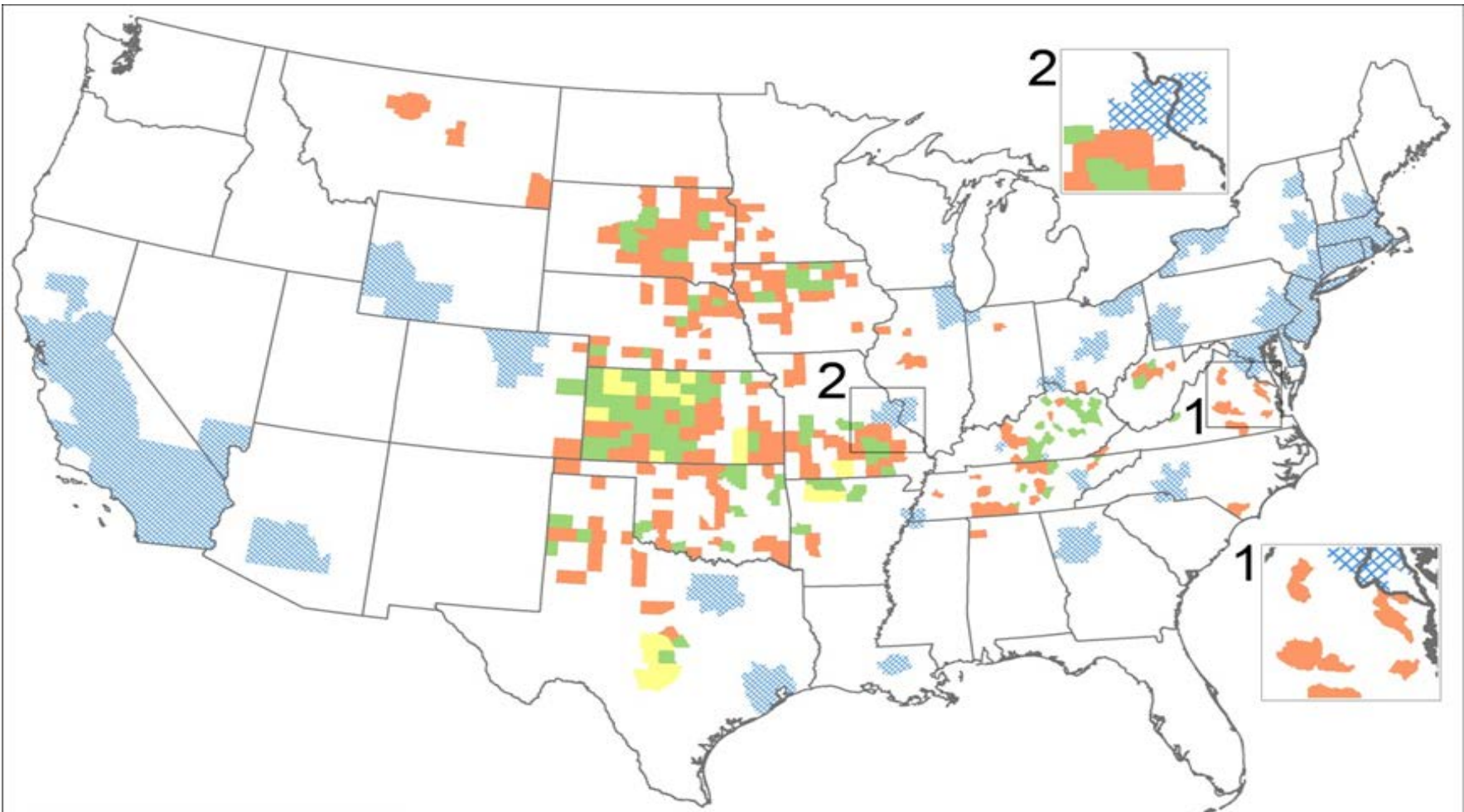
# Counties with Cellulosic Feedstock O<sub>3</sub> Precursor Emissions Exceeding 3 NEI Thresholds, Alongside Current O<sub>3</sub> Nonattainment Areas



PM <sub>2.5</sub>	Number of Counties	
	1997/2006	2012
R > 0.2	3	0
R > 0.1	13	4
R > 0.05	34	12

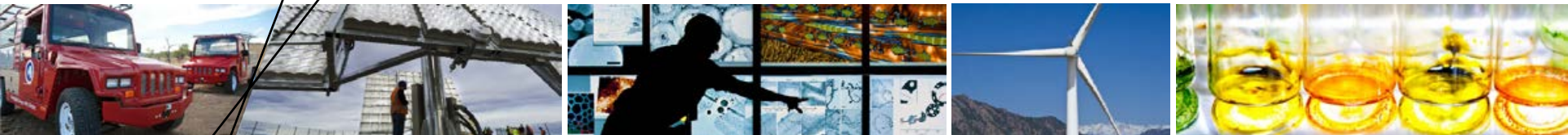
 Counties in nonattainment for 1997 or 2006 PM<sub>2.5</sub> NAAQS  
 Counties with concentration greater than 2012 PM<sub>2.5</sub> NAAQS

# Counties with Cellulosic Feedstock O<sub>3</sub> Precursor Emissions Exceeding 3 NEI Thresholds, Alongside Current O<sub>3</sub> Nonattainment Areas



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

Counties in nonattainment for 1997 or 2008 8-hr Ozone NAAQS

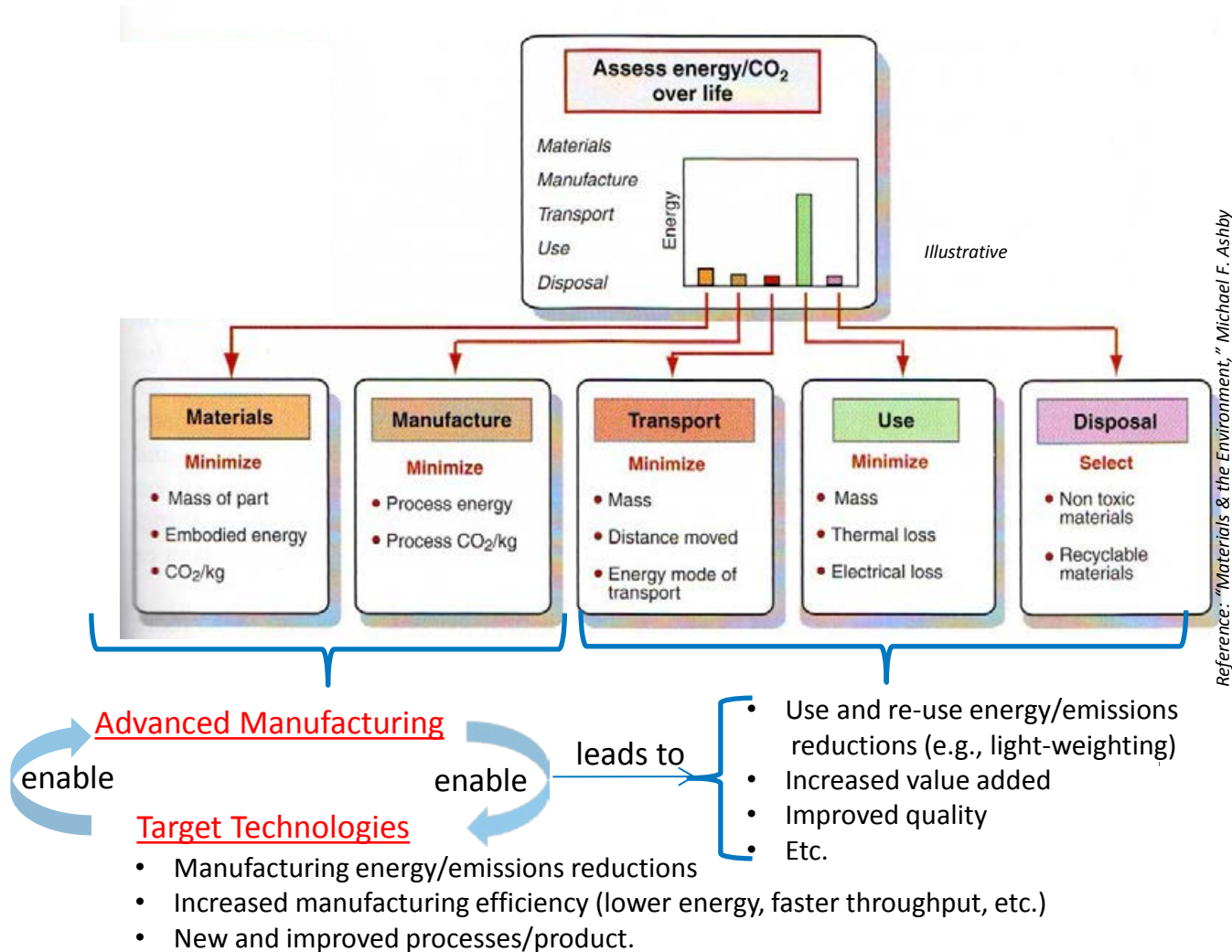


# Materials Flows through Industry (MFI) tool for energy impacts

Alberta Carpenter, Margaret Mann



# DOE AMO Life Cycle Approach



What are the opportunities for manufacturing impacts across the life cycle?

# Materials Flow through Industry (MFI) Tool

**Function:** A tool enables scenarios of changes in energy efficiency of processes, changes in materials use, changes in carbon intensity of materials:

- Process comparisons
- Material substitution
- Sector energy efficiency potential
- Grid mix evaluation
- Track energy & GHG emissions at the per unit (mass) product level

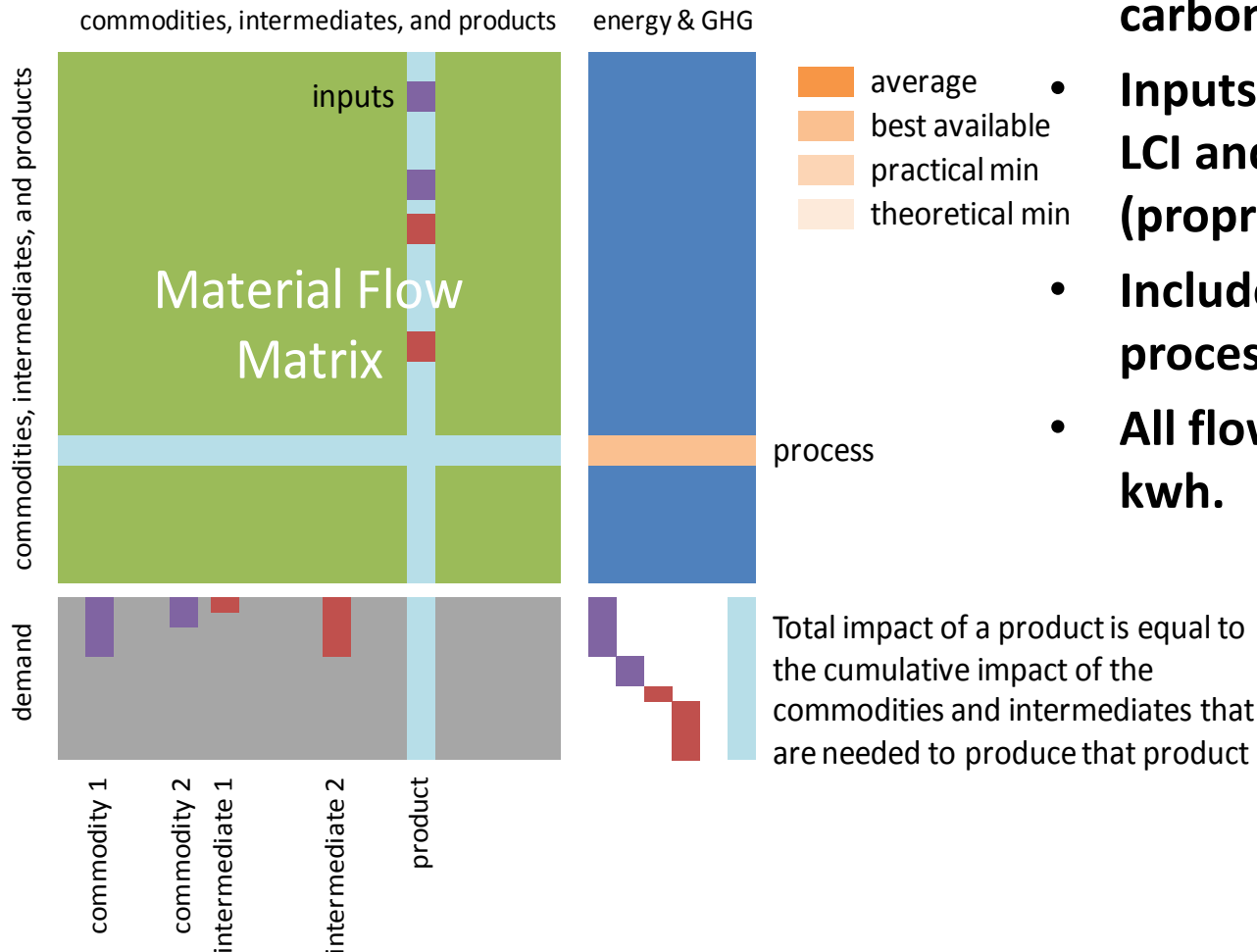
## **Data Driven:**

- Use pre-existing lifecycle (LC) data readily adopted for parts of the sector (USLCI, ecoinvent).
- Market data and recipes for over 500 products and 1200 processes
- Recipes (mass & energy balance) of the manufacturing step: raw materials; fuel inputs; product & co-product outputs; GHG emissions (SRI).

## **Output:**

- Overall material & energy balance – material flows of through supply chain.
- Energy & GHG emissions tracked at the per unit product level and at market use level.
- Tabular and graphical representation of “base case” and “scenario” (e.g. after material substitution).

# MFI Tool Structure



- IO process based matrix model
- Tracks energy and fuel derived carbon emissions
- Inputs and outputs are based on LCI and process economics data (proprietary)
- Includes 500+ products, 1200+ processes
- All flows accounted for in kg or kwh.

Source: Seungwook Ma, PhD, DOE

# Tool Inputs

1	<b>User Input Page</b>		
2			
3			
4	<b>Step 1:</b>	Select category:	NONFERROUS
5			
6			
7	<b>Step 2:</b>	Recalculate:	Recalculate
8			
9			
10	<b>Step 3:</b>	Select material:	ALUMINUM, SMELT
11			
12			
13	<b>Step 4:</b>	Recalculate:	Recalculate
14			
15			
16	<b>Step 5:</b>	Demand (KG):	1,000
17			
18			
19	<b>Step 6:</b>	Steps in the supply chain:	
20			
21		Scenario A	5
22		Scenario B	5
23		Scenario C	5
24			

# Tool Inputs

1	<b>User Input Page</b>		4	Number of		
2			5	Substitutes:	0	
3			6			<b>Replacement Factor</b>
4	<b>Step 1:</b>	Select ca	7			<b>(lb per 1 lb of ALUMINUM, SMELT)</b>
5			8	<b>Substitute</b>		<b>Low</b>
6			9			<b>High</b>
7	<b>Step 2:</b>	Recalate	10			<b>Functionality</b>
8			11			
9			12			
10	<b>Step 3:</b>	Select material:	13			
11			14			
12			15			
13	<b>Step 4:</b>	Recalculate:	16			
14			17			
15			18			
16	<b>Step 5:</b>	Demand (KG):	19			
17			20			
18			21			
19	<b>Step 6:</b>	Steps in the supply chain:	22			
20			23			
21		<b>Scenario A</b>	24			
22		<b>Scenario B</b>				
23		<b>Scenario C</b>				

# Tool Inputs

Choose Baseline, Equal Weighting or Input Own Values

Process	Baseline Weighting	Equal Weighting	Choose Baseline	Choose Baseline	Choose Baseline
			Input Own New Weighting Scenario A	Input Own New Weighting Scenario B	Input Own New Weighting Scenario C
CARBOTHERMIC	0%	17%	100%	100%	100%
CLAY CARBOCHLORINATION	0%	17%	0%	0%	0%
HH WETTED CATHODE	0%	17%	0%	0%	0%
H-H/INERT ANODE	0%	17%	0%	0%	0%
MODERN HALL HEROULT PROCESS	100%	17%	0%	0%	0%
SMELTING OF REFINED ALUMINA TO METALLIC ALUMINUM	0%	17%	0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%
			0%	0%	0%

12

13 **Step 4:** Recalculate:

14

15

16 **Step 5:** Demand (KG):

17

18

19 **Step 6:** Steps in the supply chain:

20

21 **Scenario A**

22 **Scenario B**

23 **Scenario C**

24

# Tool Inputs

						Choose Baseline, Equal Weighting or Input Own Values		
						Choose Baseline	Choose Baseline	Choose Baseline
Product: ALUMINUM, SMELT						Input Own New Weighting Scenario A	Input Own New Weighting Scenario B	Input Own New Weighting Scenario C
Process	Baseline Weighting	Equal Weighting						
CARBOTHERMIC	0%	17%	100%	100%	100%			
CLAY CARBOCHLORINATION	0%	17%	0%	0%	0%			

						Choose Baseline or Own Values		
						Choose Baseline	Choose Baseline	Input Own
Product: ALUMINUM, SMELT						Input Own New Implimentation Scenario A	Input Own New Implimentation Scenario B	Input Own New Implimentation Scenario C
Process	Baseline Implimentation							
CARBOTHERMIC	0%	100%	100%	100%				
CLAY CARBOCHLORINATION	0%	0%	0%	0%				
HH WETTED CATHODE	0%	0%	0%	0%				
H-H/INERT ANODE	0%	0%	0%	0%				
MODERN HALL HEROULT PROCESS	0%	0%	0%	0%				
SMELTING OF REFINED ALUMINA TO METALLIC ALUMINUM	0%	0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				
		0%	0%	0%				

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**Step 6:** Steps in the supply chain:

Scenario A	5
Scenario B	5
Scenario C	5

# Tool Inputs

						Choose Baseline, Equal Weighting or Input Own Values		
						Choose Baseline	Choose Baseline	Choose Baseline
Product: ALUMINUM, SMELT						Input Own New Weighting Scenario A	Input Own New Weighting Scenario B	Input Own New Weighting Scenario C
Process	Baseline Weighting	Equal Weighting						
CARBOTHERMIC	0%	17%	100%	100%	100%			
CLAY CARBOCHLORINATION	0%	17%	0%	0%	0%			
HH								
H-ion								
M								
SM								
Product: ALUMINUM, SMELT						Choose Baseline or Own Values		
						Choose Baseline	Choose Baseline	Input Own
Product: ALUMINUM, SMELT						Input Own New Implimentation Scenario A	Input Own New Implimentation Scenario B	Input Own New Implimentation Scenario C
Process	Baseline Implimentation	Equal Weighting						
CARBOTHERMIC	0%	17%	100%	100%	100%			
CLAY CARBOCHLORINATION	0%	17%	0%	0%	0%			
HH WETTED CATHODE	0%	17%	0%	0%	0%			
H-H/INERT ANODE	0%	17%	0%	0%	0%			
MODERN HALL HEROULT PROCESS	0%	17%	0%	0%	0%			
SMELTING OF REFINED ALUMINA TO METALLIC ALUMINUM	0%	17%	0%	0%	0%			

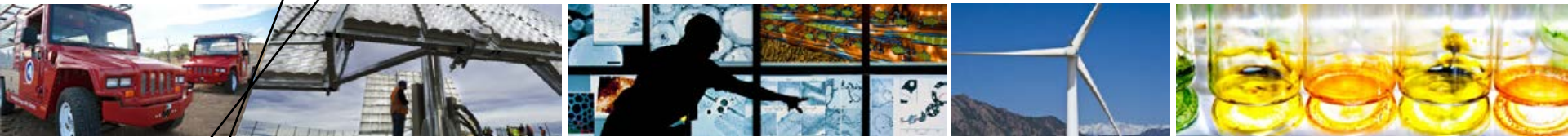
						Choose Baseline or Own Values		
						Choose Baseline	Choose Baseline	Choose Baseline
Product: ALUMINUM, SMELT						Input Own Grid Mix Scenario A	Input Own Grid Mix Scenario B	Input Own Grid Mix Scenario C
Process	Baseline Implimentation	Equal Weighting						
ELECTRICITY GRID, FRCC	0%	17%	0%	0%	0%			
ELECTRICITY GRID, MRO	0%	17%	0%	0%	0%			
ELECTRICITY GRID, NATIONAL	100%	17%	100%	100%	100%			
ELECTRICITY GRID, NPCC	0%	17%	0%	0%	0%			
ELECTRICITY GRID, RFC	0%	17%	0%	0%	0%			
ELECTRICITY GRID, SERC	0%	17%	0%	0%	0%			
ELECTRICITY GRID, SPP	0%	17%	0%	0%	0%			
ELECTRICITY GRID, TRE	0%	17%	0%	0%	0%			
ELECTRICITY GRID, WECC	0%	17%	0%	0%	0%			



# Tool Outputs

Scenario A: Results per 1000 KG of ALUMINUM, SMELT for 5 Steps													
SORTED BY DIRECT	Electricity	Coal (GJ)	Natural Gas	Diesel (GJ)	Kerosene	Fuel Oil and	Crude Oil	Primary Energy	Steam (GJ)	Mass (KG)	Carbon Dioxide	Carbon Dioxide	
TOTAL	3.08E+03	9.01E+00	9.77E+03	-4.60E+04	-2.32E+04	9.58E+03	2.20E+05	1.70E+05	0.00E+00	3.62E+05	1.28E-02	2.19E-04	
1 REFINERY GAS	1.53E+03	0.00E+00	1.07E+03	-2.78E+04	-1.47E+04	-1.01E+03	1.35E+05	9.29E+04	0.00E+00	2.04E+02	7.14E-03	1.24E-07	
2 COKE	3.67E+02	0.00E+00	2.56E+02	-6.60E+03	-3.52E+03	-2.43E+02	3.23E+04	2.22E+04	0.00E+00	4.14E+04	1.71E-03	2.51E-05	
3 KEROSENE	1.63E+02	0.00E+00	6.10E+02	-3.10E+03	0.00E+00	8.51E+02	1.19E+04	1.02E+04	0.00E+00	3.13E+04	7.66E-04	1.90E-05	
4 GASOLINE	1.42E+02	0.00E+00	3.80E+01	-3.68E+02	-1.96E+02	8.08E+03	1.80E+03	9.35E+03	0.00E+00	1.45E+05	7.01E-04	8.81E-05	
5 PETROLEUM, COPRODUCT	1.46E+02	0.00E+00	1.02E+02	-2.63E+03	-1.40E+03	-9.67E+01	1.29E+04	8.85E+03	0.00E+00	1.43E+04	6.80E-04	8.66E-06	
6 BITUMEN	1.46E+02	0.00E+00	1.02E+02	-2.68E+03	-1.40E+03	-9.67E+01	1.29E+04	8.80E+03	0.00E+00	1.02E+04	6.77E-04	6.16E-06	
7 LIQUID PETROLEUM GAS	1.45E+02	0.00E+00	1.01E+02	-2.61E+03	-1.39E+03	-9.60E+01	1.28E+04	8.78E+03	0.00E+00	6.90E+03	6.75E-04	4.19E-06	
8 DIESEL	1.92E+02	0.00E+00	6.74E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.74E+03	0.00E+00	8.77E+04	3.39E-04	5.32E-05	
9 FUEL GAS	2.02E+02	0.00E+00	7.13E+02	-5.83E+02	-4.94E+02	1.17E+03	0.00E+00	8.01E+02	0.00E+00	4.90E+03	4.82E-05	2.97E-06	
10 BUTYLENES	2.44E+01	0.00E+00	2.96E+00	0.00E+00	0.00E+00	7.69E+02	0.00E+00	7.72E+02	0.00E+00	4.03E+03	5.76E-05	2.45E-06	
11 BAUXITE	7.51E+00	0.00E+00	6.40E-02	2.54E+02	0.00E+00	4.84E+01	0.00E+00	3.03E+02	0.00E+00	5.29E+03	2.12E-05	3.21E-06	
12 NAPHTHA	9.35E-01	0.00E+00	1.07E+01	-3.84E+01	-1.08E+02	1.91E+02	0.00E+00	5.52E+01	0.00E+00	1.33E+03	4.65E-06	8.06E-07	
13 ALUMINA	8.74E-01	4.65E+00	9.09E+00	5.97E-02	0.00E+00	8.26E+00	0.00E+00	2.21E+01	0.00E+00	1.93E+03	1.50E-06	1.17E-06	
14 PROPYLENE	4.50E+00	0.00E+00	8.54E+00	0.00E+00	0.00E+00	8.29E+00	0.00E+00	1.68E+01	0.00E+00	2.76E+03	1.05E-06	1.68E-06	
15 SODIUM HYDROXIDE	9.06E-02	3.96E+00	2.45E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.99E+00	0.00E+00	1.73E+02	3.57E-07	1.05E-07	
16 C4 FRACTION	9.03E-03	0.00E+00	3.75E-01	0.00E+00	0.00E+00	2.73E+00	0.00E+00	3.11E+00	0.00E+00	7.74E+00	2.23E-07	4.70E-09	
17 NATURAL GAS, LIQUIDS, 86% E	4.64E-03	0.00E+00	2.90E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.90E+00	0.00E+00	6.47E+01	1.46E-07	3.32E-08	
18 GAS OIL, VACUUM	7.94E-03	0.00E+00	6.40E-02	-7.78E-01	0.00E+00	2.42E+00	0.00E+00	1.70E+00	0.00E+00	2.55E+02	1.30E-07	1.55E-07	
19 ISOBUTANE	1.39E-01	0.00E+00	1.33E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E+00	0.00E+00	2.17E+03	6.71E-08	1.32E-06	
20 ANODE	2.09E-01	2.82E-02	9.66E-01	4.73E-02	0.00E+00	2.14E-01	0.00E+00	1.26E+00	0.00E+00	4.50E+02	7.04E-08	2.73E-07	
21 METHANOL	0.00E+00	8.42E-02	7.23E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.07E-01	0.00E+00	2.34E+01	4.39E-08	1.42E-08	
22 XYLENES, MIXED	9.77E-02	0.00E+00	5.84E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.84E-01	0.00E+00	6.51E+02	2.94E-08	3.95E-07	
23 CALCIUM OXIDE	1.43E-02	2.75E-01	5.01E-02	2.12E-03	0.00E+00	0.00E+00	0.00E+00	3.28E-01	0.00E+00	5.87E+01	2.74E-08	3.56E-08	
24 COAL	5.26E-02	0.00E+00	7.15E-02	5.13E-02	0.00E+00	0.00E+00	0.00E+00	1.23E-01	0.00E+00	2.92E+02	7.15E-09	1.77E-07	
25 LIMESTONE	2.15E-03	1.38E-04	8.06E-04	3.16E-03	0.00E+00	0.00E+00	0.00E+00	4.10E-03	0.00E+00	1.41E+02	2.72E-10	8.57E-08	
26 IRON, PIG	0.00E+00	2.67E-03	2.32E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.69E-03	0.00E+00	1.93E-01	2.41E-10	1.17E-10	
27 FERRO NICKEL, 25% NI	2.41E-04	3.43E-04	2.55E-04	1.64E-05	0.00E+00	3.22E-05	0.00E+00	6.47E-04	0.00E+00	8.58E-03	4.72E-11	5.21E-12	
28 LIME	1.75E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E-04	0.00E+00	1.14E-04	0.00E+00	7.63E+01	8.54E-12	4.63E-08	
29 N-METHYL-2-PYRROLIDONE	3.84E-06	0.00E+00	5.03E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.03E-05	0.00E+00	6.06E-02	2.53E-12	3.67E-11	
30 FERROCHROMIUM, HIGH-CARB	3.78E-05	3.07E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.07E-05	0.00E+00	3.16E-03	2.75E-12	1.91E-12	
31 STEEL, ALLOYED	3.13E-05	9.90E-08	1.48E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.49E-05	0.00E+00	3.96E-01	7.55E-13	2.40E-10	
32 IRON, SCRAP	9.76E-07	0.00E+00	0.00E+00	2.71E-06	0.00E+00	0.00E+00	0.00E+00	2.71E-06	0.00E+00	2.71E-02	1.68E-13	1.64E-11	
33 FERROMANGANESE, HIGH-CO#	1.11E-05	1.34E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.34E-06	0.00E+00	2.98E-03	1.20E-13	1.81E-12	
34 DOLOMITE	6.90E-08	0.00E+00	0.00E+00	1.06E-08	0.00E+00	5.51E-08	0.00E+00	6.57E-08	0.00E+00	5.90E-04	4.85E-15	3.58E-13	
35	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
36	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
37	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	

- Results are still in preliminary stages
- Looking to identify which product inputs have largest energy and carbon demands.

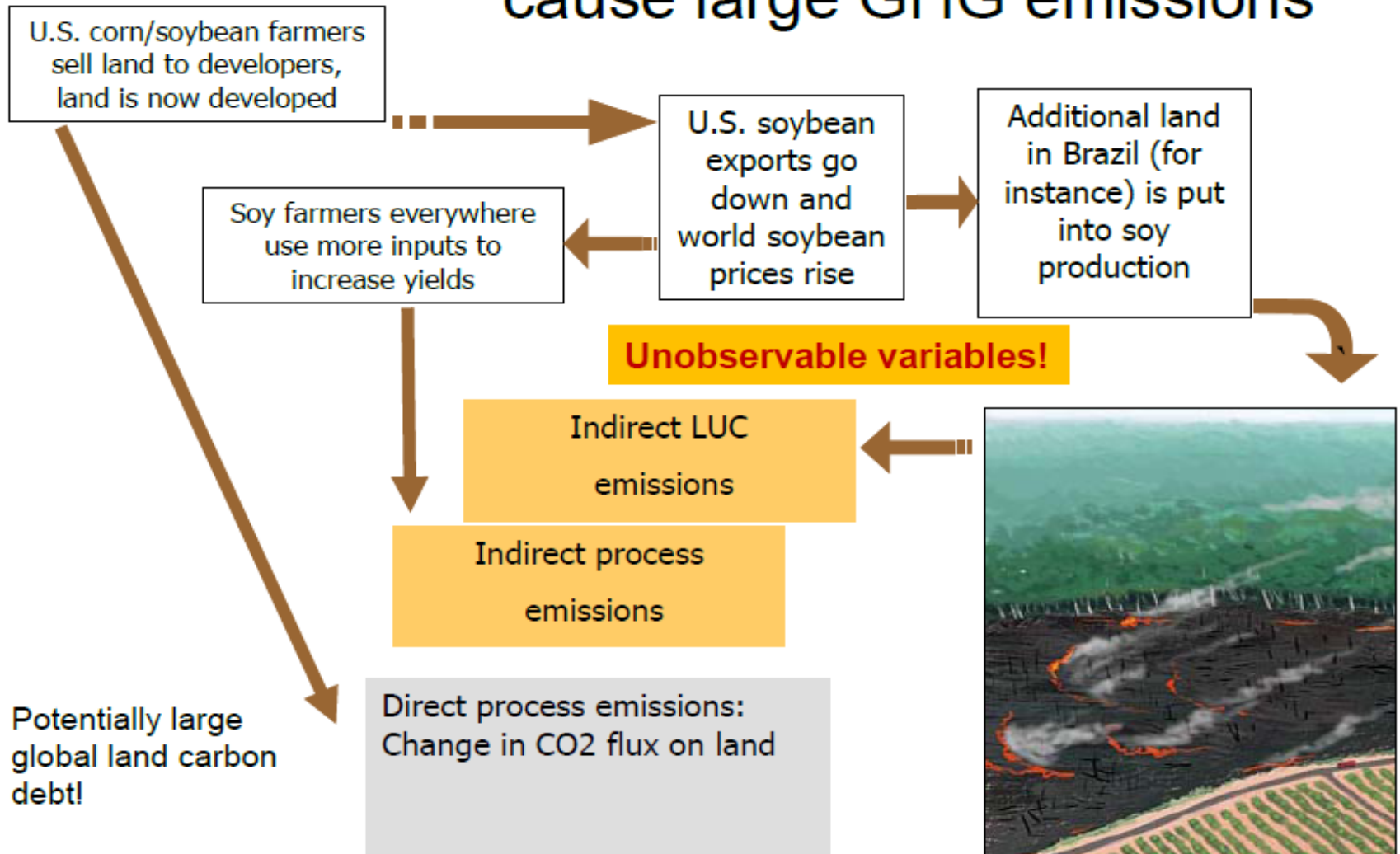


# Land use change model

Ethan Warner, Daniel Inman, Yimin Zhang

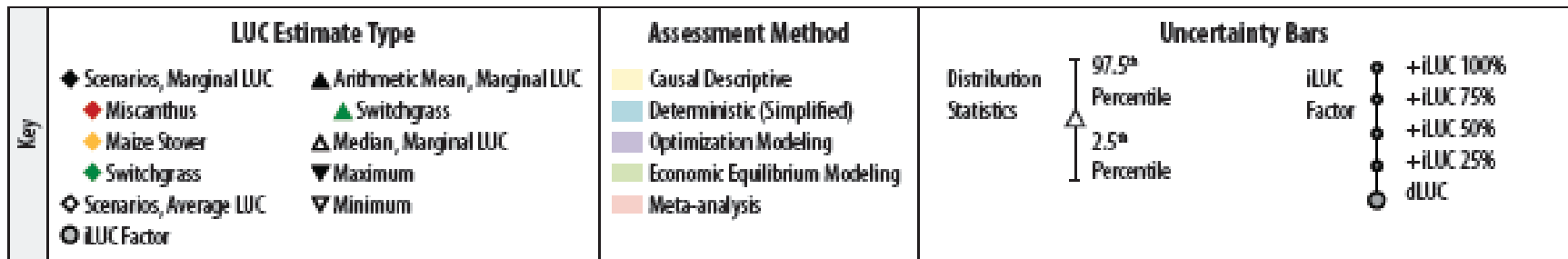
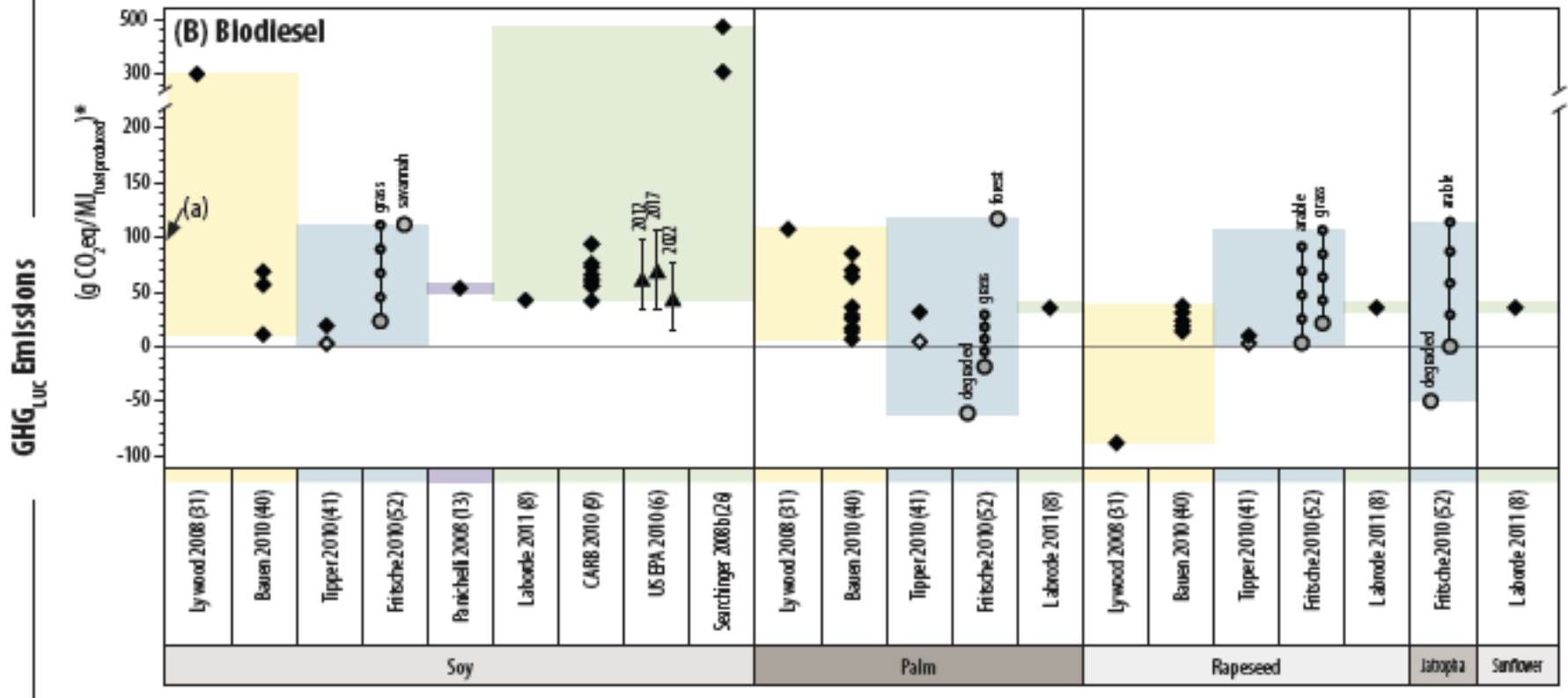
# Background

## Land use change (LUC) may cause large GHG emissions



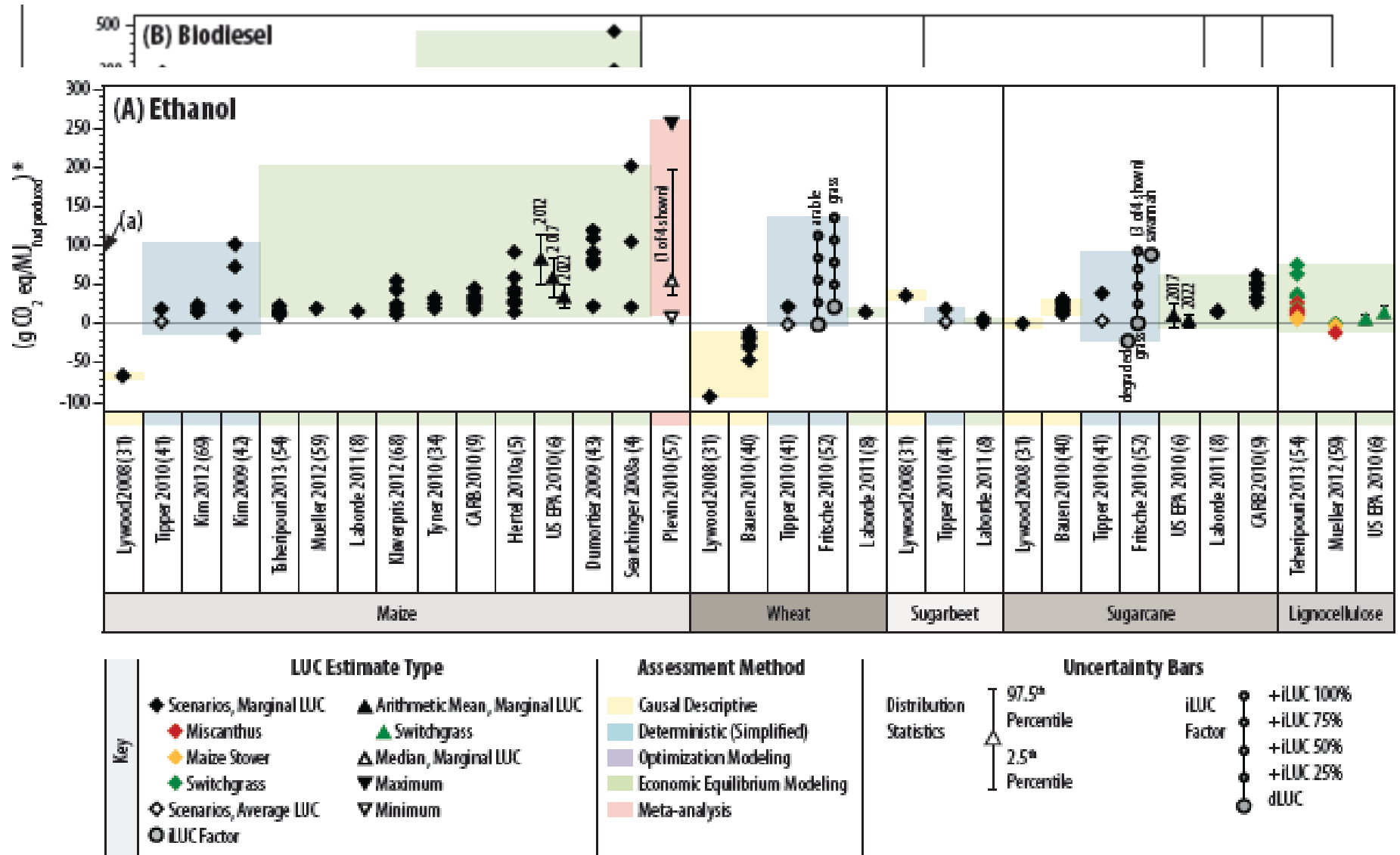
Source: Searchinger T, Heimlich R, Houghton R A, Dong F, Elobeid A, Fabiosa J, Tokgoz S, Hayes D and Yu T H 2008 Use of US croplands for biofuels increases greenhouse gases through emissions from land-use change Science 319 1238–40

# Literature Review



Source: Warner, Zhang, Inman and Heath. 2013. Challenges in the estimation of greenhouse gas emissions from biofuel-induced global land-use change. *Biofuels, Bioproducts and Biorefining*. DOI: 10.1002/bbb.1434

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# Goal Statement

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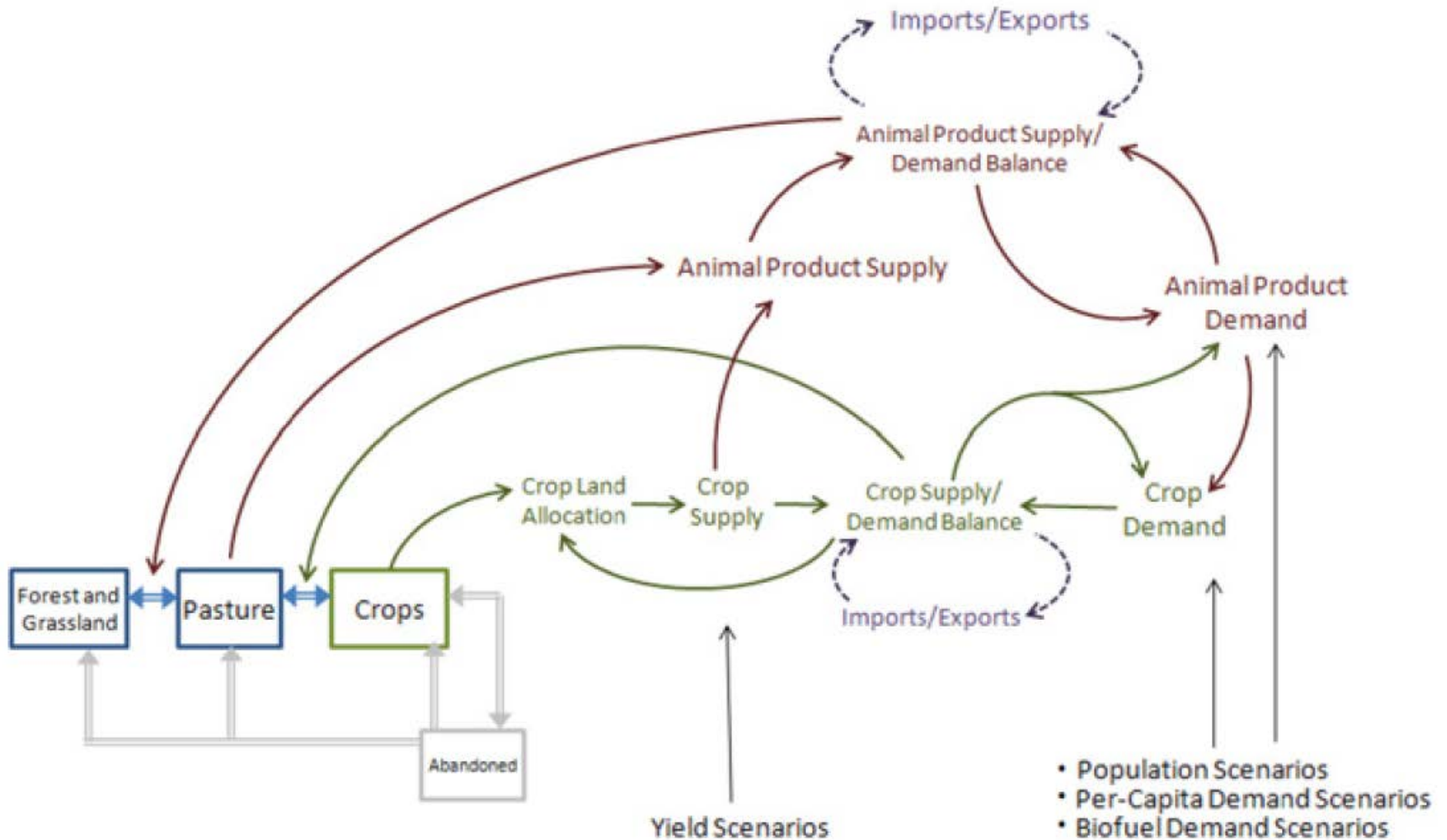
- 1. To create and utilize systems dynamics to model the key drivers of land use change, including biomass conversion and biofuels production**
- 2. To create a transparent and relatively simple model for test assumptions about land use change and to facilitate discussion about the topic area.**

# NREL's Modeling Strategy & Approach

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- **System dynamics framework**
  - Stocks/flows
  - Feedback within and across stages in supply chain.
- **Modular, “regional” model architecture**
  - “Region” can reflect world, nation, geographical region, level of development, etc.
  - Enables rapid extension of model from 1 → 2 → n regions.
- **Reliance on demographic scenarios and FAO/GTAP data to drive dynamics around population, yield, food demand**
- **Calibrate model against FAO datasets for land use and disposition**
- **Avoidance of explicit market mechanism.**

# Our Model Captures Important System Interactions



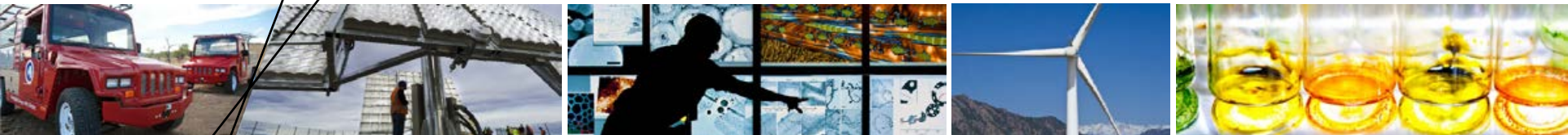
Source: Warner et al. 2013, Environ. Res. Lett. 8 015003



# Conclusions

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- **BioLUC modeling effort is focused on improving our understanding of how bioenergy and LUC interact**
- **Once complete, the model will be released publically along with processed datasets**
  - To be hosted on GitHub with links; also on Bioenergy KDF
- **We expect the model to facilitate much discussion among stakeholders and provide an accessible medium for groups to test different assumptions and datasets**
- **Having a transparent and relatively simple model (i.e., runs quickly, isn't very large, etc.) will add value to the community as a whole**
- **It is our hope that model release will stimulate an “open-source” level of interest and external development.**



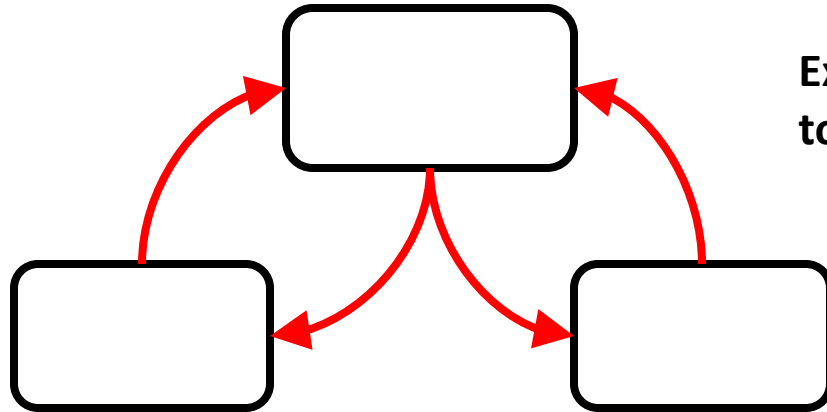
# Questions?

## LUC paper citation:

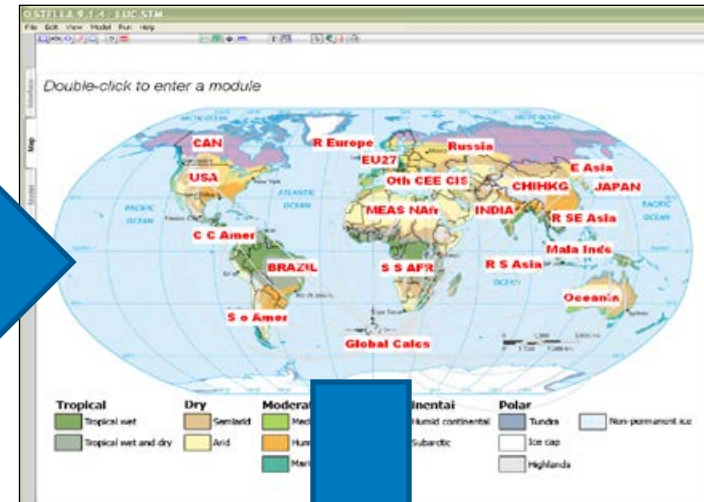
**Warner, Inman, Kunstman, Bush, Vimmerstedt, Peterson, Macknick and Zhang. 2013. Modeling biofuel expansion effects on land use change dynamics. ERL, Vol. 8, No. 1**

# Supplemental Slides

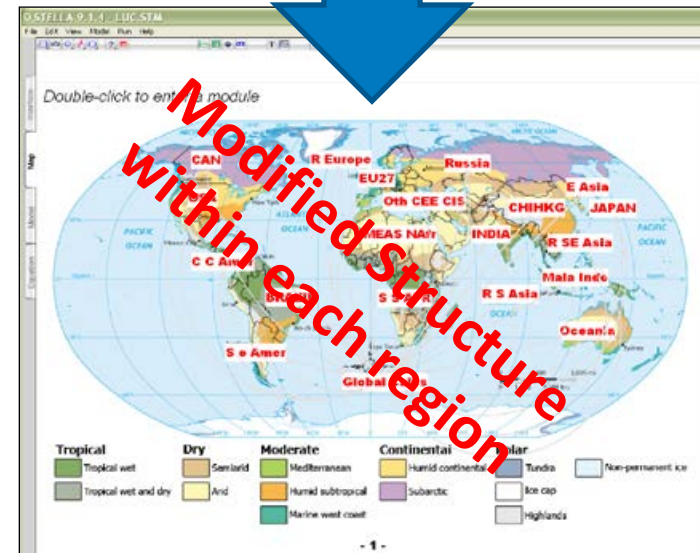
# BioLUC Model Progression



Expansion from 2 to 19 regions.



Modifications to land stocks and flows based on feedback from the ORNL workshop.



# Two-Region Insights

- **Results suggest that even in a future with high food and biofuel demands there is enough “available” land to meet both food and fuel needs.**
- **Most of the land is supplied by “pasture”**
- **Demand for land-intensive meat is difficult to supply under the high biofuel scenarios**

Base case system input per kg of product

Animal Class	Forage	Pasture	Maize	Wheat	Rice	NEC	Oil Crop	Sugar	Total kg
Cow Goat Sheep	6.1	4.9	2.6	0.1	0.0	0.0	1.1	0.0	14.8
Dairy	4.5	0.0	1.2	0.0	0.0	2.0	0.0	0.0	7.7
Pig	0.0	0.0	1.2	1.4	0.0	0.3	0.7	0.0	3.6
Poultry	0.0	0.0	1.4	0.3	0.0	0.0	0.6	0.0	2.4