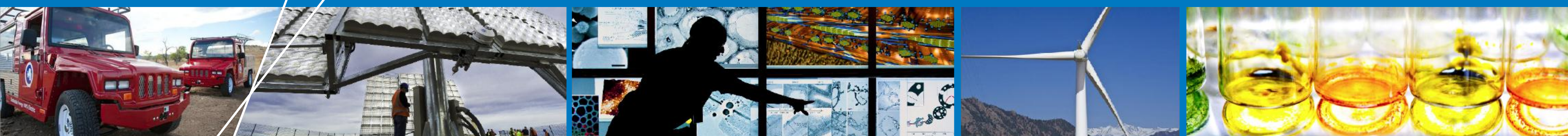
NATIONAL RENEWABLE ENERGY LABORATORY

Materials Flows through Industry (MFI) Tool – AMO Analysis Review



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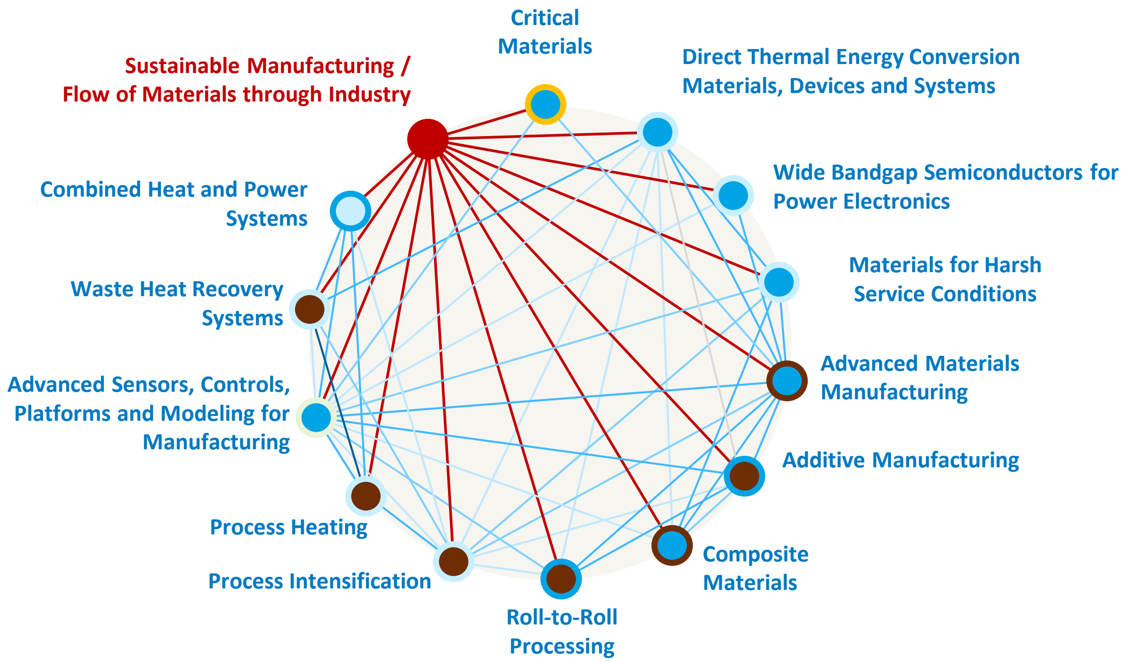
Outline

- Overview
- Description
- Methodology
- Tool structure and functionality
- Example

Overview

- Industry represents a diverse range of process technologies that use energy to take raw materials through a sequence of transformations to finished products.
- Analytically tracking the lifecycle energy impacts of current and proposed changes to the materials that flow through industry will provide a significantly more complete understanding of the energy impacts of different technologies of interest to DOE.



Description

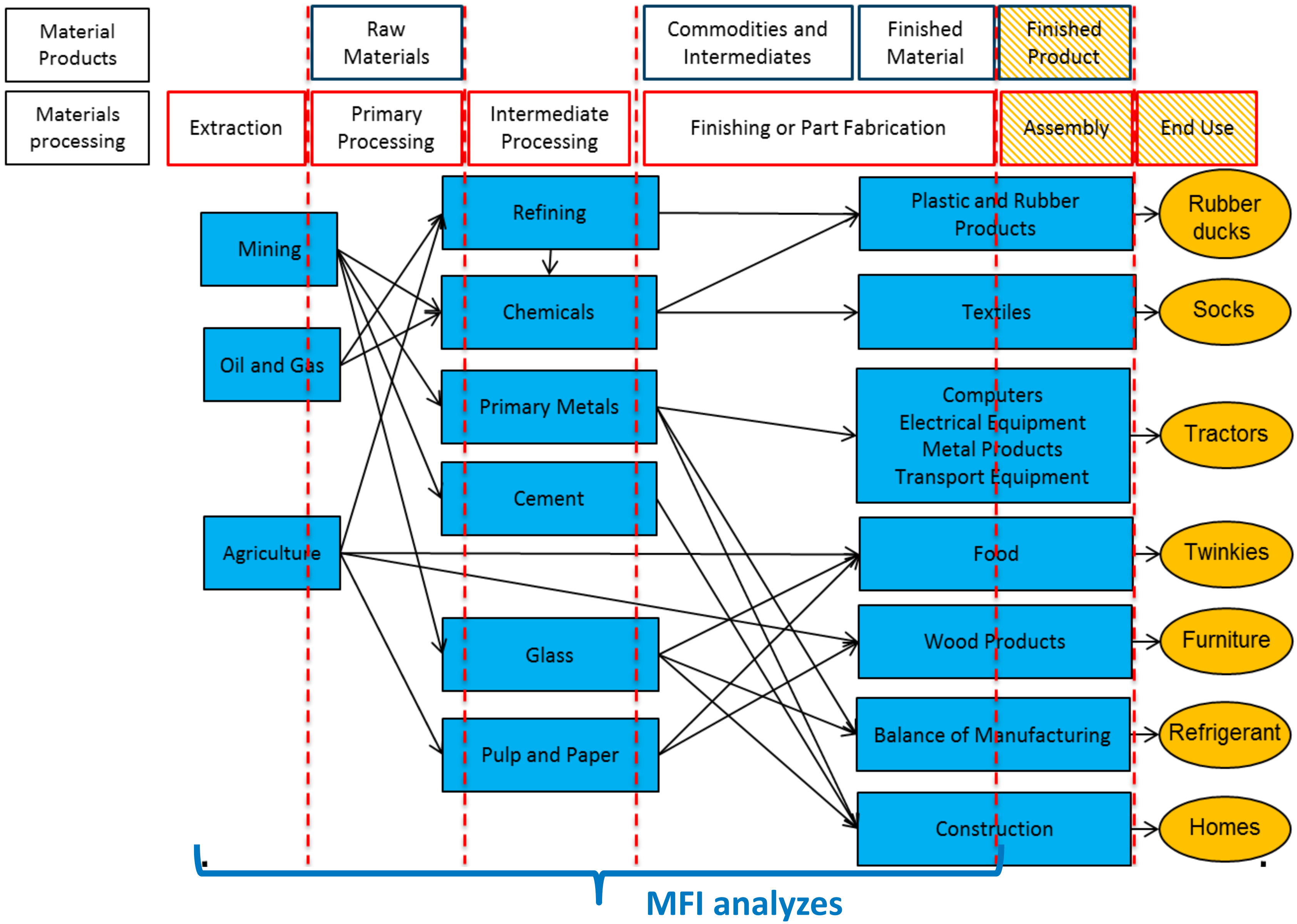
The Materials Flows through Industry (MFI) tool is a scenario tool for the evaluation of the energy use, greenhouse gas emissions, fuel costs, and macro-economic impacts of the industrial production of commodity materials

- Embodied energy and GHGs of 500 commodity products and > 1100 processes, from mine-to-product
- Process efficiency impacts within and throughout the manufacturing and chemical industry
- Impacts of novel materials (e.g., carbon fiber, biomaterials, advanced alloys) as replacements for existing manufacturing and use
- Multiple process and manufacturing pathways for industrial materials
- Cost contribution of energy use along the supply chain
- Alternative energy sources and multiple grid scenarios

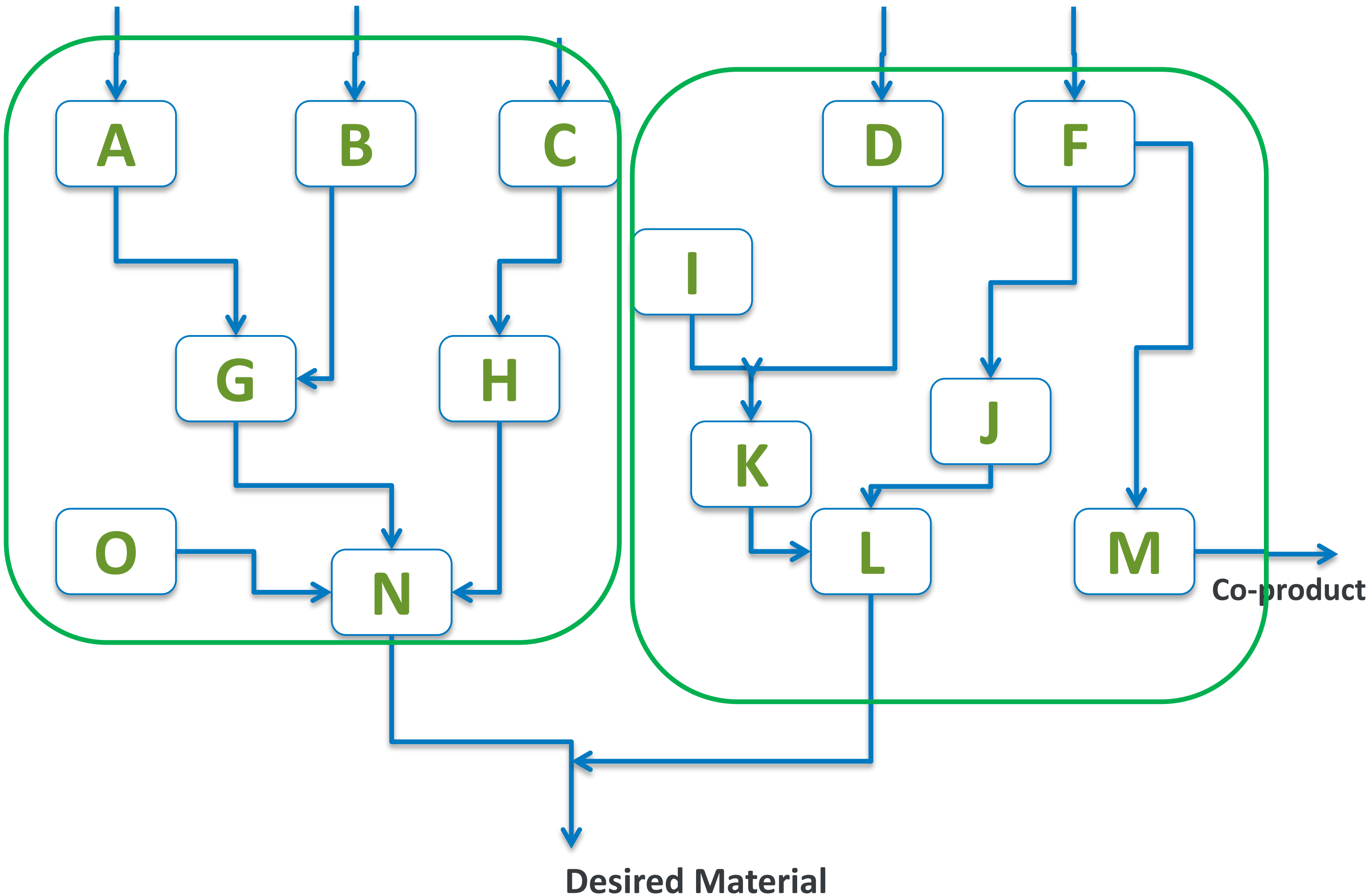
Description: Questions to answer

- What materials and energy are required in the **life cycle** to make commodities of interest in the industrial sector?
- What are the bulk materials that use the **most energy per ton** of material?
- What are the bulk materials that use the **most energy per year** (taking into account volume of production)?
- How do **process efficiency improvements** reduce energy use per material?
- What are the **NET energy and GHG savings** per unit of material substituted?
- Also can
  - What is the effect of different electricity **grid mixes?**
  - What is the effect of different process **fuel mixes**?
- Of the various ways to make a material, which are the most energy efficient?
- What are the effects of **market changes in demand**?

Methodology: Concept



Methodology: Multiple Pathways



The tool allows the user to evaluate multiple pathways up the supply chain to produce products and includes co-products.

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Methodology: approach

- **Product by material matrix (X_{pm}) is created based on inputs of process weightings (w_{ip}), sector efficiency potential (j_n) implementation and grid selection**
- $X_{pm} = \sum_{i=1}^{y_n} w_{ip} c_{ipm} j_n$
  - X = full matrix of all products (p) and materials (m)
  - p = products and m = the total number of unique products and materials
  - X_{pm} = matrix element for the m^{th} material input for the manufacture of the p^{th} product
  - c_{ipm} = the m^{th} material input for the p^{th} product by way of the i^{th} process pathway
  - w_{ip} = the i^{th} process pathway weighting for manufacturing the p^{th} product
  - y_n = the number of process pathways for manufacturing the p^{th} product
  - j_n = the percent implementation of the SEP for the p^{th} product sector.
- **The grid selection is done by process weighting the electricity product.**
- **Defaults for the grid is the national grid and for products are either market based or equally distributed amongst all available processes.**

Process ▲	Product	Owner	Process State	Proprietary	Product Process	Baseline Wtd
	aluminum, smelt					
CARBOTHERMIC	ALUMINUM, SMELT	birdie	Public	False		0.0
CLAY CARBOCHLORINATION	ALUMINUM, SMELT	birdie	Public	False		0.0
H-H/INERT ANODE	ALUMINUM, SMELT	birdie	Public	False		0.0
HH WETTED CATHODE	ALUMINUM, SMELT	birdie	Public	False		0.0
MODERN HALL HEROULT PROCESS	ALUMINUM, SMELT	birdie	Public	False		1.0
SMELTING OF REFINED ALUMINA TO METALLIC ALUMINUM	ALUMINUM, SMELT	birdie	Public	False		0.0

Methodology: energy calculations

- **For each material required in the supply chain, the energy inputs are determined based on the recipe for that material**
  - Electricity
  - Natural gas
  - Diesel
  - Kerosene
  - Fuel oil and resid
  - Crude oil
  - Refinery gas
  - Coke
  - Uranium
  - Gasoline
  - Renewables

- **The fuel energy inputs are converted to GJ for total energy demand**
- **The GJs of fuel are multiplied against GHG emissions factors (IPCC 2006) for total GHG emissions**
- **The KWH and GHG emissions for electricity are accounted for separately to avoid double counting of energy demand**

Excel Tool Structure and Functionality

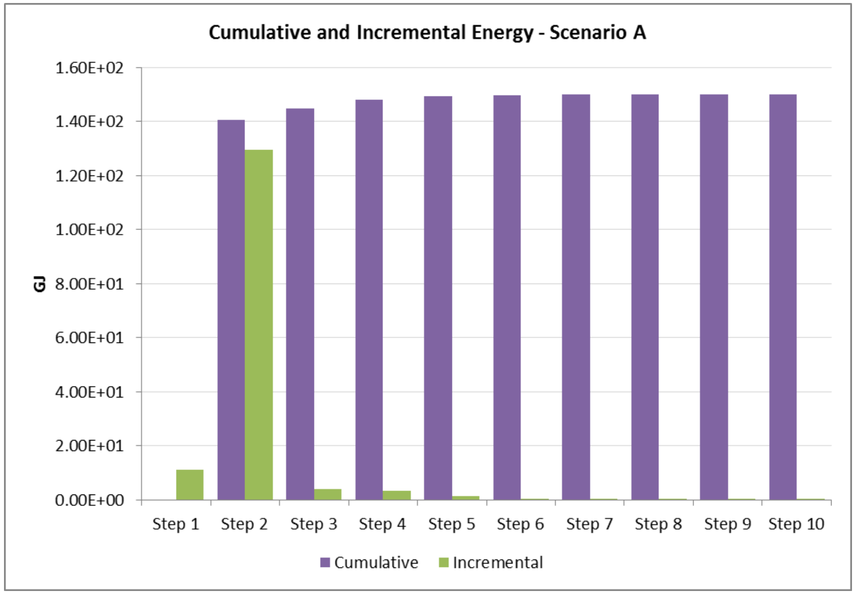
- **User Inputs**
  - Product selection and quantity
  - Process selection and allocation
  - Sector efficiency potential implementation
  - Grid selection
- **Results**
  - Electricity, mass, total energy, and carbon dioxide
  - Fuel use in manufacturing and transportation

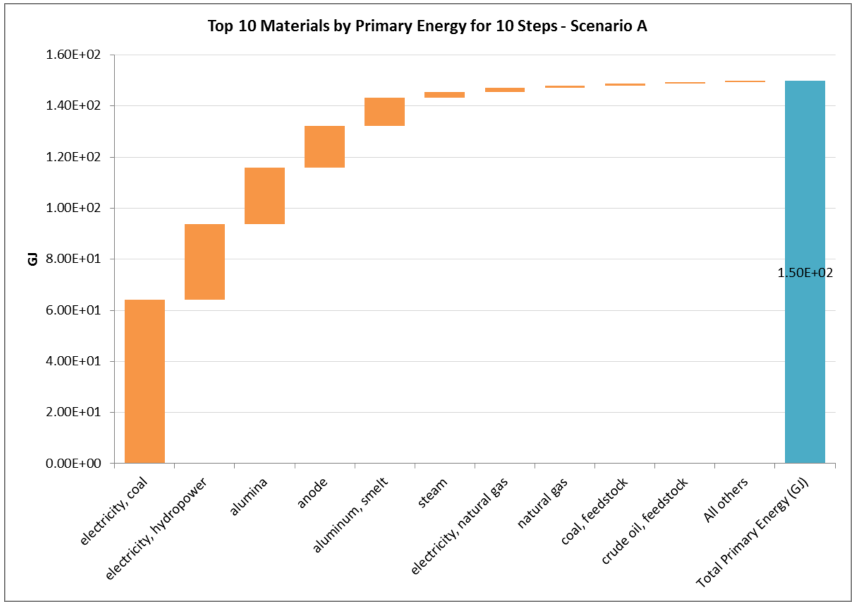
Aluminum Smelt Example Scenarios

Process, efficiency, and grid comparisons for aluminum smelt (1000 kg)

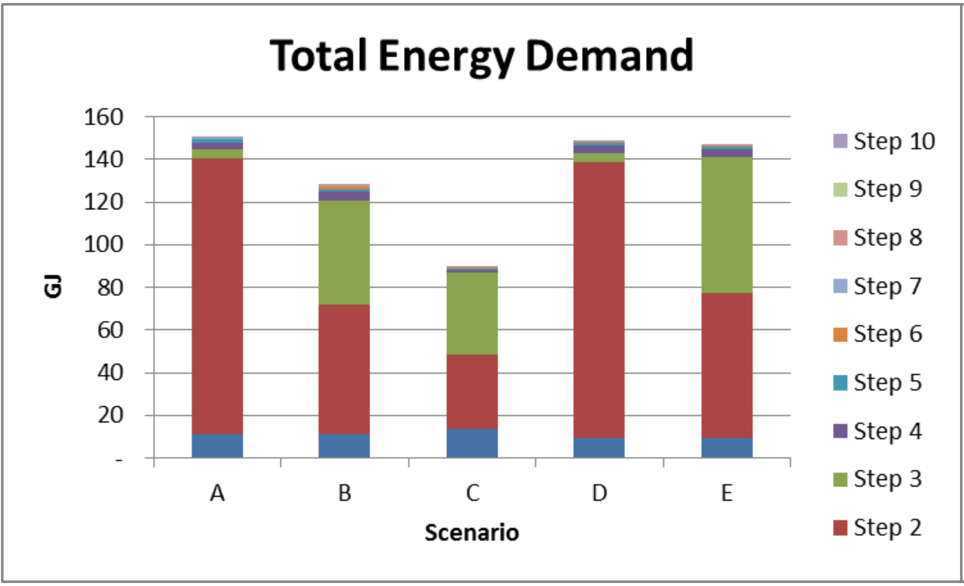
- Scenario A – Baseline (Modern Hall Heroult(MHH)); 0% SEP; national grid
- Scenario B – HH Wetted Cathode (TRL – 7) Process; 0% SEP; national grid
- Scenario C – Clay Carbochlorination (TRL – 6) Process; 0% SEP; national grid
- Scenario D – MHH process; 100% SEP; national grid
- Scenario E – MHH process; 100% SEP; 80% RE grid.

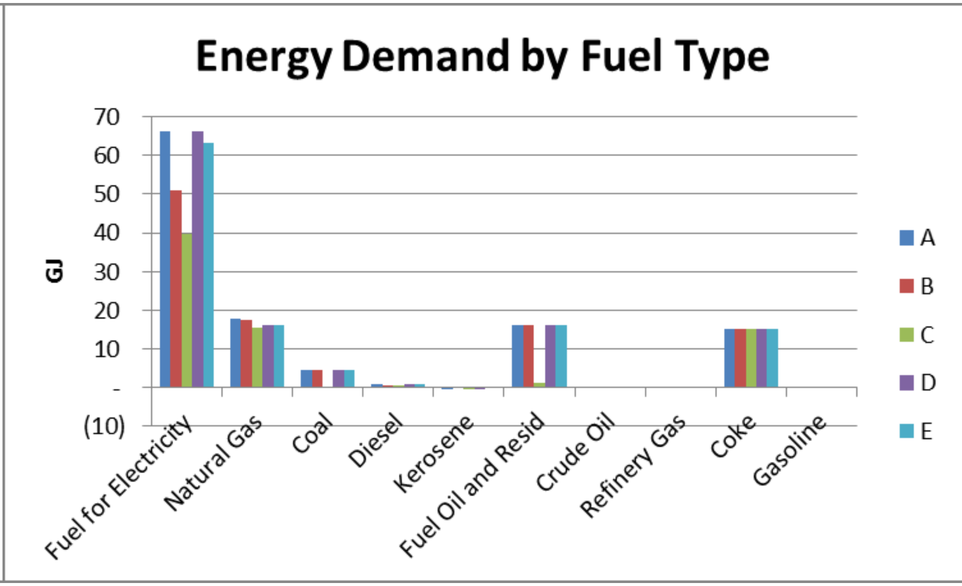
Graphical Results: Scenario A (Baseline)

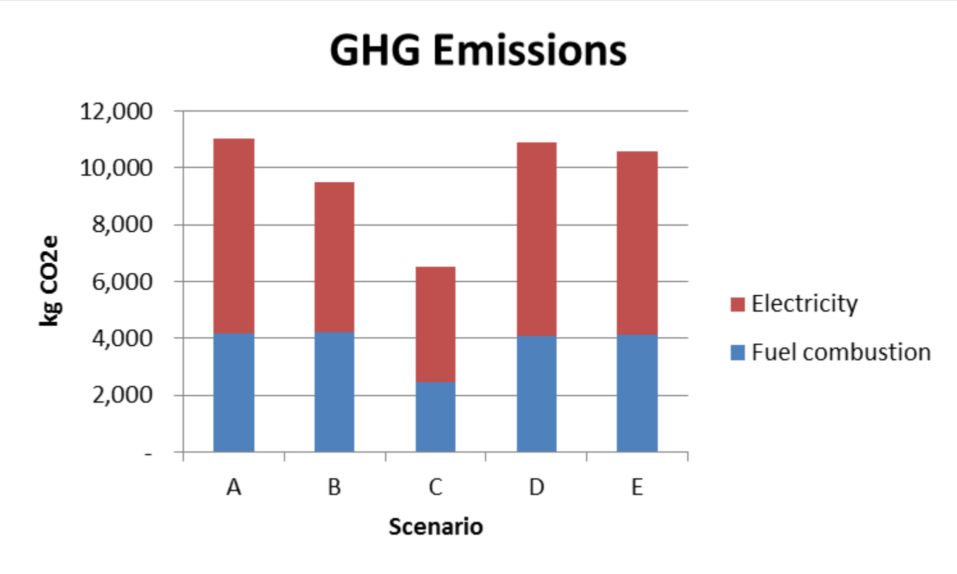


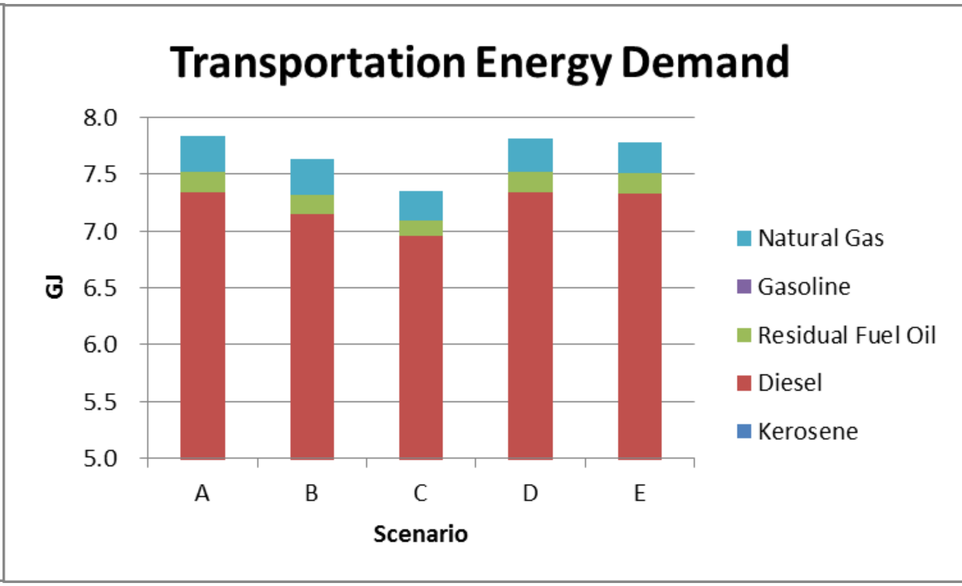


Graphical Results for Aluminum Smelt (Scenarios A – E)









Limitations

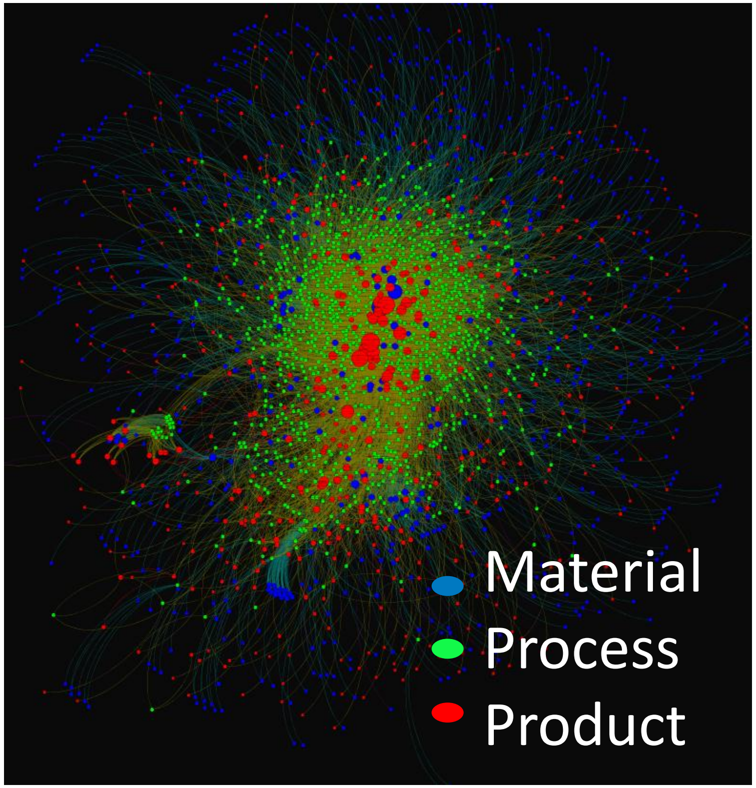
- Currently only addresses energy and energy related carbon impacts
- Currently only evaluates through the commodity product. Use phase is covered under LIGHTEnUP
- Data availability and uncertainty

Next Steps

- Peer review comments have been received and are being processed.
- Evaluation of data gaps
- Primarily the next steps will be focused on meeting goals and objectives for the Department of Energy Advanced Manufacturing Office
- Applying competitiveness metrics

Conclusions

- **Objective:** Analytically track the lifecycle energy and GHG impacts of current and proposed changes to the materials that flow through industry
- Supply chain is a complex and highly interconnected system with opportunities for energy and GHG reductions
- Supply chain analysis can provide support for next generation technologies, such as additive manufacturing



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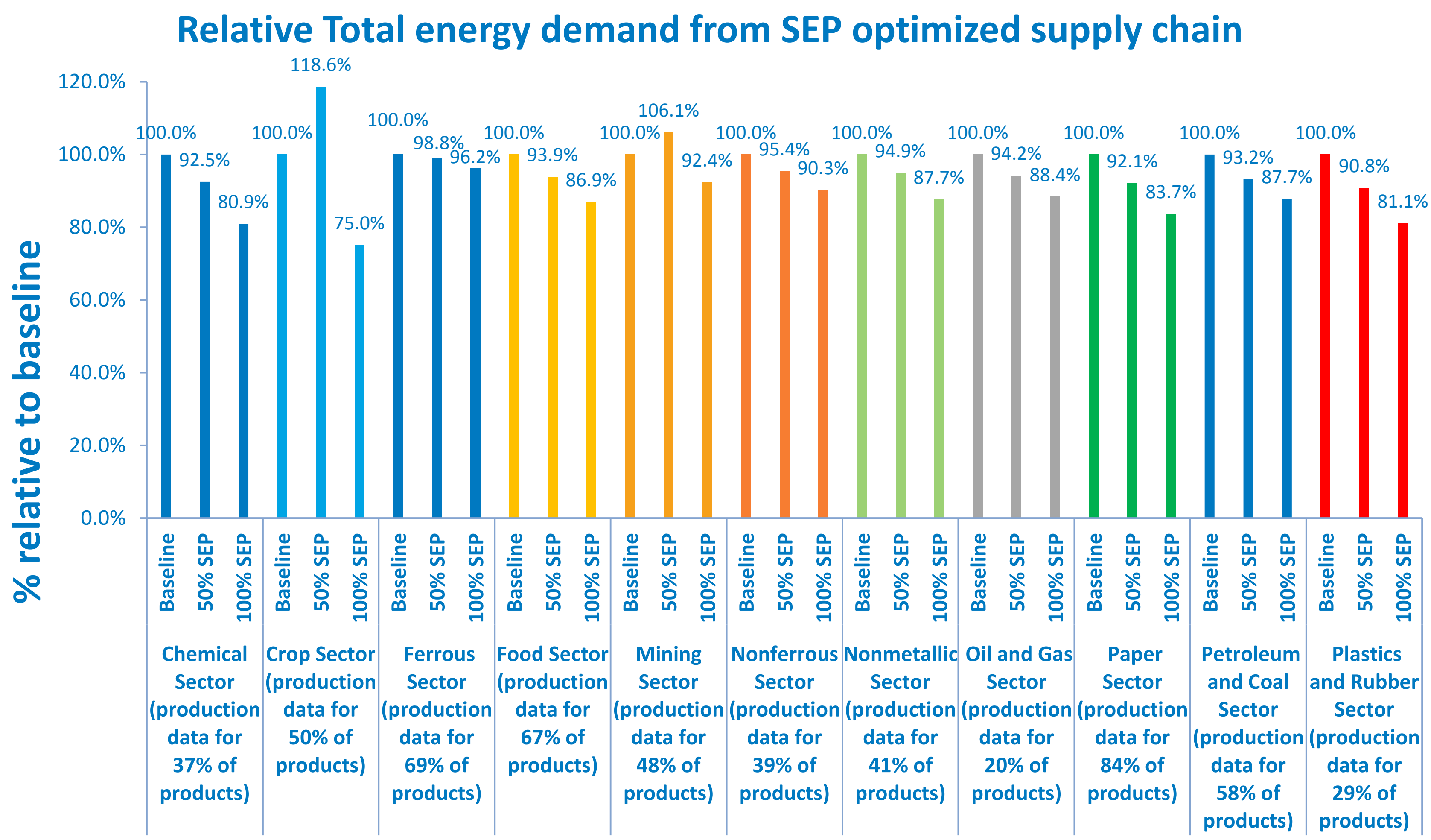
Market analysis of SEP implementation



Methodology - approach

- **Process based matrix approach**
  - Step wise calculation of material demand and associated energy and green house gas impact
  - Transportation – single aggregated calculation.
- **Matrix is constructed in a product by material structure**
  - 500+ products - any material having a recipe or upstream data
  - 1100+ materials - anything being used in a recipe
- **1200+ recipe - defines the process for manufacturing a product, inputs (energy and material) and outputs (product and co-products)**
- **Co-products are non-primary products of a process and are given a negative accounting (discussed later).**

Methodology – database / tool interface

- The calculations for the tool occur in two locations, the database and the excel tool
- The matrix is created in the database based on the user inputs (user input page in the excel tool).
- The database sends this matrix to the tool for the step wise demand vector and energy calculations.

Methodology: database

- The database holds all the recipes for the tool (see figure below), sector increased energy efficiency potential data, links to sectors and baseline process weightings and unit conversions
- Recipes can be added and modified from the database website user interface.
- Access is currently restricted to NREL users only, but will ultimately be available for external users but with restricted access due to proprietary data.

Name: 1,3-PROPANEDIOL FROM BIO-BASED PROCESS

Description:

Product: 1,3-PROPANEDIOL

Baseline Wtd: 0.111111111

Materials

Material	Material Quantity	Material Unit	Product Quantity	Product Unit	Note 1	Note 2
AMMONIA	0.015	kg	1.0	kg		ORNL
CORN	3.38	kg	1.0	kg		ORNL
ELECTRICITY	0.292	kwh	1.0	kg	FOR WET MILLING	ORNL
ELECTRICITY	0.722	kwh	1.0	kg	FOR PDO PRODUCTION	ORNL
LIME	0.00419	kg	1.0	kg		ORNL
NATURAL GAS	0.11	m3	1.0	kg	FOR WET MILLING	ORNL
NATURAL GAS	0.5775	m3	1.0	kg	FOR PDO PRODUCTION	ORNL
SODIUM HYDROXIDE	0.0177	kg	1.0	kg		ORNL
SULFUR	0.0021	kg	1.0	kg		ORNL
SULFURIC ACID	0.00697	kg	1.0	kg		ORNL
UREA	0.00697	kg	1.0	kg		ORNL

Methodology: approach

- A demand vector based on the product of interest and a user defined quantity is multiplied against the matrix to determine the material demand required and creates a demand vector for the 2nd step in the supply chain.
- This 2nd demand vector is then also multiplied by the matrix to create a 3rd demand vector.
- This is repeated for 10 steps (to represent the full supply chain).
- Each step is then added together to get the material (and energy demand) for the supply chain.
- This step wise calculation allows us to determine which step in the supply chain has the greatest energy impact.
- This final vector is in kg or kwh of product or electricity.

Methodology: Co-product management

- Co-products are included in the calculations as offsets and are considered negative inputs to recipes (see ethylene from GTL naphtha cracking example below).
- Co-products of co-products are not included due to creation of a double negative accounting.

Material	Material Quantity	Material Unit	Product Quantity	Product Unit
ALKANES	-5.3	kg	32.3	kg
BUTADIENE	-3.8	kg	32.3	kg
ELECTRICITY	3.416667	kwh	32.3	kg
OLEFINS	-8.4	kg	32.3	kg
FUEL GAS	-405.7	mj	32.3	kg
FUEL OIL AND RESID	15.7953488	kg	32.3	kg
HYDROGEN	-0.7	kg	32.3	kg
NAPHTHA, FEEDSTOCK	100.0	kg	32.3	kg
PROPYLENE	-19.1	kg	32.3	kg
REFINERY GAS	14.9333333	kg	32.3	kg

Tabular Results for Scenarios A – C

Data sources and Verification

- **Data sources:**
  - IHS/SRI Process Economics Program yearbook
  - Life cycle inventory databases
    - US LCI database – US based data
    - Simapro LCI datbase – international data
    - Journal articles
    - LBNL sector efficiency study
    - ORNL next gen process and materials data
    - Commodity Flow Survey
- **Verification**
  - Market allocation and processes verified by ICF
  - Verify against publish embodied energy
  - Reviewed by IEF team
  - Data gap analysis

Matrix values

Base recipe

MATERIAL	PRODUCT	PROCESS	INPUT	UNITS	/	OUTPUT	UNITS
COAL	SODIUM CARBONATE	SODA POWDER - ACC PLASTIC DATA	1.08E-01	KG	/	1	KG
DIESEL	SODIUM CARBONATE	SODA POWDER - ACC PLASTIC DATA	6.70E-05	L	/	1	KG
ELECTRICITY	SODIUM CARBONATE	SODA POWDER - ACC PLASTIC DATA	9.06E-02	KWH	/	1	KG
FUEL OIL AND RESID	SODIUM CARBONATE	SODA POWDER - ACC PLASTIC DATA	1.59E-03	L	/	1	KG
NATURAL GAS	SODIUM CARBONATE	SODA POWDER - ACC PLASTIC DATA	4.98E-02	M3	/	1	KG
TRONA	SODIUM CARBONATE	SODA POWDER - ACC PLASTIC DATA	1.42E+00	KG	/	1	KG

Unit conversion to kg or kwh

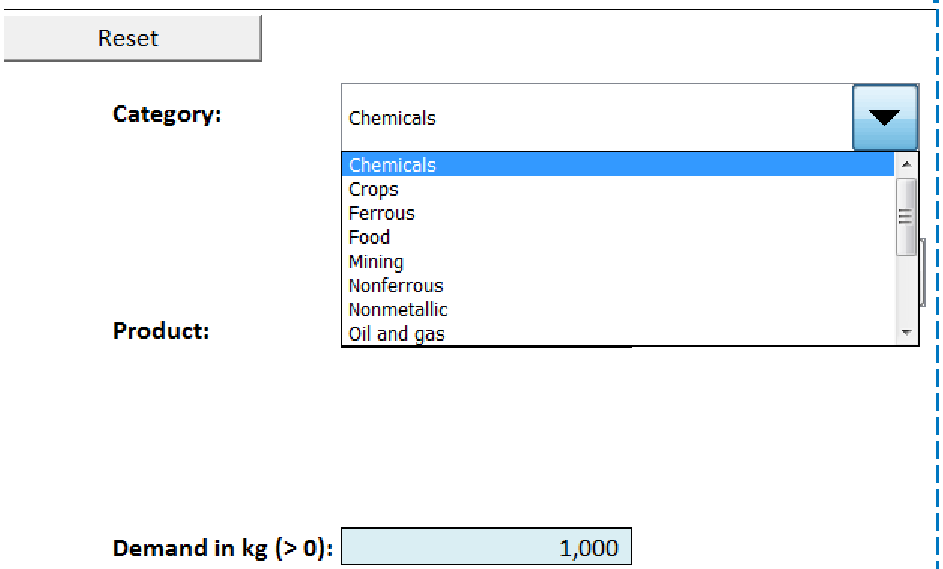
MATERIAL	CONVERSION	COEFFICIENT
COAL	1.00E+00	1.08E-01
DIESEL	8.37E-01	5.61E-05
ELECTRICITY	1.00E+00	9.06E-02
FUEL OIL AND RESID	9.91E-01	1.57E-03
NATURAL GAS	7.77E-01	3.87E-02
TRONA	1.00E+00	1.42E+00

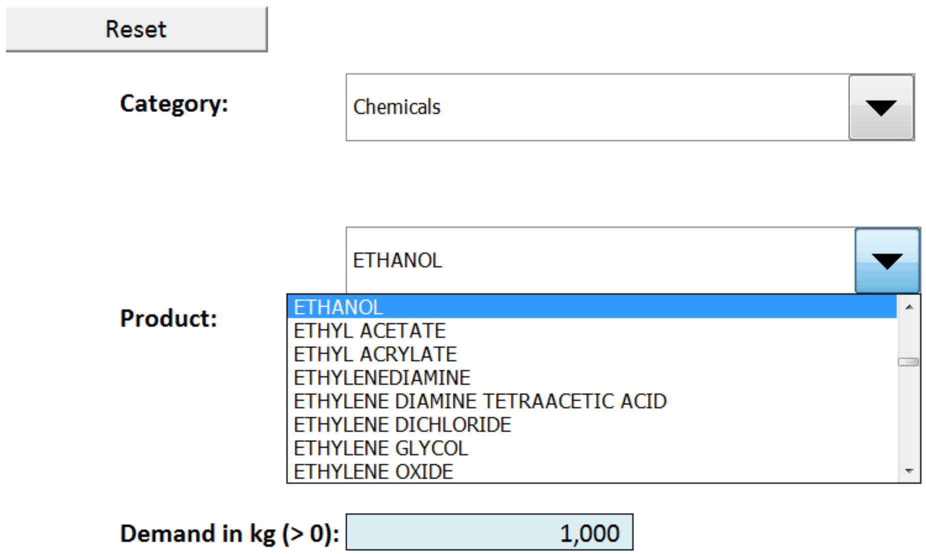
Process weighting and efficiency

Matrix values

MATERIAL	WTD COEFFICIENT A	WTD A	Efficiency A	MASANET EFFICIENCY	**A**
COAL	1.08E-01	100%	0%	12.8%	**1.08E-01**
DIESEL	5.61E-05	100%	0%	24.1%	**5.61E-05**
ELECTRICITY	9.06E-02	100%	0%	13.7%	**9.06E-02**
FUEL OIL AND RESID	1.57E-03	100%	0%	24.1%	**1.57E-03**
NATURAL GAS	3.87E-02	100%	0%	26.6%	**3.87E-02**
TRONA	1.42E+00	100%	0%	0.0%	**1.42E+00**

User Input Page – Category and Product Choice





- Users have the ability to choose from a tailored set of products based on the category they select, and drop-down menus automatically populate with updated values
- Able to define demand in kg

User Input Page – Process Weightings

Choose Baseline, Equal Weighting or Input Own Values for each scenario

Scenario A	Scenario B	Scenario C
(●) Baseline	(●) Baseline	(●) Baseline
( ) Equal Weighting	( ) Equal Weighting	( ) Equal Weighting
( ) Input Own (Below)	( ) Input Own (Below)	( ) Input Own (Below)

Product: ETHANOL

Process	Baseline Weighting	Equal Weighting	Input Own New Weighting Below for Scenario A	Input Own New Weighting Below for Scenario B	Input Own New Weighting Below for Scenario C
ETHANOL FROM CORN DRY MILL PROCESS	83%	17%	0%	0%	0%
ETHANOL FROM CORN WET MILLING	17%	17%	0%	0%	0%
ETHANOL FROM ETHYLENE BY CATALYTIC HYDRATION	0%	17%	0%	0%	0%
ETHANOL FROM MULTI OUTPUT SUGAR BEET BIOREFINERY	0%	17%	0%	0%	0%
ETHANOL FROM WHOLE CORN BIOREFINERY	0%	17%	0%	0%	0%
ETHANOL VIA HYDRATION OF ETHYLENE	0%	17%	0%	0%	0%
			0%	0%	0%

- Process choices automatically populate based on the product chosen, along with the baseline (market defined) weighting and the equal weighting percentages
- Users may choose baseline (market) weighting, equal weighting, or input a user-defined weighting for three different scenarios by using the buttons in the grey box
- Users may input their own process weightings in the blue cells

User Input Page – Efficiency Implementation

Choose Baseline or Input Own Values for each scenario

Scenario A
- ○ Baseline
- ◉ Input Own (Below)

Scenario B
- ◉ Baseline
- ○ Input Own (Below)

Scenario C
- ◉ Baseline
- ○ Input Own (Below)

Product: ETHANOL

Process	Baseline Implementation of SEP	Input Own New Implementation Scenario A	Input Own New Implementation Scenario B	Input Own New Implementation Scenario C
ETHANOL FROM CORN DRY MILL PROCESS		100%	0%	0%
ETHANOL FROM CORN WET MILLING		0%	0%	0%
ETHANOL FROM ETHYLENE BY CATALYTIC HYDRATION		0%	0%	0%
ETHANOL FROM MULTI OUTPUT SUGAR BEET BIOREFINERY		0%	0%	0%
ETHANOL FROM WHOLE CORN BIOREFINERY		0%	0%	0%
ETHANOL VIA HYDRATION OF ETHYLENE		0%	0%	0%
		0%	0%	0%

Sector Efficiency Potential (SEP) is the potential energy efficiency improvement within different sectors, assuming all possible improvements are achieved

- Users may define the percentage of the SEP that they would like to implement, or use the baseline implementation via the buttons in the grey box
- Baseline implementation is always 0% and assumes no efficiency improvements
- Selection of 50% of SEP indicates that half of the potential efficiency improvements are implemented.

User Input Page – Grid Mix

Scenario A	Scenario B	Scenario C
◉ Baseline	◉ Baseline	◉ Baseline
○ Input Own (Below)	○ Input Own (Below)	○ Input Own (Below)

Product: ALUMINUM, SMELT Electricity Grid	Baseline plementation	Input Own Grid Mix Scenario A	Input Own Grid Mix Scenario B	Input Own Grid Mix Scenario C
ELECTRICITY GRID, FRCC	0%	0%	0%	0%
ELECTRICITY GRID, MRO	0%	0%	0%	0%
ELECTRICITY GRID, NATIONAL	100%	0%	0%	0%
ELECTRICITY GRID, NPCC	0%	0%	0%	0%
ELECTRICITY GRID, RFC	0%	0%	0%	0%
ELECTRICITY GRID, SERC	0%	0%	0%	0%
ELECTRICITY GRID, SPP	0%	0%	0%	0%
ELECTRICITY GRID, TRE	0%	0%	0%	0%
ELECTRICITY GRID, WECC	0%	0%	0%	0%
ELECTRICITY, 80PCT RE CONSTRAINED TRANSMISSION	0%	0%	0%	0%
ELECTRICITY, 80% RENEWABLES CONSTRAINED RESOURCES	0%	0%	0%	0%
ELECTRICITY, 80PCT RE INCREMENTAL TECHNOLOGY IMPROVEMENTS	0%	0%	0%	0%
ELECTRICITY, 70PCT RE INCREMENTAL TECHNOLOGY IMPROVEMENTS	0%	0%	0%	0%
ELECTRICITY, 60PCT RE INCREMENTAL TECHNOLOGY IMPROVEMENTS	0%	0%	0%	0%
ELECTRICITY, 50PCT RE INCREMENTAL TECHNOLOGY IMPROVEMENTS	0%	0%	0%	0%
ELECTRICITY, 40PCT RE INCREMENTAL TECHNOLOGY IMPROVEMENTS	0%	0%	0%	0%
ELECTRICITY, 30PCT RE INCREMENTAL TECHNOLOGY IMPROVEMENTS	0%	0%	0%	0%

- Users may choose between the baseline grid mix assumption (national grid) or input their own grid mix weightings via the buttons in the grey box
- Custom grid mix weightings may be input into the blue cells