Mapping the Opportunity Space to Model the Circular Economy Using Tools Funded by the DOE Office of Energy Efficiency and Renewable Energy

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2 Argonne National Laboratory
3 U.S. Department of Energy

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

Technical Report
NREL/TP-6A20-81693
April 2022

Contract No. DE-AC36-08GO28308

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Suggested Citation
Shubhankar Upasani, Julien Walzberg, Dwarak Ravikumar, Alberta Carpenter, Garvin Heath, Ulises Gracida-Alvarez, Thathiana Benavides, et al. 2022. *Mapping the Opportunity Space to Model the Circular Economy Using Tools Funded by the DOE Office of Energy Efficiency and Renewable Energy*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-6A20-81693. https://www.nrel.gov/docs/fy22osti/81693.pdf.

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April 2022

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303-275-3000 • www.nrel.gov

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This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Advanced Manufacturing Office. The views expressed herein do not necessarily represent the views of the DOE or the U.S. Government.

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List of Acronyms and Abbreviations

ABM	agent-based model
ADOPT	Automotive Deployment Options Projection Tool
AM	Additive Manufacturing
AWARE-US	Available Water Remaining for the United States
BEAM	Behavior, Energy, Autonomy, and Mobility
BEIOM	Bio-based circular carbon economy Environmentally-extended Input-Output Model
BioAGE	Bioeconomy Air emissions Greenhouse gas emissions, and Energy use model
CE	Circular Economy
CECE	Circular Economy Capacity Expansion
CELAVI	Circular Economy Life cycle Assessment and Visualization Framework
CSV	comma-separated values
DES	Discrete event simulation
DMT	dimethyl terephthalate
DREEM	Dynamic Rare Earth Production dEMand
EEIO	environmentally extended input output
EERE	Energy Efficiency and Renewable Energy
EG	ethylene glycol
EOL	end of life
EVI-Pro	Electric Vehicle Infrastructure Projection Tool
FastSim	Future Automotive Systems Technology Simulator
GHG	greenhouse gas
GREET	Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies
GSR	GeoSpatial Roadmap
HTML	HyperText Markup Language)
ISCEM	Iron & Steel CE Model
ISO	International Organization for Standardization
kg	kilogram
LCA	life cycle assessment
LCI	life cycle inventory
LCIA	life cycle impact analysis
LDRD	Laboratory Directed Research and Development
LiAISON	Life cycle Analysis Integration into Scalable Open-source Numerical models
LIBRA	Lithium-Ion Battery Resource Assessment
MA3T	Market Acceptance of Advanced Automotive Technologies
MFA	material flow analysis
MFI	Materials Flows through Industry
MJ	megajoules
NdFeB	neodymium magnets
OR	operations research
PET	polyethylene terephthalate
PI	principal investigator

POLARIS	Planning and Operations Language for Agent-based Regional Integrated Simulation
PTA	purified terephthalic acid
PViCE	PV in the Circular Economy
ReX	re-[reduce, reuse, repurpose, repair, remanufacture, recycle, recover, et cetera]
REVISE	Regional Electric Vehicle Infrastructure Strategic Evolution
RMC	Raw Material Consumption
SD	Systems Dynamics
SIIP	Scalable Integrated Infrastructure Planning
TDO	Total Domestic Output
TMR	Total Material Requirement
TRACI	Tool for Reduction and Assessment of Chemicals and other environmental Impacts
VTO	Vehicle Technologies Office
WATER	Water Analysis Tool for Energy Resources

Executive Summary

Transitioning from a linear to a circular economy (CE) can be a way of achieving sustainable development and decarbonization goals of a society. The success of such a transition can be quantified using tools that can model relevant parameters of a CE that have been identified in literature. This work evaluated tools, models, and frameworks (collectively referred to as tools) that have been funded by the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy (EERE) to determine the extent they are able to model the CE. This report briefly introduces the reader to the concept of a CE, then lists some of the research questions that an analyst can hope to answer through a CE modeling exercise, followed by some desirable principles of a CE modeling tool. We then list a set of recommended CE parameters that an analyst can include when modeling a CE, as well as a set of auxiliary CE parameters. As a part of the tools review, we conducted an inventory of tools across different national laboratories, program offices, and research consortia by conducting a literature search and contacting experts in relevant analysis topic areas, and, then short-listed the inventory of tools to include only those that can currently or potentially model the CE. In coordination with the tool developers, we characterized the tools against a set of the previously defined recommended and auxiliary CE parameters.

A decision tree was then developed based on parameters chosen from the initial characterization and discussions with analysts working in the CE space[1] with the intent of providing analysts with a list of EERE tools as possible options to model the CE for their specific applications, by filtering the parameters (columns) of the decision tree (an Excel worksheet). Additionally, a gap analysis was performed of the reviewed EERE tools based on their ability to model the CE across the breadth of CE parameters identified in Section 1. The gap analysis provided insights into questions such as which CE strategy has the most representation in the EERE tools, which technology area has the most EERE tools, and what is the modeling ability of the EERE tools across spatial-temporal dimensions, for example. The findings of the gap analysis conveyed current and potential opportunities of EERE tools for modeling the CE. This was followed by examples of scenarios for using the decision tree to obtain a set of EERE tools as potential modeling choices.

Lastly, we discussed methodologies developed in the CE literature in response to existing research gaps and provided guiding principles for choosing a CE methodology. Two case studies are included to demonstrate recent development efforts in EERE tools that can be leveraged to CE modeling use cases - the Circular Economy Life cycle Assessment and Visualization Framework (CELAVI) from the National Renewable Energy Laboratory and the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model by Argonne National Laboratory. These case studies demonstrate where a gap in the CE modeling space was identified and closed to demonstrate ongoing efforts in the field to answer research questions and advance CE modeling capabilities.

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[1] The final list of tools we considered for the CE characterization are listed in Appendix A.

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1 The Circular Economy (CE)—Introduction, Principles, and Parameters

An increasing rate of material consumption and a growing population mean Earth's supply of natural resources is experiencing unsustainable and unprecedented demand. This forces us to find solutions that ensure the availability of resources for sustaining society in the years to come. Actors from various backgrounds are addressing these challenges from their own perspectives: for example, engineers are developing efficient manufacturing processes, designers are creating lightweight and durable products, educators are incorporating sustainable thinking in their curricula, and policymakers are finding interdisciplinary solutions that benefit society at large. The circular economy (CE) is an approach to resource use that aims to move away from the linear material use framework of "take-make-waste" to a more circular and interdependent system where product, material, and resource use is optimized to avoid unnecessary social, economic, and environmental costs (Figure 1).

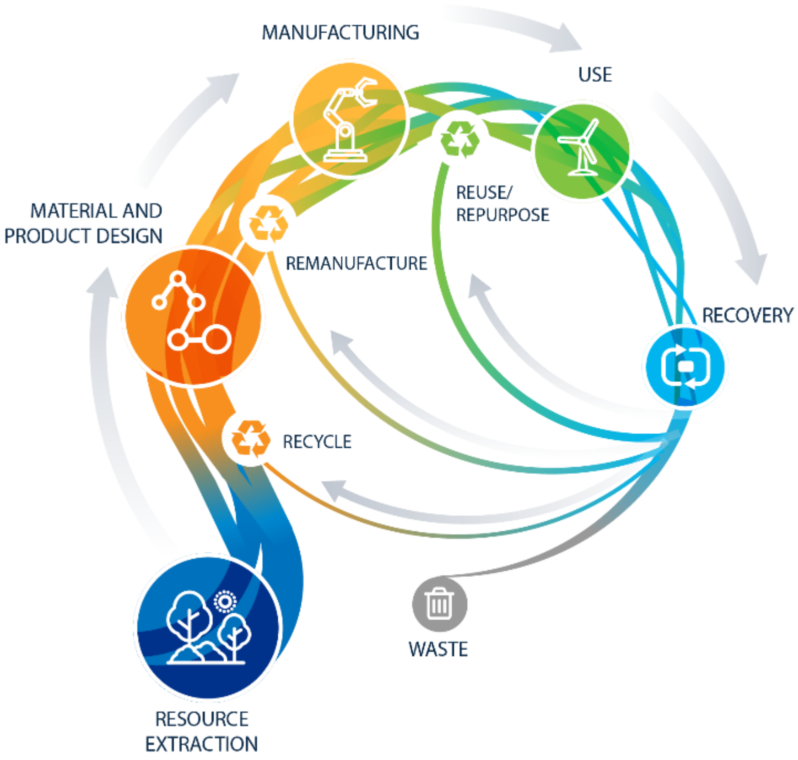

Figure 1. Idealized flow of materials in an economy applying circular strategies

Research Questions in a CE Modeling Exercise

The purpose of any analysis exercise—a circular economy (CE) analysis or any other analysis—is usually to obtain answers to a set of driving questions and make decisions that change the state of the system in a desired direction. In the case of a CE modeling analysis, the desired direction of change is moving toward a system that maximizes resource looping, minimizes waste generation, and improves resource efficiency of processes in a way that minimizes environmental, social, and economic impacts. In doing so, the objective is to effectively track, measure, and analyze the progress and translate the information into findings that communicate the success or limitations of the transition to a CE. The former part of the objective (tracking, measuring, analysis) can be performed using different tools, models, frameworks, and data management systems.[2] But a clear definition of the latter half of the objective (understanding success or limitations of the CE transition) is important when deciding which tools will be used to model and analyze the CE. A modeler can define what is the intended purpose of the analysis and then decide whether a modeling tool and the insights it provides align with the intended purpose of the analysis. In defining the intended purpose, a modeler can come up with a list of research questions that need to be answered to successfully understand the impacts associated with a CE transition. Some of these research questions can be specific to the system under consideration whereas others can be broad questions that provide insights into aspects of the CE irrespective of the system context and field of application. Examples of such broad, general, CE research questions that can be posed when framing a CE modeling exercise, and their relevance for understanding the CE are listed in Table 1.

Table 1. Examples of CE Research Questions and Their Relevance to Understanding CE

CE Research Question	Relevance
What is the goal for transitioning toward a CE?	A CE analysis can provide an assessment of whether the objective of the CE transition was met and to what extent.
How does transitioning toward a CE directly impact the rate of virgin material consumption in the system?	A CE analysis should be able to quantify the decrease (or increase) of the use of virgin materials, especially those that are constrained in supply or are vulnerable to supply risks (e.g., critical materials).
How does transitioning toward a CE improve the efficiency of processes and reduce waste production?	A CE analysis should be scoped to be able to quantify the impacts of CE strategies on process efficiency improvements and waste minimization.
How can implementing one or more CE strategies that require additional infrastructure and technology costs for the implementation be achievable?	A CE analysis should account for competing use of resources or increased materials demand in auxiliary sectors that are due to the implementation of CE strategies.
How does implementing one or more CE strategies affect social factors such as equity, jobs, healthy living and working conditions? Or does it disproportionately affect certain groups and communities while the benefits are realized elsewhere?	A CE analysis should consider the societal impacts on those who directly benefit from or are harmed by the implementation of CE strategies in a technology sector. An understanding of the positive and negative impacts on society provides a starting point for devising solutions that provide equitable benefits.
How does implementing one or more CE strategies impact the sustainability performance of the system? Does it shift negative sustainability impacts outside the system of study?	Implementing a CE strategy for the sake of CE will not always result in improving the sustainability of the system. CE is intended to be a tool to improve the sustainability of the system, and not the end goal. An understanding of the sustainability performance and tradeoffs of implementing CE strategies helps improve decision-making.

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[2] In this review, we evaluated a range of tools, models, and frameworks (as defined by the principal investigators). In this report, we collectively refer to them as tools.

CE Research Question	Relevance
How does implementing one or more CE strategies affect key players in the value chain of the system? What are the tradeoffs from the perspective of different stakeholders?	Implementing a CE strategy requires systemic change from actors along the value chain of a technology.

Principles of a CE Modeling Tool

For a CE modeling exercise, there are several principles to which the tool should adhere, and which can help determine whether the tool is suitable for a user's specific purposes. Some of those principles are adopted from the ISO 14040 standard for life cycle assessment (*ISO 14040:2006: Environmental Management—Life Cycle Assessment—Principles and Framework*, n.d.). The principles that can be applied during the tool selection process include:

1. **Coherence:** The tool should be able to do a circularity assessment of the modeled system in a systemic and consistent manner. The assumptions made in the model development and the type of data that needs to be used in the tool should be clear.
2. **Comparability:** The tool should provide metrics that can enable comparison of products, processes, or systems within a single assessment.
3. **Traceability:** The tool should be formulated so that the resource flows and associated data required can be traced through the history and future of the resources, materials, and products involved in the system so that the circularity of a system can be practically verified. Traceability can extend across different life cycle stages of the value chain and the associated impacts on the technological and ecological systems involved in the modeled system.
4. **Transparency:** The tool, model, or framework developed as well as the data sources used in them should be transparent and unambiguous. They should be available to all interested parties wherever possible and should keep account of confidentiality where appropriate. Uncertainty or volatility in data, and any estimations and assumptions made should be declared. Ensuring transparency permits comparative analysis, consistent documentation of data, reporting of data collection, data calculation and data quality by specifying and structuring relevant information. Where uncertainties exist or assumptions have been made, sufficient data should be provided in any analysis or result to enable third-party calculation of alternative scenarios following different assumptions or applying different data.
5. **Data Reliability:** Data required for the tool should be accurate, complete, stable, repeatable, and precise, publicly accessible wherever possible, credible, and verifiable, thus reflecting the best state of knowledge available from measurement or calculation. All data used must have undergone objective expert review in accordance with standards[3] and the source of the data provided, and all data should be referenced and traceable. The data and information used should be as complete and consistent as reasonably practical (e.g., from well-developed data sets and well-maintained databases where these exist). Any lower-quality data sources used, or assumptions made in an analysis should be

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[3] A CE ISO standard is under development (https://www.iso.org/standard/80648.html)

carefully managed, considered and reported along with a quantitative assessment of the uncertainties these introduce to the results and the identification of data sources or assumptions that represent key sensitivities in the analysis and the potential uncertainty in the overall result.

6. **Completeness:** The tool should account for all resources and resource flows required for a specified circularity system and within appropriate system boundaries and through the entire life of a product or system.

CE Parameters

When modeling the CE, several parameters can be used to determine the scope and the level of circularity of the modeled system and consequently the amount and type of data required to do so. In this work, we use several parameters to characterize the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy (EERE)-funded tools included in the review process. To help analysts make better decisions when selecting a tool to model a CE application, we divide the parameters into two categories: *recommended* CE parameters and *auxiliary* CE parameters. We suggest (1) recommended CE parameters should ideally be included in a CE modeling exercise and (2) auxiliary CE parameters could be included in CE modeling if the modeler has considerable knowledge and decision-making ability. The choice of recommended CE parameters is driven by their ability to:

- Measure and assess the effect of adopting a CE
- Perform a holistic evaluation of the system
- Reveal unintended consequences from implementing a CE strategy.

Recommended CE Parameters

The recommended CE parameters are detailed in this section.

ReX or CE Strategies

The CE can be modeled according to several different approaches depending on whether the focus is on the inputs to the system, the product itself, the number of times the product is used, the number of people that use the product, whether the product can be used as a service (i.e., a “product-service” system), how well is the product designed for disassembly, and whether the product can be repaired or refurbished, for example. The focus of these approaches is on material consumption and making the economy more circular. Such approaches are called a CE strategy or a ReX strategy.

According to Potting et al. (Potting, et al. 2017), ReX strategies serve as an actionable means of transitioning from a linear to a circular system. ReX strategies are characterized by their R-number: the X in ReX stands for a number from 0 to 9; hence the R-number ranges from R0 to R9. As a convention, the lower (lesser) the R number, higher the degree of circularity of the ReX strategy. For instance, R7 (Repurpose) has a lower degree of circularity than R6 (Remanufacture) (Potting, et al. 2017). This illustrates that although recycling (R8) is an important piece of a CE, an ideal CE involves many other circularity strategies. The ReX strategies are explained in detail in Figure 2 and the section below:

- **R0—Refuse:** From the perspective of a product designer, refuse is the avoidance of toxic materials and the design of processes to eliminate material waste (e.g., eliminating plastic packaging).
- **R1—Rethink:** The product is made more use-intensive (e.g., car sharing).
- **R2—Reduce:** Reduce refers to decreasing the consumption of the use of virgin materials and avoiding waste in the manufacturing processes of the product so that it provides the same functionality but consumes less resources.
- **R3—Reuse:** This is the reuse of a product by a second consumer for the same functionality or purpose without an additional external treatment or processing.
- **R4—Repair:** Repair addresses specific defects, broken parts, or malfunctioning components in a product with the overall goal of extending the lifetime of the product.
- **R5—Refurbish:** Refurbishing involves improving the working condition, quality, or functionality of a multicomponent product. Refurbishing extends beyond addressing minor defects and results in "upgrading" the product or bringing it up to the state of the art.
- **R6—Remanufacture:** The components in an existing product are disassembled, checked for quality standards, and reused in a new product with the same functionality. Activities in remanufacture can include one or more of the following: disassembly, inspection, cleaning, and testing.
- **R7—Repurpose:** Repurposing is reusing a discarded product or its parts in another function, thus ensuring the materials in the product get a new life.
- **R8—Recycle:** Recycling is the recovery of materials from the product after its end of life (EOL). The recovered materials do not maintain any of the product's structure and can be used in the original or any alternate application at the same grade or a lower grade.
- **R9—Recover:** Recovery involves the recovery of energy from the EOL waste of a product (e.g., through incineration).

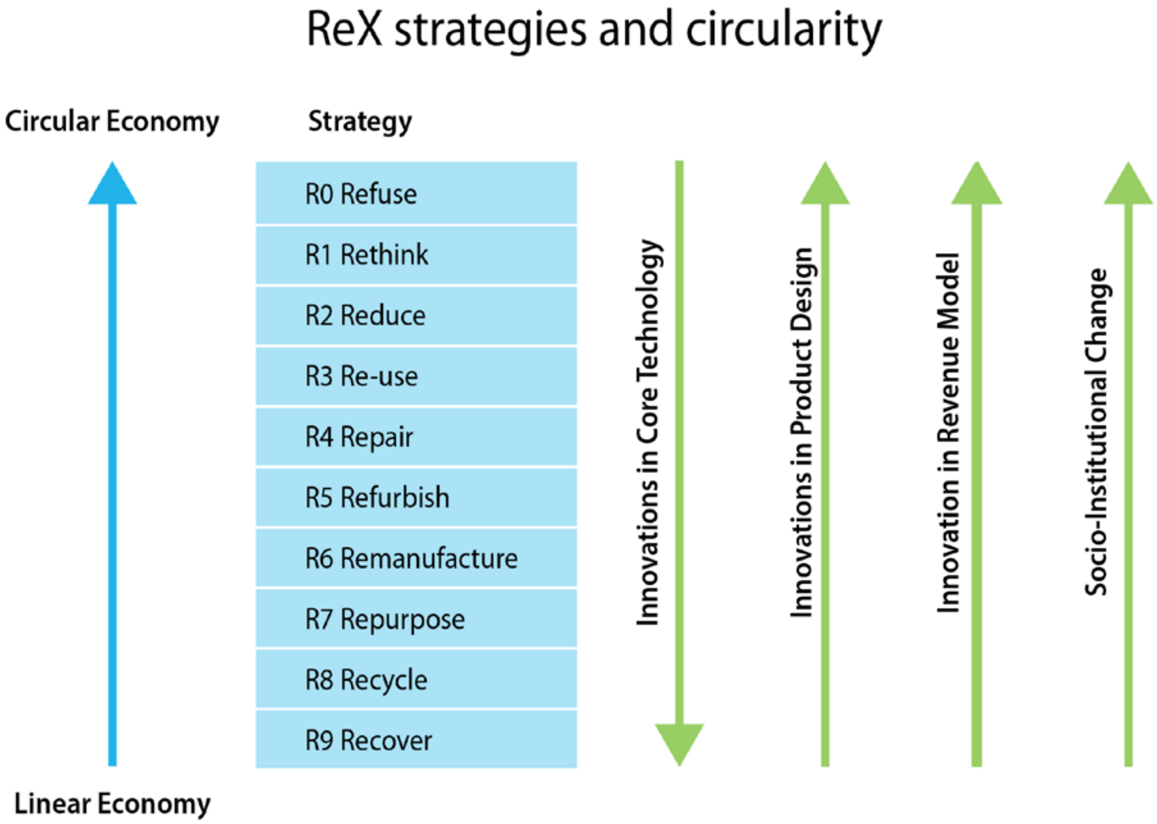

Figure 2. ReX strategies and circularity

After Potting et al. (2017) which is based on RLI (2015)

Sustainability Indicators

Implementation of a circularity strategy needs to be carefully assessed and evaluated for its effect on a system's sustainability performance. In other words, circularity itself is not the end goal but rather a means of achieving the goal of sustainability. Sustainability indicators assess the broader burdens or benefits of implementing CE strategies by quantifying their social, economic, and environmental impacts. When selecting a tool to model the CE, it is important to know exactly which of the three categories of sustainability indicators the tool can provide.

Circularity Indices

Circularity indices quantify or measure the effectiveness of applying a CE strategy to a system through a score (Saidani, et al. 2019). The score typically ranges from 0 (no circularity) to 100% (complete circularity), and it can be applied at the level of a product, organization, economic sector, or region. The scores are quantified based on material reuse or economic value. For example, the product-level circularity metric quantifies the ratio of the economic value of the recirculated parts in a product to the overall economic value of all the parts in the product (Linder, Sarasini and van Loon 2017).

Technology Area

The choice of tool to model a system is often limited by the technology-specific application area the modeler wants to analyze. Some tools are developed to be more general and can model systems belonging to a variety of technology areas. Other tools can model only specific technologies (and thus require data, assumptions, parameters relevant to that technology only), and these are more suited to CE modeling applications that fall within the same technology space. In some cases, certain tools might have initially been developed using a specific technology as a demonstrative example, but that does not necessarily mean the tool cannot be extended to model other technology systems. For example, such cases potentially present the opportunity for collaboration and tools integration across different research groups, organizations, and industries.

Auxiliary CE Parameters

The *auxiliary* CE parameters used to further characterize the EERE tools are explained in this section.

Levels of the CE Analysis

A given tool can provide a level of CE analysis that spans the categories in Figure 3 (page 7), which include

- **Nano:** The tool models the CE strategy at the level of a product
- **Micro:** The tool models the CE strategy at the level of an industrial facility, or an enterprise
- **Meso:** The tool models the CE strategy at the level of an industrial park with collaboration by multiple enterprises.
- **Macro:** The tool models the CE strategy at the city, state, country, or global level.

It is up to the modeler to choose the level of analysis they want to conduct while modeling the CE and accordingly to select a tool that fulfills the desired level of analysis.

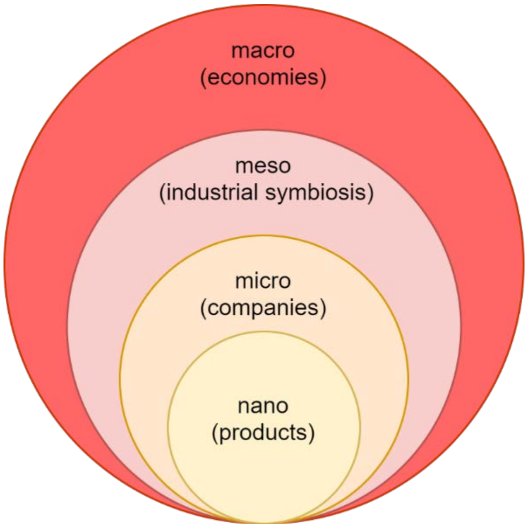

Figure 3. Levels of a CE analysis

Data Requirements

The amount of data that the tools require can be categorized as high, medium, or low. For example, the tool might apply a life cycle assessment (LCA) methodology to quantify environmental impacts, which typically means the data requirement is high; this is because an LCA requires detailed material and energy inventory data to quantify the environmental footprint of the product. Conversely, a tool might only model the CE at the product level or the organization level and might require a less data to represent the system being considered.

Data Granularity

The data required by the tool to conduct the analysis can either be highly aggregated (low granularity) or disaggregated (highly granularity). For example, an LCA necessitates data at the disaggregated level of individual inventory items and processes required to manufacture a product; consequently, a tool that conducts an LCA has a high data granularity requirement. Conversely, a tool that models interactions of aggregated entities, such as trade flows across economic sectors or mobility patterns of a region can be categorized as having a high or medium granularity of data, respectively.

Temporal Resolution

The transition to a CE by implementing circular strategies is a deliberate process that occurs over a period of time. Accordingly, if one wants to model the CE and understand the impacts associated with adopting a CE strategy, being able to obtain results that have a dimension of time variability becomes important. A CE tool might model the considered system in only a point of time (static) or over a period of time (dynamic) with varied resolution (e.g., hourly, daily, weekly, monthly, or yearly). The final choice of which time resolution best represents the system under study rests with the modeler, and it depends on the scope of the analysis and the desired outputs of the modeling exercise. For example, a CE modeling exercise intended to understand the impacts of a CE strategy on the material efficiency of economic sectors of a region might be best modeled by a tool that provides a yearly or monthly time resolution. In contrast, an organization looking to track its circularity performance after implementing CE strategies in different business units might benefit from using a tool that provides a daily or weekly time resolution.

Life Cycle Stages Covered

The life cycle stages of a product system are the design phase, raw material extraction, manufacturing (processing), use phase, and EOL. A tool might only model one of the life cycle stages and thus provide metrics that inform about material impacts in the corresponding life cycle stage or stages. Depending on the scope of the analysis, the modeler can decide whether being able to model certain—or all—life cycle stages is a priority. Table 2 summarizes the recommended CE parameters and the auxiliary CE parameters and provides examples of the values different parameters can take in the context of a CE.

Table 2. Parameters in CE Modeling

Parameter Category	CE Parameters	Examples of Parameter Values
Recommended CE parameters[a]	ReX strategies	• Reduce, Reuse, Recycle, Refurbish, et cetera (R0–R9) (See Figure 2, page 6)
	Sustainability indicators	• Environmental (e.g., greenhouse gas emissions and waste) • Economic (e.g., net present value and profit) • Social (e.g., jobs, and well-being)
	Technology area	• Industry • Energy storage • Transportation
Auxiliary CE parameters	Scope	• Nano (product) • Micro (organization) • Meso (industrial symbiosis) • Macro (economic sectors, countries, global)
	Data requirements	• Low (simplified process models, can focus on a specific set of metrics) • Medium (disaggregated material flows, can focus on a specific set of metrics) • High (detailed process models, can focus on a wide range of metrics)
	Data granularity	• Low (sectoral or regional data of a material flow) • Medium (material flow data disaggregated by technology or service) • High (detailed material flow data of a single technology or service)
	Temporal resolution	• Dynamic (Hourly, Daily, Weekly, Monthly, Yearly) • Static
	Life cycle stages covered	• Design • Raw material extraction • Manufacturing/Processing • Use • EOL

[a] The term "parameter" is used here to describe the different tool characteristics to be considered.

2 Review of EERE-Funded Tools for Modeling the CE

The National Renewable Energy Laboratory was asked to evaluate how the tools that have been funded by U.S. Department of Energy Office of Energy Efficiency and Renewable Energy (EERE) can be used to model the CE. This section briefly describes our approach, which is illustrated in Figure 4, in identifying, characterizing, and understanding the EERE-funded tools for their ability to model the CE. We started by developing an inventory of tools and models funded by EERE across different national laboratories, program offices, and research consortia by conducting a literature search and contacting experts in relevant analysis topic areas, summarized in Appendix B. We then short-listed the inventory of tools to include only those that can currently or potentially model the CE. We did an internal initial characterization of the tools against a set of CE characterization criteria identified by Walzberg et al. (Walzberg, et al. 2021) and then contacted the tool developers to confirm our initial characterization and obtain feedback where needed.

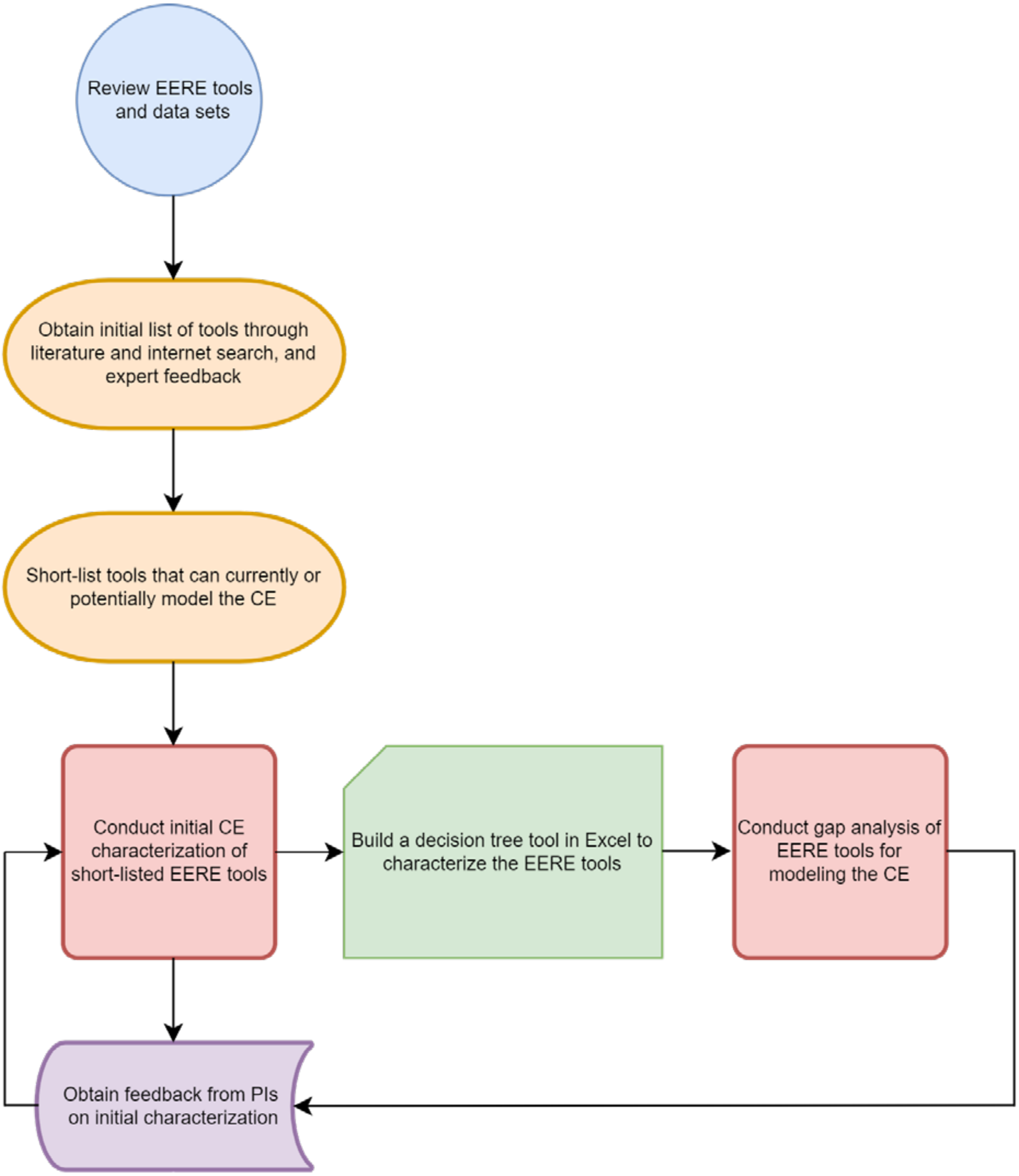

Figure 4. Flowchart depicting the process of characterizing EERE tools for CE modeling capability

PIs = principal investigators

Next, we developed a decision tree based on parameters chosen from the initial characterization and discussions with analysts working in the CE space.[4] The decision tree was designed to provide analysts with a list of EERE tools as possible options to model the CE for their specific applications, which tools users achieve by filtering the parameters (columns) of the decision tree (an Excel worksheet). We also performed a gap analysis of the reviewed EERE tools based on their ability to model the CE across the breadth of CE parameters we identified in Section 1. The gap analysis provided insights into questions such as which CE strategy has the most representation in the EERE tools, which technology area has the most EERE tools, and what is the modeling ability of the EERE tools across spatial-temporal dimensions, for example.

Finally, we summarized our findings in this report, which is intended to be used as a guiding document for researchers across EERE who are looking to identify tools from the EERE tools portfolio that can be used in their specific CE modeling application. Keeping in mind that many readers might be unfamiliar with the CE, we introduce the concept of the CE and associated terminology in Section 1. We also convey the relevance of CE parameters from a modeling perspective and highlight important research questions that one should answer in a CE modeling analysis. This is intended to prime analysts to better understand the choices available in the decision tree when using it for their project/application. In Section 3, we communicate the findings of the gap analysis using upset plots to convey current and potential opportunities of EERE tools for modeling the CE. This is followed by examples of scenarios for using the decision tree to obtain a set of EERE tools as potential modeling choices. Here, scenarios where the current EERE portfolio does not match any decision criteria supplied by the user are also explored.

In Section 4, we provide guiding principles for choosing a CE methodology, and in Section 5 we include some examples of case studies to demonstrate some recent development efforts in EERE tools that can be leveraged to CE modeling use cases. Using the Circular Economy Life cycle Assessment and Visualization Framework (CELAVI) from the National Renewable Energy Laboratory as a case study, we point to methodologies and publications in the CE literature where a gap in the CE modeling space was identified and closed to demonstrate ongoing efforts in the field to answer research questions and advance CE modeling capabilities. This effort will serve as a starting point for tools users to engage with researchers currently working on CE and will provide them with methodological choices in cases where the EERE tools portfolio does not provide them with a tool for their project application. A second case study uses the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model from Argonne National Laboratory. For this case study, researchers at Argonne National Laboratory developed a CE analysis framework for measuring the environmental impact of recycling technologies enabling circularity of plastic packaging. This case study provides an example of the reasoning behind the inclusion and integration of methodologies, pathway and process stages definitions, and election of environmental and circularity metrics. The results from the analysis of the framework are included in Section 4 to provide a complete perspective to readers.

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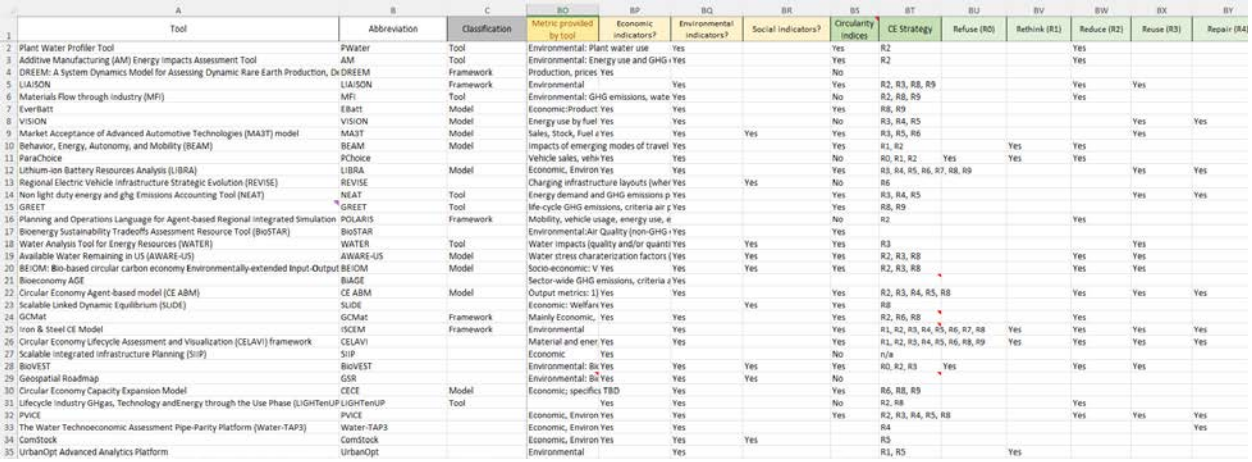
[4] The final list of tools we considered for the CE characterization are listed in Appendix A.

3 Decision Tree Tool and Gap Analysis

The decision tree analysis is intended to help analysts identify the EERE-funded tools, models, or frameworks that are best-aligned with the requirements for their CE capability assessments. The decision tree analysis consists of an Excel spreadsheet (shown in Figure 5) containing a series of questions that are presented in Table 3 (center column). Each question has multiple alternatives (Table 3, right column), and tool users answer each question by selecting a Yes or a No for each alternative in the Excel spreadsheet. Depending on the specificity of their CE analysis requirements, analysts can answer one or more questions in any order. The alternatives represent the requirements for the CE capability assessment. The requirements can be entered in the CE characterization Excel data template by selecting a Yes or No in the column corresponding to the alternative.



	A	B	C	BO	BP	BQ	BR	BS	BT	BU	BV	BW	BX	BY
1	Tool	Abbreviation	Classification	Metric provided by tool	Economic indicators?	Environmental indicators?	Social indicators?	Circularity indices	CE Strategy	Refuse (R0)	Rethink (R1)	Reduce (R2)	Reuse (R3)	Repair (R4)
2	Plant Water Profiler Tool	PWater	Tool	Environmental: Plant water use		Yes		Yes	R2			Yes		
3	Additive Manufacturing (AM) Energy Impacts Assessment Tool	AM	Tool	Environmental: Energy use and GHG		Yes		Yes	R2			Yes		
4	DREEM: A System Dynamics Model for Assessing Dynamic Rare Earth Production, D	DREEM	Framework	Production, prices	Yes			No						
5	LIAISON	LIAISON	Framework	Environmental		Yes		Yes	R2, R3, R8, R9			Yes	Yes	
6	Materials Flow through Industry (MFI)	MFI	Tool	Environmental: GHG emissions, wate		Yes		No	R2, R8, R9			Yes		
7	EverBatt	EBatt	Model	Economic:Product	Yes	Yes		Yes	R8, R9					
8	VISION	VISION	Model	Energy use by fuel	Yes	Yes		No	R3, R4, R5				Yes	Yes
9	Market Acceptance of Advanced Automotive Technologies (MA3T) model	MA3T	Model	Sales, Stock, Fuel a	Yes	Yes	Yes	Yes	R3, R5, R6				Yes	
10	Behavior, Energy, Autonomy, and Mobility (BEAM)	BEAM	Model	Impacts of emerging modes of travel		Yes		Yes	R1, R2		Yes	Yes		
11	ParaChoice	PChoice		Vehicle sales, vehi	Yes	Yes		No	R0, R1, R2	Yes	Yes	Yes		
12	Lithium-ion Battery Resources Analysis (LIBRA)	LIBRA	Model	Economic, Environ	Yes	Yes		Yes	R3, R4, R5, R6, R7, R8, R9				Yes	Yes
13	Regional Electric Vehicle Infrastructure Strategic Evolution (REVISE)	REVISE		Charging infrastructure layouts (wher		Yes	Yes	No	R6					
14	Non light duty energy and ghg Emissions Accounting Tool (NEAT)	NEAT	Tool	Energy demand and GHG emissions p		Yes		Yes	R3, R4, R5				Yes	Yes
15	GREET	GREET	Tool	life-cycle GHG emissions, criteria air p		Yes		Yes	R8, R9					
16	Planning and Operations Language for Agent-based Regional Integrated Simulation	POLARIS	Framework	Mobility, vehicle usage, energy use, e				No	R2			Yes		
17	Bioenergy Sustainability Tradeoffs Assessment Resource Tool (BioSTAR)	BioSTAR		Environmental:Air Quality (non-GHG		Yes		Yes						
18	Water Analysis Tool for Energy Resources (WATER)	WATER	Tool	Water impacts (quality and/or quanti		Yes	Yes	Yes	R3				Yes	
19	Available Water Remaining in US (AWARE-US)	AWARE-US	Model	Water stress charaterization factors (		Yes	Yes	Yes	R2, R3, R8			Yes	Yes	
20	BEIOM: Bio-based circular carbon economy Environmentally-extended Input-Output	BEIOM	Model	Socio-economic: V	Yes	Yes	Yes	Yes	R2, R3, R8			Yes	Yes	
21	Bioeconomy AGE	BIAGE		Sector-wide GHG emissions, criteria a		Yes								
22	Circular Economy Agent-based model (CE ABM)	CE ABM	Model	Output metrics: 1)	Yes	Yes		Yes	R2, R3, R4, R5, R8			Yes	Yes	Yes
23	Scalable Linked Dynamic Equilibrium (SLiDE)	SLiDE		Economic: Welfare	Yes		Yes	Yes	R8					
24	GCMat	GCMat	Framework	Mainly Economic,	Yes	Yes		Yes	R2, R6, R8			Yes		
25	Iron & Steel CE Model	ISCEM	Framework	Environmental		Yes		Yes	R1, R2, R3, R4, R5, R6, R7, R8		Yes	Yes	Yes	Yes
26	Circular Economy Lifecycle Assessment and Visualization (CELAVI) framework	CELAVI		Material and ener	Yes	Yes		Yes	R1, R2, R3, R4, R5, R6, R8, R9		Yes	Yes	Yes	Yes
27	Scalable Integrated Infrastructure Planning (SIIP)	SIIP		Economic	Yes			No	n/a					
28	BioVEST	BioVEST		Environmental: Bi	Yes	Yes	Yes	Yes	R0, R2, R3	Yes		Yes	Yes	
29	Geospatial Roadmap	GSR		Environmental: Bi	Yes	Yes	Yes	No						
30	Circular Economy Capacity Expansion Model	CECE	Model	Economic; specifics	TBD	Yes		Yes	R6, R8, R9					
31	Lifecycle Industry GHgas, Technology andEnergy through the Use Phase (LIGHTenUP	LIGHTenUP	Tool		Yes	Yes		No	R2, R8			Yes		
32	PVICE	PVICE		Economic, Environ	Yes	Yes		Yes	R2, R3, R4, R5, R8			Yes	Yes	Yes
33	The Water Technoeconomic Assessment Pipe-Parity Platform (Water-TAP3)	Water-TAP3		Economic, Environ	Yes	Yes			R4					Yes
34	ComStock	ComStock		Economic, Environ	Yes	Yes	Yes		R5					
35	UrbanOpt Advanced Analytics Platform	UrbanOpt		Environmental		Yes			R1, R5		Yes			

Figure 5. The decision tree as a spreadsheet tool for selecting a CE tool which meets the analyst's CE requirements

Table 3. The Decision Tree Analysis to Identify the Tool That Is Best Suited to Meet Analysts' CE Analysis Requirements

The decision tree consists of a series of questions (center column) and alternatives for each question (right column), which the user can answer by selecting a Yes or No in the Excel worksheet.

Question Number	Question	Alternatives to Each Question The user can enter a Yes or No for each alternative.
1	Which EERE office or program do you want to include as a part of the CE analysis?	• Advanced Manufacturing Office • Bioenergy Technologies Office • Building Technologies Office • Federal Energy Management Program • Hydrogen and Fuel Cell Technologies Office • Laboratory Directed Research and Development • Office of Strategic Programs • Solar Energy Technologies Office • Vehicle Technologies Office

Question Number	Question	**Alternatives to Each Question** The user can enter a Yes or No for each alternative.
		• Wind Energy Technologies Office • Water Power Technologies Office • Combined or undefined
2	For which technology, technologies, or sector do you seek to conduct the CE analysis?	• Industry • Additive Manufacturing • Rare Earth and Critical Materials • Biofuels and bioproducts • Energy Storage • Vehicles • Transportation • Buildings • Photovoltaics • Wind • Infrastructure • Geospatial Planning and Evaluation • Market Systems
3	What is your preference for the data requirements for the CE analysis?	• High • Medium • Low
4	What is your preference for the data granularity for the CE analysis?	• High • Medium • Low
5	Would you like to import data in a specific format into the platform of analysis?	• Excel • CSV
6	Would you like to export data in a specific format from the platform of analysis?	• Excel • CSV • HTML
7	Can the platform of analysis be integrated with other tools?	• Planned • None • Soft-linked
8	What is your preference for the granularity of time when conducting the CE analysis?	• Hourly • Daily • Weekly • Monthly • Yearly • Static

Question Number	Question	Alternatives to Each Question The user can enter a Yes or No for each alternative.
9	What is your preference for the geographical scope when conducting the CE analysis?	• City • County • State • Country • Global • Undefined Geographical Scope
10	What is your preference for the scope of the CE analysis?	• Nano • Micro • Meso • Macro
11	Do you require the use of sustainability indicators when conducting the CE analysis?	• Economic • Environmental • Social
12	Do you require the use of circularity indices when conducting the CE analysis?	• Yes • No
13	Which CE strategies would you require as a part of the analysis?	• Reuse (R0) • Rethink (R1) • Reduce (R2) • Reuse (R3) • Repair (R4) • Refurbish (R5) • Remanufacture (R6) • Repurpose (R7) • Recycle (R8) • Recover (R9)
14	What is your preference for the temporal frame when conducting the CE analysis?	• Ex ante (before) • Ex durante (during) • Ex post (after)
15	What is your preference for the life cycle stages which need to be included when conducting the CE analysis?	• Design • Raw material extraction • Manufacturing/processing • Use • EOL
16	What is your preference for the accessibility of the tool?	• Public • Private • Limited

Question Number	Question	**Alternatives to Each Question** The user can enter a Yes or No for each alternative.
17	What is your preference for the user interface of the tool?	• Web-based • Excel • GitHub • Another interface

We illustrate the application of the decision tree analysis through two scenario examples. In the first scenario, the analyst seeks to understand the circularity indices, social indicators, environmental indicators, economic indicators, and CE strategies covered by CE tools from the Vehicle Technologies Office (VTO). As a result, the analyst will select Yes for VTO in Question 2 in Table 3. Scenario 1 results are depicted in Figure 6. The bottom row indicates seven CE tools for vehicles are available from VTO. The horizontal bars with the orange heading indicate the number of VTO tools with circularity indices, social indicators, environmental indicators, and economic indicators. Similarly, the horizontal bars with the green heading indicate the number of VTO tools with the various CE strategies.

In the second example, the analyst seeks to understand the circularity indices, social indicators, environmental indicators, economic indicators covered by CE tools from VTO and which account for Repair as a CE strategy. As a result, the analyst first selects Yes for VTO in Question 2 in Table 3 and then selects Yes for Repair in Question 15 in Table 3. The results for the VTO case study are depicted in Figure 6.

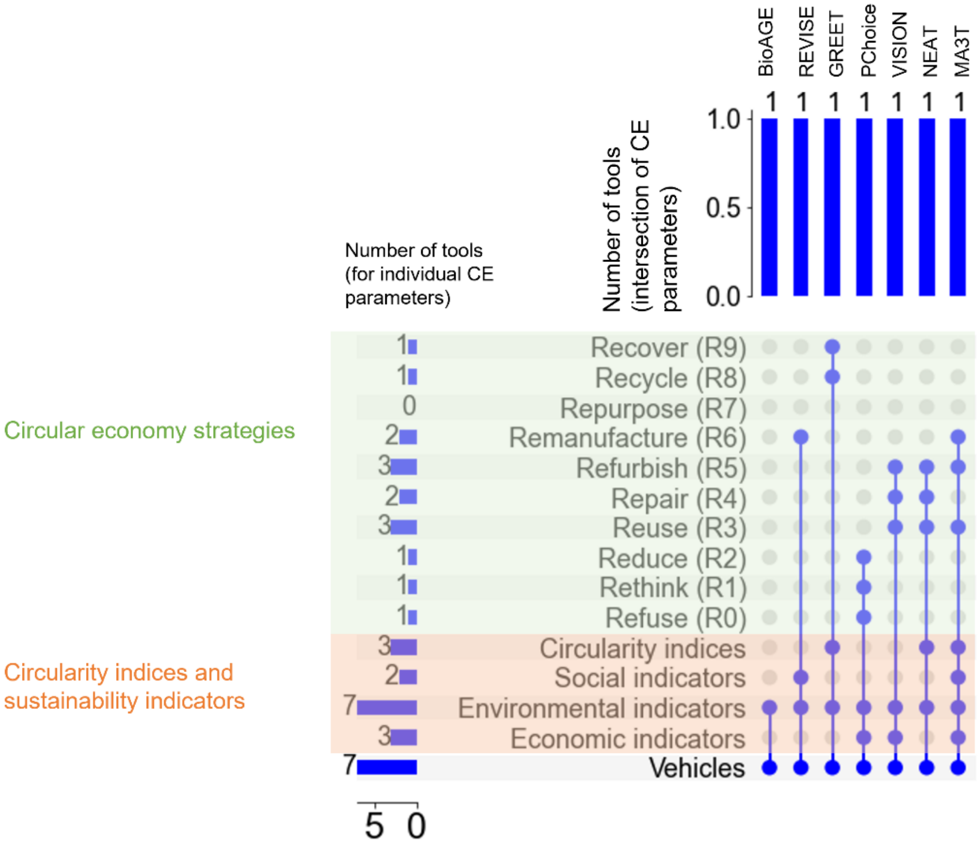


Figure 6. Results from the decision tree analysis with which the analyst seeks to understand the CE strategy, circularity indices, social indicators, environmental indicators, and economic indicators capabilities in CE tools from VTO

The horizontal bars represent the number of tools that provide an individual CE parameter. For example, the second horizontal bar from the bottom indicates three tools include economic indicators. The vertical bars represent the number of tools with an intersection of individual CE strategies, circularity indices and social, environmental, and economic indicators corresponding to the solid blue circles. For example, the first vertical bar from the right indicates only one CE tool from VTO includes circularity indices, social, environmental, and economic indicators, and accounts for reuse, refurbish and remanufacture CE strategies.

BioAGE = Bioeconomy AGE, PChoice= ParaChoice, REVISE = Regional Electric Vehicle Infrastructure Strategic Evolution, GREET = Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies, NEAT = Non-Light Duty Energy and GHG Emissions Accounting Tool, MA3T = Market Acceptance of Advanced Automotive Technologies

The horizontal bar in the first row from the top in the results in Figure 7 indicates only two CE tools from VTO include Repair as a CE strategy. The solid blue circles in the second and third columns from the right identifies the two tools as VISION and the Non-Light Duty Energy and GHG Emissions Accounting Tool (NEAT). A further inspection of the second and third columns reveals no solid blue circles correspond to the social indicators row, which indicates the two VTO CE tools that account for Repair as a CE strategy do not account for social indicators.

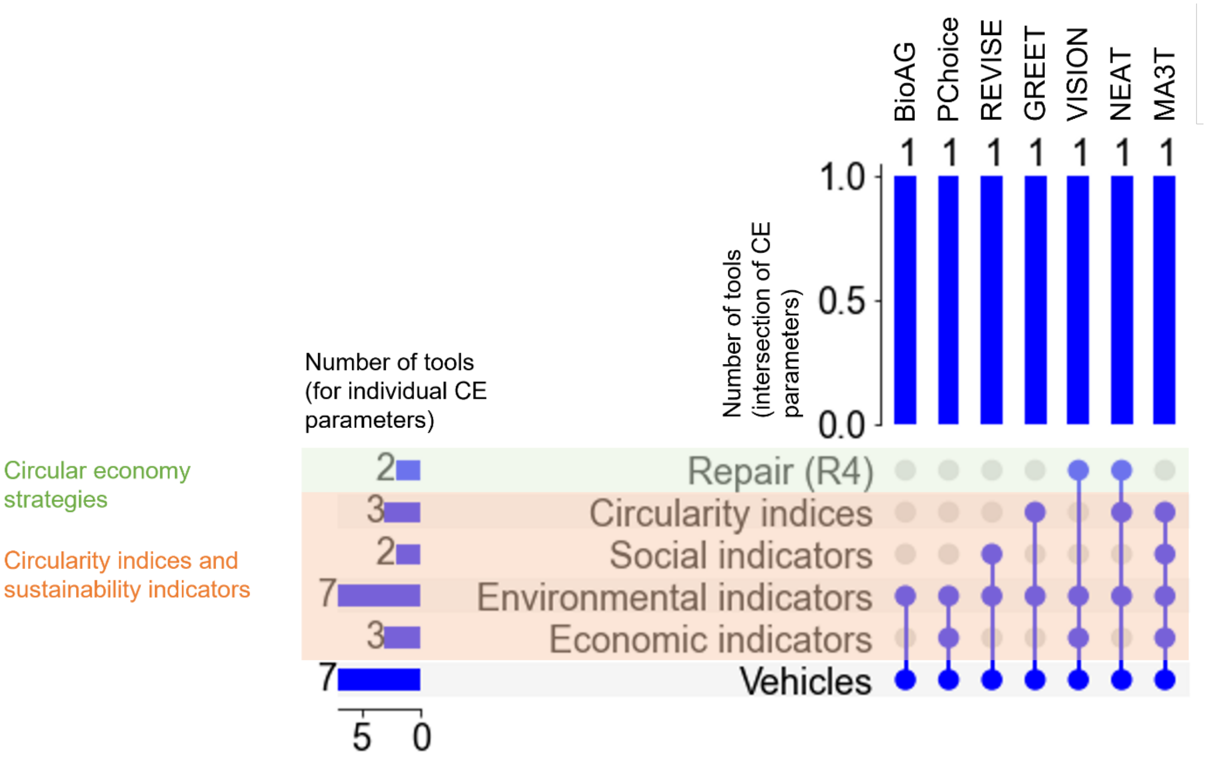


Figure 7. Results from the decision tree analysis with which the analyst seeks to identify the CE strategy, circularity indices, social indicators, environmental indicators, and economic indicators capabilities in CE tools from VTO and which include Repair as a CE strategy

BioAGE = Bioeconomy AGE, PChoice= ParaChoice, REVISE = Regional Electric Vehicle Infrastructure Strategic Evolution, GREET = Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies, NEAT = Non-Light Duty Energy and GHG Emissions Accounting Tool, MA3T = Market Acceptance of Advanced Automotive Technologies

The decision tree analysis helps analysts limit the lists of tools to those most closely aligned with their requirements. Analysts can also explore the features available in each of the tools in the narrowed lists and assess whether available features available are sufficient or whether they must be amended to conduct a CE analysis. In addition, the results from the decision tree analysis can help users understand broader trends for CE tools across different technology areas. The decision tree analysis can identify gaps in the modeling capabilities for CE across the various tools, which can be addressed through future research.

Figure 8 depicts the results of a decision tree analysis that includes all the technologies and accounts for the prevalence of various CE strategies and circularity and sustainability indices. The horizontal bars in the green box for the CE strategies shows that Reduce and Recycle strategies are widely accounted for and are included in 16 and 15 tools respectively, followed by Reuse in 13 tools. Similarly, the horizontal bars in the orange-labeled rows show that the social indicators are underrepresented and account for only nine tools. Furthermore, the solid blue circles in the first, second, third, sixth, and seventh columns show that CELAVI, NREL’s circular economy agent-based model (CE ABM), Iron & Steel CE Model (ISCEM), the Lithium-Ion Battery Resource Assessment (LIBRA) tool, and the PV in the Circular Economy (PViCE) tool have broader modeling capabilities than the rest of the tools, as they account for five or more CE strategies.

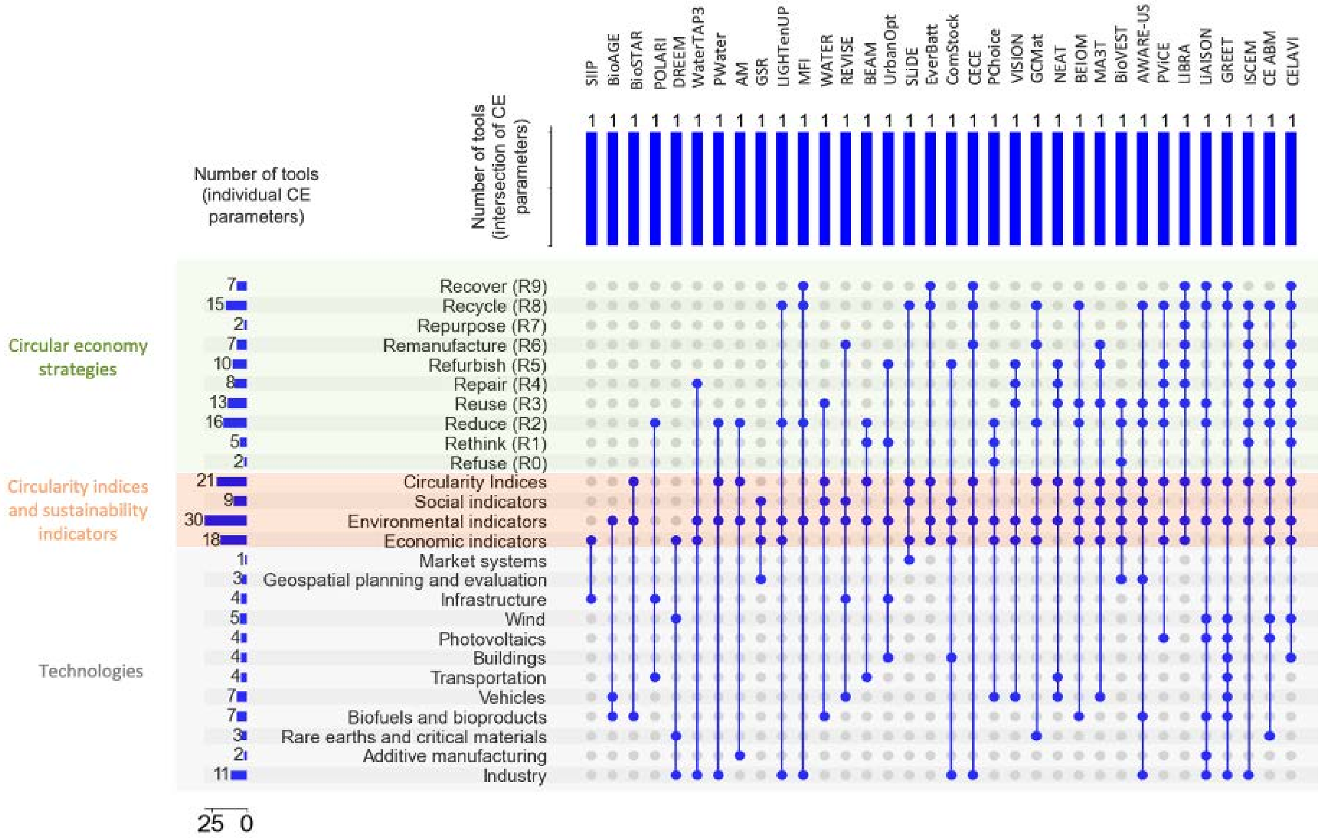


Figure 8. Results from the decision tree analysis with which the user seeks to understand the prevalence of the various CE strategies (in green), the use of circularity indices and sustainability indicators (in orange) in CE tools across different technology areas (in gray)

SIIP = Scalable Integrated Infrastructure Planning, BioAGE = Bioeconomy AGE, BioSTAR = Bioenergy Sustainability Tradeoffs Assessment Resource tool, POLARIS = Planning and Operations Language for Agent-based Regional Integrated Simulation, DREEM = A System Dynamics Model for Assessing Dynamic Rare Earth Production, Demand and U.S. Wind Energy Demand, WaterTAP3 = The Water Technoeconomic Assessment Pipe-Parity Platform, PWater = Plant Water Profiler Tool, AM = Additive Manufacturing energy impacts assessment tool, GSR = Geospatial Roadmap, LIGHTenUP = Life cycle Industry GHgas, Technology and Energy through the Use Phase, MFI = Materials Flows through Industry tool, WATER = Water Analysis Tool for Energy Resources, REVISE = Regional Electric Vehicle Infrastructure Strategic Evolution, BEAM = Behavior, Energy, Autonomy, and Mobility, UrbanOpt = UrbanOpt Advanced Analytics Platform, SLiDE = Scalable Linked Dynamic Equilibrium, EverBatt = EverBatt model, ComStock = ComStock model, CECE = Circular Economy Capacity Expansion model, PChoice = ParaChoice model, VISION = VISION model, GCMat = Global Critical Materials model, NEAT = Non-Light Duty Energy and GHG Emissions Accounting Tool, BEIOM = Bio-based circular carbon economy Environmentally-extended Input-Output Model, MA3T = Market Acceptance of Advanced Automotive Technologies, BioVEST = BioVEST model, AWARE-US = Available Water Remaining in U.S., PViCE = PV in the Circular Economy tool, LIBRA = Lithium-ion Battery Resources Analysis, LIAISON = Life cycle Assessment Integration into Scalable Open source Numerical models, GREET = Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies, ISCEM = Iron and Steel Circular Economy Model, CE ABM = Circular Economy Agent Based Model, CELAVI = Circular Economy Life cycle Assessment and Visualization framework REVISE = Regional Electric Vehicle Infrastructure Strategic Evolution

Appendix Table 2 includes a comprehensive list of the characterized tools along with a, brief description, and hyperlinks from where the reader can download or read more about them.

4 Beyond the EERE Tools: Choosing a CE Methodology

Researchers and practitioners can develop their own tools or analysis based on their research question and requirements when no tools are available for any previously identified scenarios. However, choosing the right tool or methodology to assess circularity can be challenging. On a microscale (e.g., when designing or rethinking a product), simple tools providing circularity and environmental indicators may be sufficient (e.g., LCA, material circularity indicator) (Moraga, et al. 2019). Because the transition from a linear economy to a CE represents a systemic and dynamic change in social and economic structures that is difficult to capture with a single methodology (Walzberg, et al. 2021), several studies have attempted to provide guidance on choosing a suitable methodology.

Merli, Preziosi, and Acampora (2018) reviewed more than 500 journal articles to characterize how CE research was conducted. They found that decision-making tools and models are most prevalently employed—compared to business and management, process engineering, policy, and economic frameworks—and often at a macro scope. However, Merli, Preziosi, and Acampora note that most scholars forgo the social implications of the circularity transition, and that more attention should be devoted to rethinking new approaches to production and consumption. And the Rethink strategy of the R9 framework (Potting, et al. 2017) has the most potential to create value and achieve a truly circular economic system, according to Merli, Preziosi, and Acampora (2018) and Morseletto (2020).

Singh et al. (2021) also reviewed the CE literature to identify the key methodological challenges arising when measuring CE outcomes. These authors point to the weaknesses of existing industrial ecology methods. Data quality and availability, how to choose the type of LCA to perform (i.e., consequential versus attributional LCA), and limited scope of analysis limit the insights that can be gained when studying CE systems with LCA. Like LCA, data quality and availability limit the use of material flow analysis (MFA). Moreover, MFA is usually a static tool that prevents modeling the circularity transition, which calls for methods that account for change over time. The use of monetary—rather than physical—flows and their limited ability to represent waste flows are two of the limits of environmentally extended input-output (EEIO) for measuring circularity. The authors conclude that future research should focus on applying the consequential approach of LCA to more CE systems, conducting dynamic MFA, (e.g., by combining the method with system dynamics models), and developing physical EEIO models.

Sassanelli et al. (2019) reviewed how different methods to assess circularity have been combined, their variables (e.g., energy, materials, and pollutants), their inclusion of life cycle stages, and their coverage of the triple bottom line (i.e., accounting for environmental, social and economic impacts) in a sample of 45 CE studies. In addition to confirming findings from Merli, Preziosi and Acampora (2018) and Morseletto (2020) regarding the lack of studies including social aspects, Sassanelli et al. conclude a holistic methodology able to systematically measure the circularity degree of a given system (accounting for all resources involved in its life cycle) may be needed.

More recently, Moraga et al. (2019) attempted to more clearly provide guidance concerning the methodology choice in CE studies. According to the authors, combining methods—especially from the fields of complex systems science and industrial ecology—could enable the inclusion of several key aspects of the circularity transition, such as the abilities to represent stakeholder decisions, model the system dynamically, incorporate a comprehensive spatial resolution, and represent environmental, economic, and social externalities.

Given the different philosophies, output metrics, and scope of the research methodologies applied to study the CE, the appropriate method or combination of methods to use will depend on the research question being asked (Walzberg, et al. 2021, Corona, et al. 2019). Table 4 presents the different methodologies, the research questions they seek to answer, and some of their possible output metrics (according to our own research).

Within industrial ecology, life cycle sustainability assessment and EEIO can answer questions about the environmental, economic, and social benefits of a more circular product or economy (Walzberg, et al. 2021). MFA can detail material flows in a system and track stocks, while life cycle sustainability assessment and EEIO do not. Therefore, the MFA method can answer a range of questions regarding circularity, including how long it can take for a material to recirculate after it has been used (Walzberg, et al. 2021). Complex systems science methods can simulate the transition of complex socio-technical systems, answering questions regarding the dynamics of those systems (Walzberg, et al. 2021). The type of questions answered by system dynamics (SD) models is related to how the causal structures of the CE system and its feedback loops influence its behavior. Taking a bottom-up approach, agent-based modeling (ABM) highlights how interactions among the CE systems' parts (e.g., stakeholders) drive its overall behavior. Discrete event simulation (DES) is best at answering questions regarding the sequence of events that may lead to increased circularity. Finally, operations research (OR) can answer a broad range of CE-related questions, such as choosing a particular CE solution in the face of conflicting information and choosing the best CE solution depending on the system's constraints.

Boyer et al. (Boyer, et al. 2021), however, argue that regardless of the specific method or metrics chosen, any CE study should report the contribution of the CE system along three dimensions: material recirculation, utilization, and endurance. Therefore, in this framework, a CE would aim to maximize these three dimensions. Maximizing the first dimension, material recirculation, ensures CE systems use material recovered from prior use (e.g., reused, remanufactured, or recycled) instead of virgin materials. The utilization aims to encourage products to be used frequently rather than staying unused. Finally, the endurance dimension predicates that CE systems should retain their value over time rather than become physically degraded or socially obsolete. According to the Boyer et al., such a heuristic would provide a common ground for CE studies sufficiently wide to include diverse sectors, scales, and geographies and sufficiently structured to ensure CE initiatives contribute to coherent ends. Reporting the CE dimensions separately would ensure potential trade-offs are captured in the analysis.

The CE literature has also dedicated much attention to circularity metrics (Moraga, et al. 2019, Ghisellini, Cialani and Ulgiati 2016, Merli, Preziosi and Acampora 2018, Iacovidou, et al. 2017), (Moraga, et al. 2019, Ghisellini, Cialani and Ulgiati 2016, Merli, Preziosi and Acampora 2018, Iacovidou, et al. 2017, Saidani, et al. 2019, Parchomenko, et al. 2019, Kristensen and Mosgaard 2020). Because metrics are generated from methods (Walzberg, et al. 2021), they are also a key parameter to consider when devising a research approach. Different metrics have different dimensions (e.g., material circularity, environmental sustainability, economic sustainability, and social sustainability (Hanes, et al. 2021)) that depend on the methods that generate them. Thus, choosing a method or combination of methods will necessarily affect the assessed metrics.

Table 4. Typical Output Metrics (Nonexhaustive) and Methods That Can Be Used To Evaluate Aspects of a CE

Table adapted from Walzberg, et al. (2021). LCA = life cycle assessment; EEIO = environmentally extended input-output; MFA = material flow analysis; ABM = agent-based modeling; SD = system dynamics; DES = discrete event simulation; OR = operations research

Method	**Research Question**	**Possible Output Metrics** (sample metrics only; not an exhaustive list)
LCA	What are the environmental impacts related to a product or system?	• Environmental interventions (life cycle inventory) • Environmental impact (life cycle impact analysis) • Raw material consumption
EEIO	What are the environmental impacts related to an economic system?	• Circularity gap index • Environmental impact (life cycle impact analysis) • Environmental interventions (life cycle inventory) • Material footprint • Raw material consumption • Waste ratio
MFA	What are the material (or energy) flows and stocks related to a system?	• Direct material input • Domestic material consumption • Material footprint • Net addition to stock • Processed material • Raw material consumption • Total domestic output • Total material requirement
ABM	What are the interactions among a systems' individual parts and how do they drive its overall behavior?	• Decoupling factor • EOL rates • Raw material consumption • Value added at factor cost • Waste and recycling per capita • Waste ratio
SD	How do underlying system structures influence the behavior of complex dynamic systems (e.g., systems with interdependence, mutual interaction, information feedback, and circular causality)?	• Decoupling factor • EOL rates • Net addition to stock • Raw material consumption • Value added at factor cost • Waste and recycling per capita • Waste ratio

Method	Research Question	Possible Output Metrics (sample metrics only; not an exhaustive list)
DES	What is the sequence of (eventually stochastic) events that triggers the dynamics of a system?	• Decoupling factor • Raw material consumption • Value added at factor cost • Waste ratio
OR	What is the best solution for a decision-making problem?	• Decoupling factor • EOL (e.g., recycling and reusing) rates • Raw material consumption • Value added at factor cost • Waste ratio

5 How to Choose a Method or Combination of Methods: Two Case Studies

In this section, we provide two case studies to demonstrate recent development efforts for EERE tools that can be leveraged to CE modeling use cases. First, a case study of the Circular Economy Life cycle Assessment and Visualization (CELAVI) Framework is intended to serve as a starting point for engaging with researchers working on CE and to provide them with methodological choices when the EERE tools portfolio does not provide a tool that meets their needs. Next, a case study using the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) tool provides an example of the reasoning behind the inclusion and integration of methodologies, pathway and process stages definitions, and election of environmental and circularity metrics.

CE Life Cycle Assessment and Visualization (CELAVI) framework

The EERE Circular Economy Life cycle Assessment and Visualization (CELAVI) framework from the National Renewable Energy Laboratory illustrates how different research methodologies are chosen and combined (Corona, et al. 2019).

Development of CELAVI

Starting with a research question—*how the impacts of supply chains might change over time and space as circularity increases*—the CELAVI developers reviewed different methods used in the CE context. Then, a mapping was undertaken to determine which critical aspects of the CE are captured by existing methods and how well these methods satisfy the requirements needed to answer the research question (Table 4). The CELAVI developers examined these methods with respect to three main categories of requirements: capabilities (e.g., ability to model externalities and uncertainties), resolution (e.g., temporal, and spatial resolution), and scope (e.g., temporal, and spatial scope).

Capability Requirements

To answer CELAVI's primary research question, a CE tool needs to be able to incorporate environmental, economic, and social externalities; model the techno-economic and market potentials of material efficiency; assess circularity; account for uncertainty; and be flexible enough that the scope of the analysis includes systems indirectly affected by the circularity transition (Walzberg, et al. 2021, Ghisellini, Cialani and Ulgiati 2016).

The ability to capture environmental, economic, and social externalities is a required capability in this application because doing so is essential to being able to quantify changes in impacts. Due to the dynamic and holistic nature of the circularity transition, such externalities should be captured at the highest resolution and largest scale relevant to stakeholders. As described in the previous section, a single method does not seem sufficient to reach this objective.

The technical potential of CE systems is the highest level at which they can be deployed free of any constraints. The economic potential excludes economically ineffective systems and is, therefore, smaller than the technical potential. Finally, the market potential is often smaller than the economic potential and depends on how individuals and businesses adopt the CE systems in practice. This last level of analysis is crucial to model the social changes implied by the CE. For instance, the new business models implied by the sharing economy may not be adopted by the overall population and, thus, remain at a niche level or vanish. Therefore, to address CELAVI's application, the CE tool must be able to model stakeholders' behaviors and the nonlinearities linked to the adoption process to account for the market potential of the circularity transition.

The technologies, business models, and consumption patterns developed and adopted during a future circularity transition are uncertain, and so are the parameters underlying those developments. Therefore, the CELAVI developers require the CE method to incorporate uncertainty, for instance, by using probability distributions or scenarios.

One last capability that a CE tool must demonstrate for utility in CELAVI's application is flexibility in scope. CE systems implemented in a specific supply chain may affect other supply chains, for instance, through recycling or repurposing. In addition, the exchange of secondary materials between economic sectors is a fundamental part of the CE. Therefore, the CE tools used in this application should model those exchanges and their potential environmental, social, and economic drawbacks and benefits.

Resolution Requirements

CELAVI's primary research question also requires the CE tools to include temporal aspects, enable the analysis of a country or a region, and model technologies individually.

Transitioning from a linear economy to a CE may only take place over many years. Decisions about circularity may be made annually, and implementing new recycling technologies, business models, or product designs may take several years. During this time frame, socioeconomic and technology changes may occur, and stakeholders may make different decisions, accelerating or hindering the transition. Therefore, to understand how the impacts of supply chains change over time, CE tools must incorporate temporal aspects, either continuously or discretely (e.g., modeling the system year by year). The exact temporal scale will depend on the exact research question and the analyzed CE system.

The circularity transition also needs to happen at multiple scales—products, supply-chains, and the economy—to be viable (Merli, Preziosi and Acampora 2018, Parchomenko, et al. 2019). During the transition, shifts in transportation, material processing, services, and recycling activities will occur between industrial sectors and across regions. Hence, a high spatial resolution is needed for CE tools to capture the impacts of such shifts.

CE tools should also be able to model individual technologies because CE strategies such as reusing products or recycling materials require adapting existing technologies and business models or developing new ones.

Scope Requirements

To study circularity transitions in the CELAVI application, a CE tool also needs to satisfy three scope requirements: a temporal scope spanning several years, a national economic scope, and a national spatial scope. Following a similar rationale to the temporal resolution requirement, CE tools must adopt a long temporal scope because of the multiple years a circularity transition may take. The exact temporal scope should be estimated by the relevant stakeholders of the studied CE project. To answer CELAVI's research question, CE tools' spatial and economic scopes should be national for a similar reason. Circular supply chains will, indeed, most likely increase connections between industries and regions. A wide spatial scope will, thus, ensure critical environmental, economic, and social aspects of the studied CE systems are captured.

Mapping Tools Characteristics and Requirements for Circularity Transition Modeling

After reviewing the requirements needed to model the circularity transition and its impacts, the next step in the CELAVI framework development was identifying methods capable of capturing those requirements. These methods include LCA, EEIO, MFA, ABM, SD, DES, and OR.

Table 5 illustrates how well each method satisfies the CELAVI CE modeling requirements and shows that no single method can satisfy all requirements. For example, LCA cannot capture the market potential, dynamics of the circularity transition, or a wide spatial scope; moreover, consequential LCA—using either partial or computable general equilibrium models—lacks technology resolution and may misrepresent the market potential of CE systems. EEIO and MFA are aggregated methods that cannot represent individual technologies appropriately; moreover, those methods cannot include the market potential in the analysis and do not account for temporal aspects.

Table 5. Examples of Requirements Met by Diverse CE Methods, as Evaluated for Satisfying the Primary Research Question Posed by the EERE's CELAVI tool

Circularity transition modeling requirements		LCA	EEIO	MFA	ABM	SD	DES	OR
Capabilities:	Modeling externalities	🟩	🟩	🟨	🟧	🟧	🟧	🟧
	Modeling the market potential	🟧	🟧	🟧	🟩	🟩	🟨	🟨
	Modeling uncertainties	🟧	🟧	🟨	🟩	🟨	🟩	🟩
	Flexible scope	🟨	🟨	🟨	🟧	🟩	🟧	🟨
Resolution:	Inclusion of temporal aspects	🟧	🟧	🟧	🟩	🟩	🟩	🟩
	High spatial definition	🟧	🟨	🟩	🟨	🟩	🟨	🟨
	Individual technologies	🟩	🟨	🟨	🟩	🟨	🟩	🟩
Scope:	Wide spatial	🟧	🟩	🟩	🟨	🟩	🟨	🟨
	Wide economic	🟨	🟩	🟩	🟧	🟩	🟨	🟨
	Several years	🟧	🟧	🟧	🟩	🟩	🟩	🟩

Orange = the method does not meet the requirement; yellow = the method partially meets the requirement; green = the method fully meets the requirements

LCA = life cycle assessment; EEIO = environmentally extended input-output; MFA = material flow analysis; ABM = agent-based modeling; SD = system dynamics; DES = discrete event simulation; OR = operations research

Table recreated from Hanes et al. (2021) and Walzberg et al. (2021).

In contrast, ABM, SD, and DES are dynamic (although not continuous) methods that can assess the CE transition over multiple years and include the CE system's market potential. However, those methods cannot model environmental, economic, or social externalities. Moreover, a trade-off often occurs between spatial resolution and spatial and economic scope when using ABM due to high computational requirements. On the contrary, the spatial and economic scope of SD may be wide, but its ability to model individual technologies is moderate. The DES method excels at representing industrial processes and thus individual technologies, but it cannot capture the social dynamics of CE systems, such as technology adoption.

Finally, OR has a narrow spatial resolution and a limited ability to represent externalities. Moreover, due to computational limitations, OR algorithms may not find the optimal solution to the research question when the modeled CE systems present nonlinearities.

The CELAVI developers determined LCA and DES were the best methods to combine in order to answer the research question—*how might the impacts of supply chains change over time and space as circularity increases*—that is targeted by the CELAVI framework. Indeed, the DES method enables detailed supply chains modeling, including a high technological and temporal resolution. Moreover, DES can model various decisions affecting the modeled supply chain during the simulation. On the other hand, LCA enables the quantification of externalities along the supply chain. The combination of LCA with DES means externalities can be computed at each time step of the simulation, providing a temporal account of the supply chain's environmental impacts.

Though Table 5 is useful to illustrate the approach set out by the CELAVI developers, it must be understood as a subjective exercise that depends on the project, the research question, and researchers' skills and backgrounds. For instance, seasoned LCA practitioners may have no difficulties modeling uncertainties in LCA and regard the method as fully meeting the modeling uncertainty requirements. The level of detail of the research question also informs on the type of method to use. For instance, if the research question focuses on distributed solar photovoltaics, ABM may be a suitable method. But if the research question is concerned about the effect of CE strategies on economic flows, EEIO could be more appropriate. Furthermore, Table 5 is not exhaustive and other approaches—particularly qualitative ones—could be added. Thus, CE researchers are encouraged to consider Table 5 as a process rather than an answer and to adapt the table to suit their own research questions and skills.

Finally, although all the capabilities, level of resolution and scope elements needed for a project may affect the chosen type of methods—and thus the assessed metrics—the type of externalities that each method can model is an important parameter in determining what output metrics CE researchers will be able to assess. Table 6 presents some of the typical output metrics from the CE methods presented in Table 5.

In summary, building on the approach used by the CELAVI developers, CE researchers could consider adopting the following stepwise progression when needing to choose a method or combination of methods:

1. Define the research question.
2. Identify the capabilities, level of resolution, and scope needed to appropriately answer the research question.
3. Based on the project, research question and researchers' skills, map how existing CE methods answer the needs in capabilities, level of resolution and scope.

Following this process, researchers may find that several methods should be combined to appropriately answer the research question (such as for the CELAVI tool) or that a single method is sufficient.

CELAVI Overview

The CELAVI tool, which was recently developed, is still under active development. It is designed to provide a framework for modeling how externalities of energy systems could change as supply chains transition from linearity toward circularity and support stakeholder decisions about circularity transitions. An alpha version of the tool is available on GitHub,[5] and additional documentation can be found in Hanes et al. (2021).

The current version of CELAVI combines two modeling perspectives: DES and LCA. The result is a dynamic and flexible multiscale tool. The DES module models detailed and dynamic supply chains, which are then linked to background life cycle processes via the LCA module. The CELAVI framework also represents technological and economic changes (e.g., the learning effect). Although the tool's first case study focused on wind power systems, the framework is being developed in a flexible and modular manner to allow for adaption to other applications

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[5] https://github.com/NREL/celavi

(but it has not yet been applied outside the wind industry). CELAVI can explore questions such as how much learning effect is required for a recycling supply chain to be on cost-parity with landfilling, how much investment is needed to reach a certain level of circularity, or how increasing circularity affects the environmental impacts of the system.

The intended audience of the tool includes governing bodies, corporations, and nongovernmental organizations. Figure 9 presents an overview of the CELAVI tool, and Table 6 summarizes the CELAVI tool's characteristics.

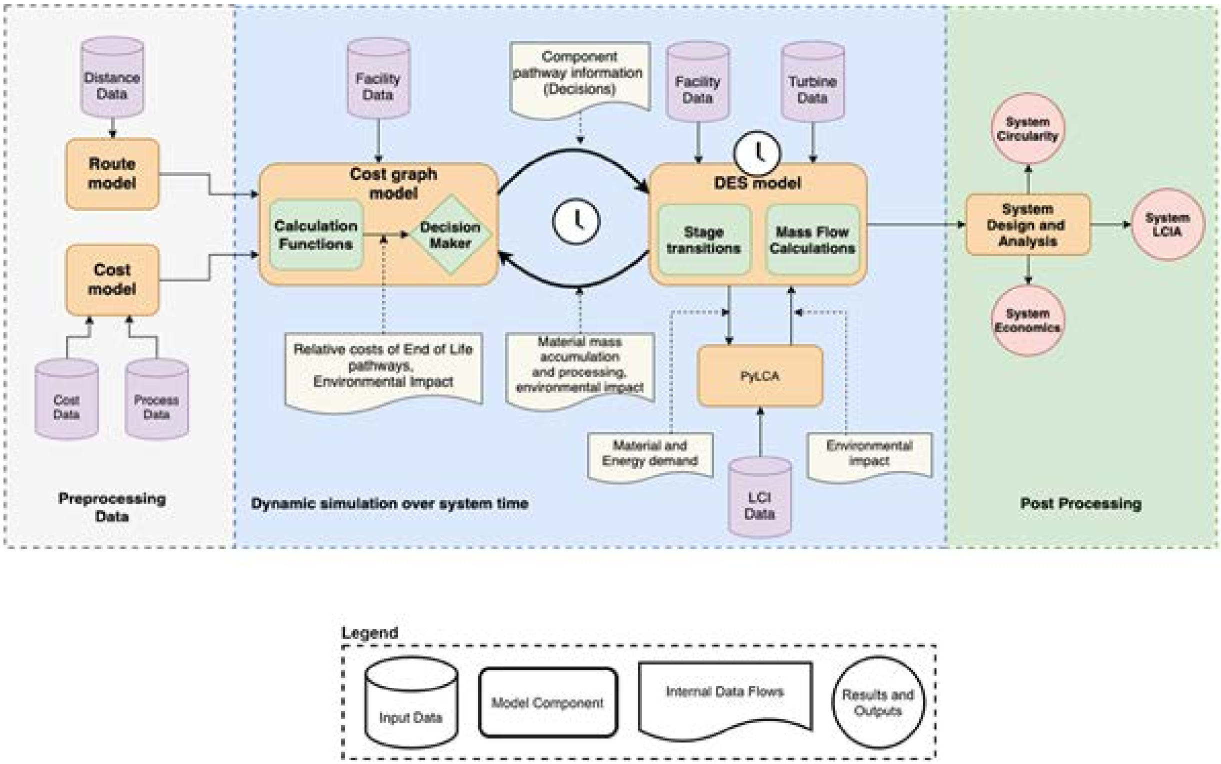

Figure 9. Overview of the CELAVI tool

LCI = life cycle inventory, LCIA = life cycle impact analysis
Based on Hanes et al. (2021)

Based on discussion with CELAVI's principal investigator, detailed characteristics of the tool were documented. They include the following:

- **Life Cycle Stages Covered:** The CELAVI tool models "cradle-to-grave" systems, including raw material extraction, manufacturing, use, EOL, and transportation activities. Thus far, the framework has only been applied to analyze wind power systems.
- **ReX Strategies Modeled:** Apart from the Refuse (R0) and Repurpose (R7) strategies, the CELAVI framework can model seven of the nine ReX strategies usually defined in the CE literature by Morseletto (2020): Rethink (R1), Reduce (R2), Reuse (R3), Repair (R4), Refurbish (R5), Remanufacture (R6), Recycle (R8), and Recover (R9). Although the refuse and repurpose strategies may not be the most relevant in the wind power case study, model modifications could enable the inclusion of those strategies if they were relevant to the studied CE system.

- **Output Metrics/Indicators:** The material and energy flow rates for all modeled ReX strategies and all life cycle stages, the percentage of in-flow and out-flow circularity and the environmental impacts covered by the Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI) are the main outputs of CELAVI. Outputs are generated at each time step of the simulation, which enables the visualization of results as a time series.
- **Scope:** The DES component of CELAVI enables the analysis of a system at the nano (materials), micro (components), and meso (supply chain) scales. Although using another method such as SD could enable modeling the macroscale, doing so would be at the expense of a finer material resolution, which was needed to feed the LCA model. CELAVI developers are currently considering other approaches that might allow for the inclusion of macro-scale components.
- **Time Resolution:** The time resolution of CELAVI is a month to a year, depending on the simulation parameters. Though a finer temporal resolution is theoretically possible, it may not always be coherent to increase the temporal resolution because stakeholders' decisions about circularity may take months to years.
- **Data Requirements:** CELAVI requires a large quantity of data. Data for the DES model includes the costs and capacity of each EOL pathway, the system's material and energy demand, and the locations of facilities throughout the supply chain (e.g., recycling sites or landfills). Data for the LCA are the outputs of the DES model, background life cycle inventory data, and life cycle impact assessment characterization factors.
- **Data Granularity:** The data granularity of the CELAVI tool is high. Few of the data used in the tool are aggregates or proxy values (e.g., averages). However, proxy values could be used instead of more-detailed data depending on data availability. Sensitivity analyses can be conducted with CELAVI to quantify uncertainty.
- **Material Efficiency Potential:** CELAVI includes the technical and economic potentials of the ReX strategies, but it currently does not account for the market potential, as stakeholders' behaviors are not modeled. Future releases of the framework will include a stakeholder decision model to account for the market potential (Ghisellini, Cialani and Ulgiati 2016).
- **Pillars of Sustainability:** Environmental and economic externalities are modeled by the CELAVI tool. Although social impacts are unaccounted for, the spatial resolution of CELAVI could allow the tool to be used to conduct a regional LCA, providing, for instance, information about the populations affected by transportation or recycling activities is available; also, the number and type of jobs at each stage in the supply chain could be incorporated, assuming such data were available.

Table 6. Summary of CELAVI Tool's Characteristics

General	Name	Circular Economy Life cycle Assessment and Visualization (CELAVI)
	Primary developer	National Renewable Energy Laboratory
	Description	CELAVI hybridizes existing methods to meet the demands of modeling circularity transitions and associated impacts.
	Access to tool	Available on GitHub at https://github.com/NREL/celavi

Life Cycle Stages	Raw material extraction	Yes
	Manufacturing	Yes
	Use	Yes
	EOL	Yes
	Transportation activities	Yes
ReX Strategies Modeled	Refuse (R0)	No, but could be included
	Rethink (R1)	Yes
	Reduce(R2)	Yes
	Reuse (R3)	Yes
	Repair (R4)	Yes
	Refurbish (R5)	Yes
	Remanufacture (R6)	Yes
	Repurpose (R7)	No, but could be included
	Recycle (R8)	Yes
	Recover (R9)	Yes
Technology Area	n/a	Wind power
Output Metrics/ Indicators	Circularity metrics	Yes
	Material flows	Yes
	Energy flows	Yes
	Environmental impacts	Yes
	Costs/revenue	Yes
	Social indicators	No, but could be included
Scope	Nano (materials)	Yes
	Micro (components)	Yes
	Meso (supply chains)	Yes
	Macro (economy)	No, but could be included
Time Resolution	Hourly	No
	Daily	No
	Weekly	No
	Monthly	Yes
	Yearly	Yes
	Static	No
Data Requirement	Low	No
	Medium	No
	High	Yes

Material Efficiency Potentials	Technical	Yes
	Economic	Yes
	Market	No, but could be included
Pillars of Sustainability	One or two	Yes
	All three pillars	No, but could be included

Example of CELAVI Usage

In this section, we describe how we applied the CELAVI tool to a case study of the tracking of wind blade material quantities in Iowa and Missouri from manufacturing through EOL pathways from 2000 to 2050. This information can be used by wind plant owners, recyclers, municipalities, and other stakeholders to assess potential EOL management challenges under different circularity cost and wind capacity expansion scenarios.

As Table 6 indicates, several life cycle stages and materials are included in the model. For example, Figure 10 presents the number of wind blades in each EOL pathway over time under two circularity cost scenarios: moderate circularity cost and high circularity cost. In this example, CELAVI includes three EOL pathways: landfilling, mechanical recycling, and cement coprocessing. The selection of EOL pathways, and other aspects of the CELAVI case study parameters (e.g., circularity costs and capacity expansion assumptions), can be modified or expanded in other applications. As shown in Figure 10, under Scenario B (high circularity cost) more blades end up in landfills than in Scenario A (low circularity cost).

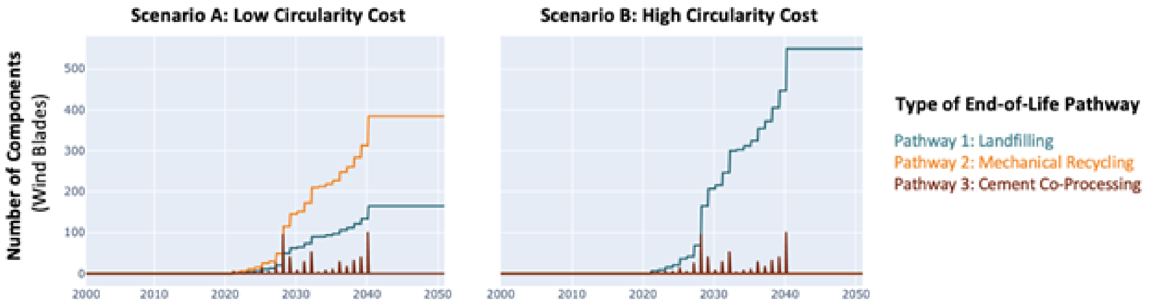

Figure 10. Example of output from CELAVI Iowa and Missouri wind blade case study illustrating the number of components (wind blades) by EOL pathway for two scenarios: low circularity cost and high circularity cost

In addition to tracking materials quantities across life cycle stages, the CELAVI tool is capable of computing environmental impacts (as indicated in Table 6). Figure 11 shows wind blade global warming potential for 2000–2050. As illustrated in Figure 11, wind blade manufacturing is the primary source of global warming potential (see blue curves of manufacturing facilities in Figure 11). Toward the end of the studied period, however, impact from EOL management starts to also contribute to global warming potential as more wind blades are decommissioned, although to a much lower extent than manufacturing (see purple, green, and orange curves of EOL facilities in Figure 11).

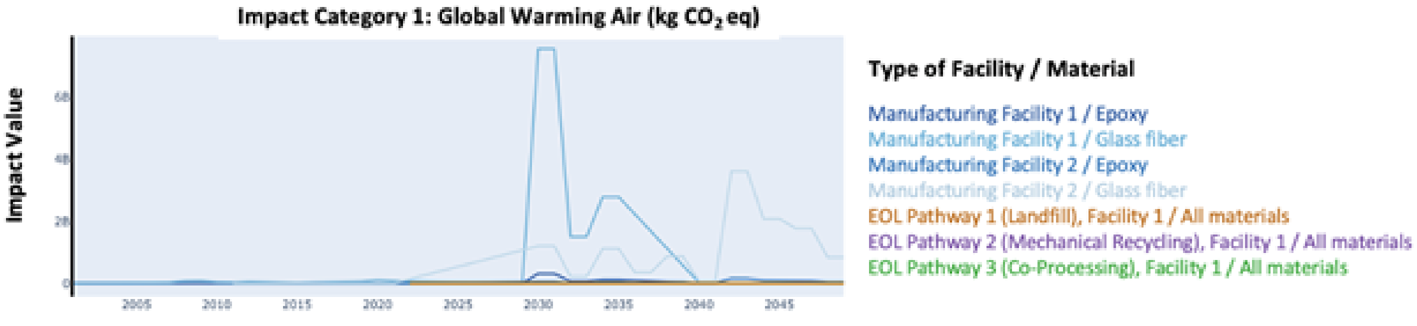

Figure 11. Example of output for one scenario from CELAVI Iowa and Missouri wind blade case study illustrating results for one environmental impact category: global warming potential.

Figure 12 illustrates another capability of the CELAVI framework: spatially explicit results that show how material and energy flows, economic indicators, and environmental impacts are distributed regionally. The figure shows that in the first two decades of the model run, most of the smog impacts are due to manufacturing wind blades and are caused by the two manufacturing facilities in Iowa (blue histograms in Figure 12-a). As more and more blades reach end of life, EOL management facilities also cause smog impacts in Iowa and Missouri (purple, green, and orange histograms in Figure 12), although manufacturing remains the dominant source of impacts.

Figure 12. Example of output for one scenario from CELAVI Iowa and Missouri wind blade case study illustrating spatially varying smog impacts for three different years: 2011 (a), 2029 (b), and 2039 (c)

In alignment with CELAVI's goal of using transparent and open-source data, the framework uses the U.S. Life Cycle Inventory database and the compatible impact methodology TRACI tool, which has a low regional resolution. Therefore, although CELAVI tracks the locations of emissions sources, environmental impacts are not fully regionalized. Using an impact methodology such as Impact World+ (which accounts for the regional dynamics of environmental impacts such as smog and acidification) could further enhance the framework, but such a modification would require using other (likely proprietary) life cycle inventory data.

Figure 12 was directly taken from the CELAVI visualization dashboard (shown in Figure 13), which is under development. Once completed, the dashboard will be freely available online for the intended audience of the tool (e.g., governing bodies, corporations, and nongovernmental organizations) to use.

Figure 13. CELAVI visualization dashboard

CE Sustainability Analysis Framework for Plastics Based on the GREET Life Cycle Analysis Model and a Material Flow Analysis

Increasing the recovery of materials in economic systems is a main motivation for transitioning from a linear economy to a CE. In recent years, the concept of a CE has gained increasing attention in the European Union and around the world, partly as the result of promotions by the Ellen MacArthur Foundation and the Government of the United Kingdom (Moraga, et al. 2019). Unlike with a linear economy, the implementation of strategies and technologies that promote circularity can reduce pollution caused by waste and slow the use of nonrenewable resources (Ellen MacArthur Foundation, Granta Design 2015). By recycling, a CE can also increase the value of materials through their reincorporation after their use phase.

For the plastics sector, current industry practices lead to low recycling and re-use rates. According to the U.S. Environmental Protection Agency (EPA 2020), only 9% of plastics used in the U.S. market are recycled, and the remainder is sent to landfills (75%) or incinerated (16%). Common barriers to a high plastics recycling rate include a low waste collection rate, lack of infrastructure for more efficient plastics recycling (e.g., material recovery facilities are not optimized to improve resin recovery), and lack of sufficient policy and economic incentives for greater use of recycled resin. Also, recycling rates vary with the type of plastic. For the packaging sector, polyethylene terephthalate (PET) is the resin with the highest recycling rate in the United States, though the overall recycling rate is still lower than 19% (NAPCOR, APR 2018). With current industry practices, most PET resins are recycled from used bottles through a mechanical recycling process, which includes collecting, sorting, washing, flake production, and pelletizing. Scaling up mechanical recycling, along with a higher waste collection rate, could improve circularity for plastics packaging, but mechanical recycling has its limitations. Owing to quality degradation that occurs during mechanical recycling, resins can only be recycled a few times. In addition, producing high-quality PET resin via mechanical recycling can face technical and cost challenges, as removal of contaminants (e.g., fine particles, adhesives, and pigments) is difficult. As a result, most recycled PET pellets (80%) go to low-value applications (e.g., fibers and films).

To address the challenges facing mechanical recycling, various chemical recycling technologies have been developed as an alternative option. The chemical recycling category includes several routes, such as depolymerization, pyrolysis, and dissolution. The depolymerization route aims to reproduce virgin-like resins that meet the more stringent requirements of high-value applications such as clear bottles and food-grade containers. Depolymerization processes (e.g., hydrolysis and methanolysis) break down polymers into smaller molecules, known as monomers, which are indistinguishable from those used to produce virgin polymers. Therefore, the quality of the chemically recycled resins is comparable to that of virgin resins. Another advantage is that chemical recycling allows the use of plastic waste with a higher content of pigments and impurities because the monomers produced from the decomposition are purified before their use in resin production. Although chemical recycling shows the potential to reduce the EOL management of waste plastics, energy and chemicals are needed for the conversion process, and there is a concern the net environmental benefits of chemical recycling do not exceed the net environmental benefits of mechanical recycling. In particular, CE strategies should be implemented in a manner consistent with decarbonization goals. The technologies promoting circularity do not necessarily have a lower carbon footprint than state-of-the-art technologies (Lonca, et al. 2020, Rigamonti and Mancini 2021). Therefore, it is important to incorporate the assessment of environmental impacts into the evaluation of CE strategies.

Components of a CE Sustainability Analysis Framework

To support the successful transition to a circular economy, identifying the key process stages or barriers is critical to recognizing opportunities and unlocking the full potential of CE strategies. Like that of the virgin material production, the supply chain for a CE would also involve multiple stakeholders and processes, such as waste collection, sorting, and resin recovery. Each of these process stages has certain requirements for energy and materials that contribute to the overall environmental impact of the CE system. The characteristics of the circularity strategy under analysis (e.g., type of feedstock and targeted application of recycled resin) will define the process stages involved and the type and quantity of material and energy resources. The definitions of these process stages influence not only the overall recovery rate of materials in the system but also the environmental impacts derived from the implementation of the circularity strategy.

Though the CE concept focuses on increasing material retention rate to reduce waste and pollution, a successful CE should also consider environmental impacts (e.g., energy use, greenhouse gas [GHG] emissions). Earlier studies suggested circularity does not equal sustainability (Abokersh, et al. 2021). For example, if recycling turns out to be more energy- and carbon-intensive than virgin pathways, higher circularity does not improve sustainability. This observation indicates that the pathway to achieving higher circularity is very important, and an appropriate modeling framework that considers both circularity and sustainability performance is needed to support robust environmental impact analysis. However, the simultaneous assessment of circularity and environmental impacts is challenging, as it requires the integration of different tools addressing specific aspects of either circularity or environmental evaluation.

To help in the selection of tools for circularity analysis, this section presents principles and considerations for developing a CE sustainability analysis framework to evaluate the environmental impacts and circularity metrics of plastic packaging. The scenarios analyzed here focus on the production of PET bottles and the impacts that the modification of material factors and the inclusion of different recycling technologies can have on the resource consumption, carbon footprint, and solid waste generation of PET resins and bottles.

Life cycle assessment (LCA) is an appropriate method for assessing the environmental impacts of circularity-enabling technologies. It incorporates different phases of a product life cycle, and, depending on the granularity of the data, it can identify the critical process stages that influence the environmental impact of the system. LCA methods, which have been developed over the past 30 years, focus on providing fair, apples-to-apples comparisons of technologies and identifying environmental impact hotspots within the life cycle and supply chains of technologies. It is an effective way to benchmark alternative technologies relative to their conventional counterparts. In the development of new technologies, LCA hotspot analysis can help identify key opportunities for process improvement. It enables technology developers to set specific targets for improving the environmental performance of the system. LCA can also include other indicators, apart from environmental impacts, which amplify the perspective of circularity evaluation.

Evaluating material recovery in the implementation of circularity strategies analysis is important. Therefore, an analysis framework for circularity needs to account for the flows of post-use materials that are diverted from EOL management and incorporated back into the system. The extent of these closed-loop flows establishes the contribution of each recycling technology to the environmental impact of the system. The estimation of material recovery in CE strategies required the incorporation of material flow analysis (MFA) in the study. MFA also estimates the solid waste generated, material losses, flows of upcycled and downcycled materials, and requirements of the system for virgin material. All these parameters cover important aspects of circularity that now can be incorporated into LCA. We integrated these two tools—LCA and MFA—into the CE sustainability analysis framework developed for this case study.

Framework Structure

The framework for this case study employed the Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET) model (ANL n.d.) to perform the environmental assessment in the case study. GREET is a well-established tool for LCA because of its extensive life cycle inventory database and its methods for estimating the energy use, water consumption, and air pollutant emissions. Five production pathways for PET resin, including virgin and recycling pathways, were incorporated into the framework. Two of these technologies represented the fossil-based production pathways of PET resin: esterification of purified terephthalic acid (PTA) with mono ethylene glycol and transesterification of dimethyl terephthalate (DMT) with ethylene glycol. These virgin production pathways, which do not incorporate recycling streams, represent the current linear economy employed in PET resin manufacturing.

The three recycling technologies considered here are mechanical recycling, enzymatic hydrolysis (the base process for chemical recycling), and methanolysis (the base process for upcycling). Enzymatic hydrolysis decomposes PET bottles into PTA and mono-ethylene glycol, and methanolysis converts PET fibers into DMT and mono-ethylene glycol, which are the feedstock materials for PET resin production in the virgin pathways. Data on the life cycle inventories of the technologies were obtained from the literature (Singh, et al. 2021, Franklin Associates 2018, PE Americas 2009) and from industry partners. Figure 13 presents the process stages involved in each of the five production pathways Major operations in the recycling pathways include the collection of waste PET from the source of generation, sorting PET from the collected stream, reclaiming operations that reduce the size of the waste PET and clean it, the production of the recycled resin through the different technologies, and bottle manufacturing by injection stretch blow molding. Detailed information on inventory data, assumptions, and considerations for the LCA will be provided in a forthcoming publication (Gracida-Alvarez, et al. Forthcoming). Total energy consumption, water consumption, and GHG emissions were the metrics calculated from the LCA, as they reflect the impacts on the use of natural resources and the carbon footprint.

MFA was incorporated into the modeling framework by using and defining material factors that aided in the estimation of recycling flows and material losses in the system. A complete list of the factors along with their definitions is presented in Table 7, and their relationship with the different process stages of the recycling technologies can be seen in Figure 14. The calculation of the material factors used data from U.S. government agencies (EPA 2020), a research paper (Singh, et al. 2021), LCA reports (Franklin Associates 2018, PE Americas 2009), and industry partners. The material losses (represented by the acronym ML in Figure 14) were estimated at each process stage. The addition of all these material losses proportionated the total solid waste generation of the system. The flows of recovered materials (PET bottles, carpets, and textiles) were tracked along process stages to account for the amount of incoming material from the three PET recycling technologies. The amount of virgin material used in the system is obtained from the difference between the total demand for bottles and the amount of bottle material that can be produced through recycling technologies. These results from the MFA defined two circularity metrics in the framework—solid waste generation and virgin material use—which are directly related to the extent of the flows of recovered materials in the system. The correlation between the LCA metrics and the material flows at each process stage in the framework served to incorporate the effects of circularity principles to the LCA in GREET.

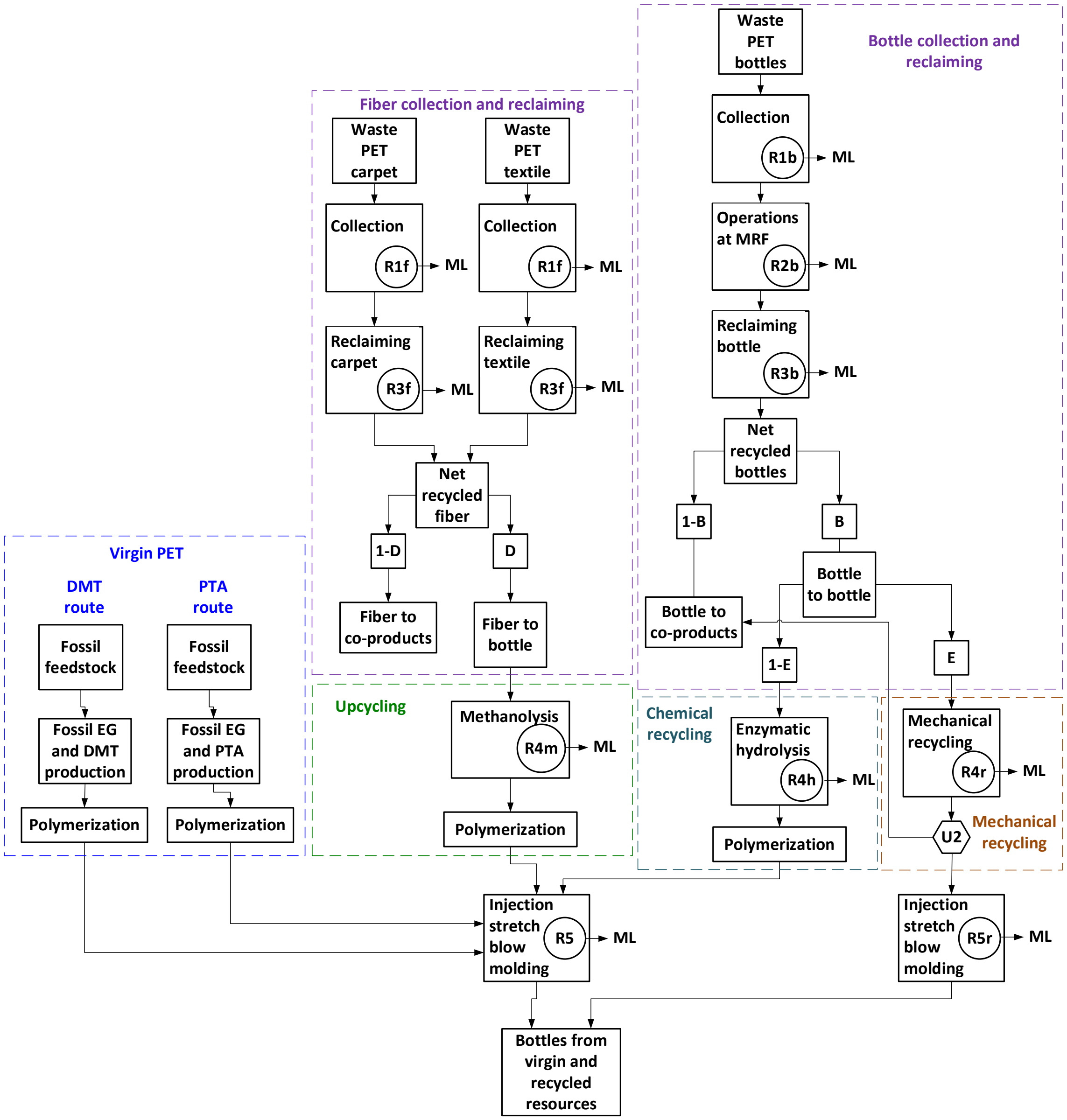

Figure 14. Process stages and material flow factors of the technologies incorporated in the framework

B: Percentage of recycled flakes to bottle production
D: percentage of densified fiber to bottle production
DMT: Dimethyl terephthalate
E: Percentage of flakes to mechanical recycling
EG: Mono-ethylene glycol
ML: Material losses from the system
PTA: Purified terephthalic acid
R1b: Recycling rate of bottles
R1f: Recycling rate of fiber
R2b: Yield of sorting at material recovery facility
R3b: Yield of bale-to-flake processing
R3f: Yield of fiber reclaiming
R4h: Yield of enzymatic hydrolysis
R4m: Yield of methanolysis
R4r: Yield of mechanical recycling
R5: Yield of bottle manufacturing from virgin and chemically recycled resin
R5r: Yield of bottle manufacturing from mechanically recycled resin
U2: Recycled-content limit of mechanical recycling

Table 7. Material Factors Used in the Framework

Flow Factor	Description
R1b	Fraction of recycled waste bottles after collection
R1f	Fraction of recycled fiber after collected
U2	Maximum percentage of mechanically recycled resin used in bottle production
R2b	Fraction of PET bottles at material recovery facilities ending up in PET bales
R3b	Yield of PET flakes obtained from baled PET bottles
R3f	Yield of densified fiber from collected waste PET fiber
R4r	Yield of mechanically recycled resin from PET bottle flakes
R4h	Yield of chemically recycled resin from PET bottle flakes
R4m	Yield of upcycled PET resin from densified PET fiber
R5	Yield of bottle production from virgin and chemically recycled PET resin
R5r	Yield of bottle production from mechanically recycled PET resin
B	Fraction of PET flakes diverted to bottle recycling
E	Fraction of PET flakes in bottle-to-bottle recycling processed through mechanical recycling
D	Fraction of densified PET fiber diverted to bottle recycling

Analysis Approaches

Our first application of the framework employed a cradle-to-gate approach to compare the five production pathways using a functional unit of 1 kg of PET resin, as proposed by Gracida-Alvarez et al. (Forthcoming). In addition to the resource consumption and GHG emissions from each process stage, this comparison included the avoided impacts from diverting 1 kg of waste materials from traditional EOL management. The modeling of EOL assumed 80% of the waste is stored in landfills and the remaining 20% is incinerated with energy recovery (EPA 2020). The energy obtained from the incinerated PET waste is converted to electricity, assuming an efficiency of 25% (ANL n.d.), and it displaces electricity from the U.S. average grid mix. The net values of resource consumption and GHG emissions of each technology were obtained by subtracting the environmental impacts from the process and the avoided impacts from EOL management.

The second approach considered a system-level analysis, based on 2.6 million tonnes of bottles supplied to the U.S. market in 2017 (NAPCOR, APR 2018). After disposal, only 29% of the bottles are recycled and only 3% are recycled back to beverage bottles (NAPCOR, APR 2018). The 2017 state was chosen as the reference scenario for comparison of the environmental and circularity metrics of different circularity strategies. As the system was based on the mass of bottles supplied, the environmental and circularity metrics were reported on a per-bottle basis. The modeling of these strategies was set through scenarios that considered modifications of material factors, like recycling rates, and the inclusion of chemical recycling and upcycling technologies. The descriptions of the scenarios are presented in Table 8. Each scenario represented the implementation of a particular circularity strategy. For example, Scenario 2 analyzed the effect of increasing the recycling rate (R1b) to 90% through improved collection practices, as reported by the Oregon Beverage Recycling Cooperative (Bailey 2020). Scenario 3 looked at the substitution of chemical for mechanical recycling, while Scenario 4 integrated both. Scenarios 5 and 6 introduced resin produced from waste PET fibers to the system. The impacts of EOL management, as stated by the U.S. Environmental Protection Agency (EPA 2020), of the solid waste generated in the system were incorporated through comparisons of Scenarios 2–7 with Scenario 1, which has the highest solid waste generation and, therefore, the most electricity generated from combustion. The comparison accounted for the impacts of producing make-up electricity in Scenarios 2–7 to match the amount generated in Scenario 1 and the impacts of the management of waste that is not converted to electricity. Figure 15 presents a scheme of the elements incorporated in the framework for the system analysis.

Table 8. Scenarios Used in the Systems Analysis

Scenario	Description	Relevant Characteristics
1	Current state (reference Scenario)	Recycling rate (R1b) of 29% (Walzberg, et al. 2021) Waste is processed through mechanical recycling.
2	Increased mechanical recycling	Increasing recycling rate (R1b) from 29% to 90% (Iacovidou, et al. 2017) Waste is processed through mechanical recycling.
3	Increased chemical recycling	Increasing recycling rate (R1b) from 29% to 90% Waste is processed through chemical recycling.
4	Mechanical and chemical recycling	Increasing recycling rate (R1b) from 29% to 90% 50% of waste is processed through mechanical recycling and 50% through chemical recycling.
5	Mechanical recycling and upcycling	Upcycling is added to increased mechanical recycling technology (Scenario 2). Recycling rate of fibers (estimated): 20%
6	Mechanical recycling, chemical recycling and upcycling	Upcycling is added to increased mechanical and chemical recycling (Scenario 4). Recycling rate of fibers (estimated): 20%
7	Substitution of upcycling for virgin feedstock	Recycling rate is increased to avoid the use of virgin materials.

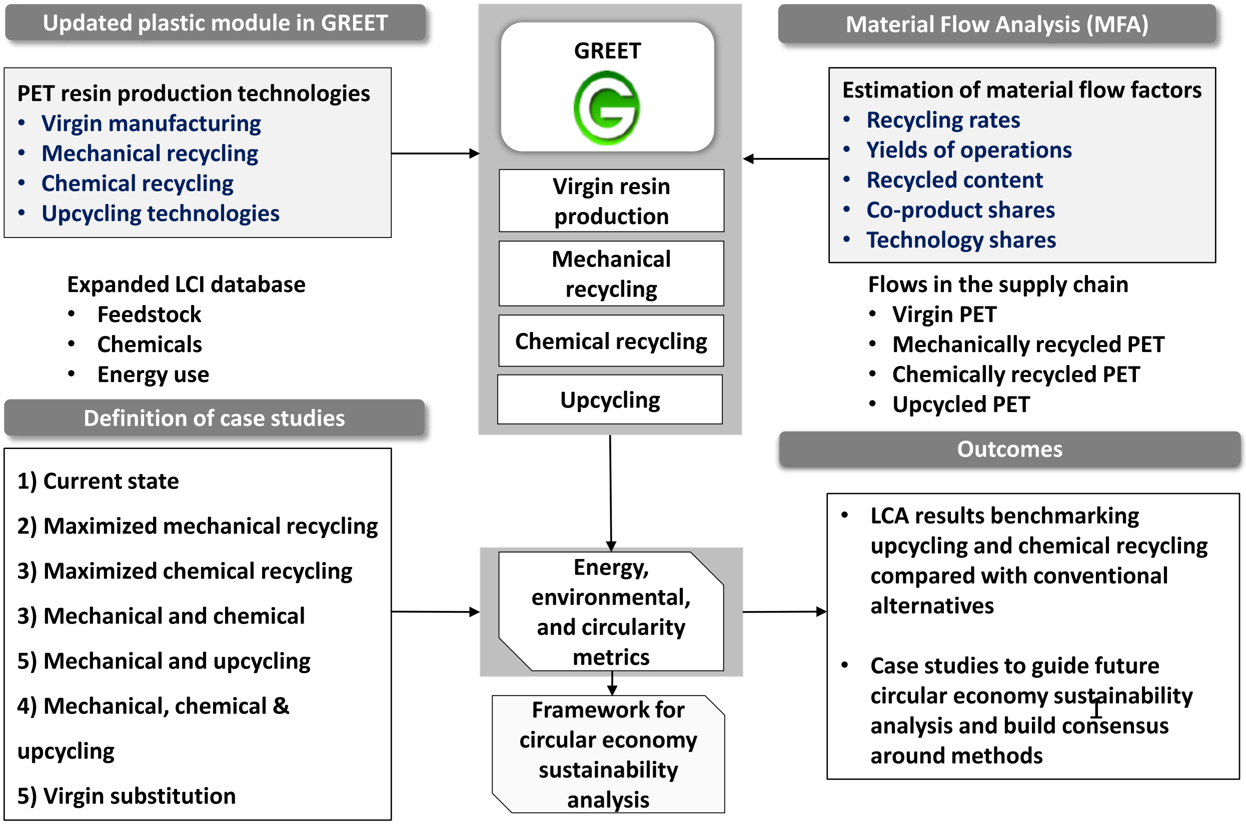

Figure 15. Integration of LCA and MFA in the CE sustainability analysis framework

Case Study Results

The results from the cradle-to-gate analysis are presented in Figure 16. The comparison of the total energy use shows that the production of virgin PET through the DMT route has the highest energy consumption (80 MJ/kg). This value is 24% higher than that of the virgin PET production route (esterification of PTA). Chemical recycling uses 61 MJ/kg of PET produced, which is 31% and 78% higher than upcycling and mechanical recycling respectively. According to Figure 16, the chemical recycling stage with the greatest contribution to total energy use (60% of the energy used) is the enzymatic hydrolysis, which requires energy for purification processes (i.e., distillation).

Chemical recycling is the PET production pathway with the highest net GHG emissions; they are 12% higher than in the DMT route and 27% higher than in the PTA route. Similarly, with respect to the total energy use, the stage with the highest contributions are enzymatic hydrolysis (64%) and polymerization (15%). In enzymatic hydrolysis, the GHG emissions are distributed as follows: 37% from natural gas, 31% from electricity, and 32% from chemicals (sodium hydroxide and sulfuric acid). The analysis of upcycling revealed that its net GHG emissions are 6% and 22% lower than virgin PET production from the PTA and DMT routes respectively. Mechanical recycling is the technology with the lowest GHG emissions of the group (84% lower than chemical recycling). In terms of water consumption, chemical recycling consumes three times the water of each virgin production as the enzymatic hydrolysis reaction takes place in an aqueous medium from which only 52% of the water is recycled.

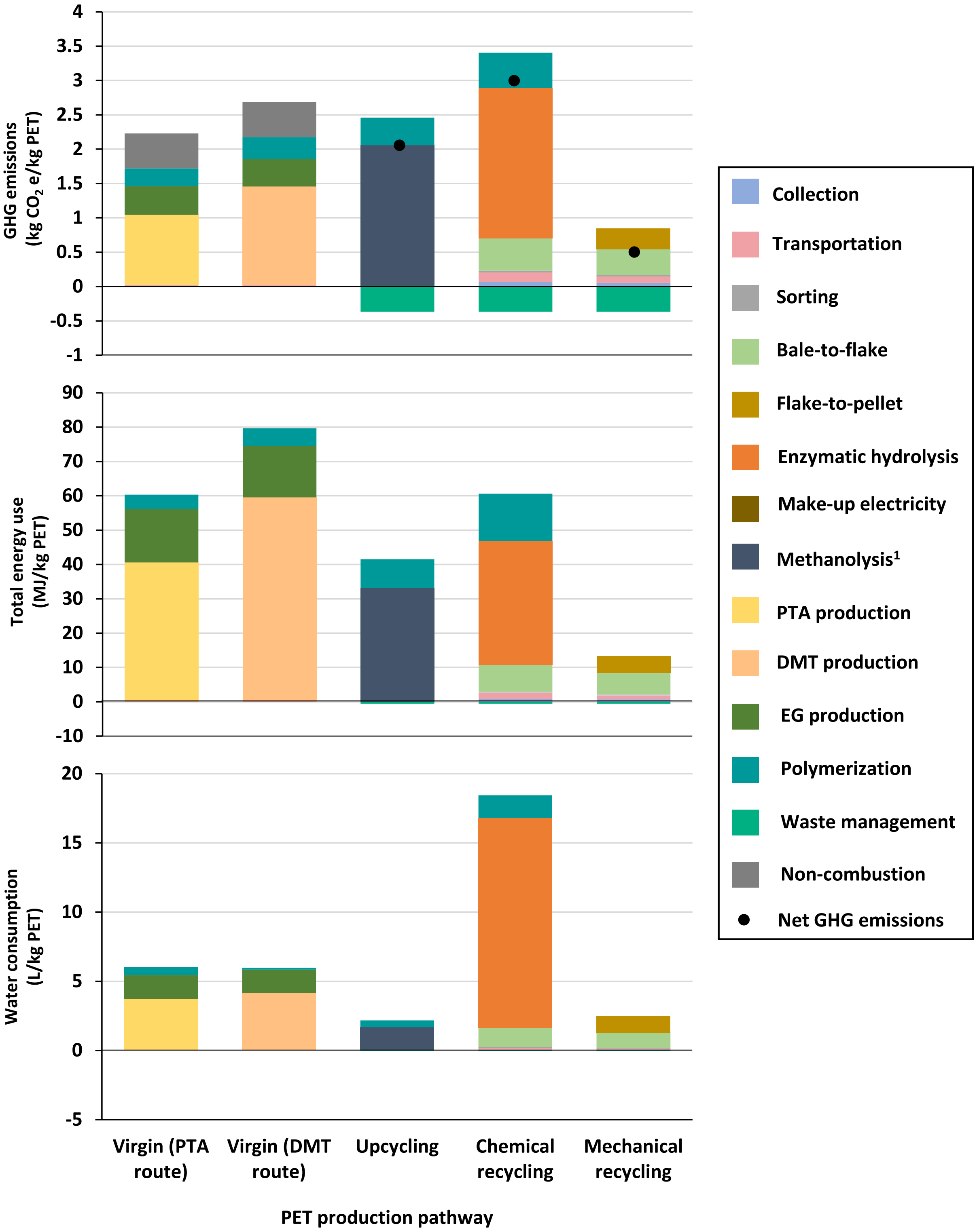

Figure 16. Comparison of the LCA metrics of the different PET production pathways

Methanolysis data have been aggregated to maintain confidentiality.
EG = ethylene glycol

Sankey diagrams generated from the MFA in the systems analysis (Figure 16) show a 16% decrease in both solid waste generation and virgin material use if the U.S. market for PET bottles shifts from the current linear economy (Scenario 1) to an economy where mechanical recycling is maximized and chemical recycling and upcycling are implemented (Scenario 6). When the analysis is narrowed to the bottle production supply chain (production of food-grade PET resin), the solid waste generation is reduced from 2.1 to 1.1 million tonnes (48% reduction) and the use of virgin materials from 2.9 to 1.3 million tonnes (56% reduction). Most of the material losses in both Scenarios 1 and 6 occur before the recycling operations as a result of the recycling rates and the yields of the sorting and reclaiming operations. After the use phase, 24% and 66% of the bottles are sent to EOL management in Scenario 1 and 6 respectively. Therefore, not only the recycling rate but also the yields of the different recycling operations have an important role in improving material restoration of the system.

The LCA results for the systems analysis are shown in Figure 18. The U.S. average virgin production assumes 90% of PET resin is produced from the PTA route and 10% of it is produced from the DMT route (Wang, et al. 2021). A comparison of the current state (Scenario 1) with other scenarios indicates that total energy use is similar to Scenario 3 and that Scenarios 7 and 5 have the lowest total energy consumption of all the scenarios (25% and 40% lower, respectively, than Scenario 1). The systems analysis indicates that the GHG emissions (43 g CO_2 e/bottle) of Scenario 3 are the highest of all scenarios because this scenario includes the two technologies with the highest GHG emissions (chemical recycling and virgin production). This value is 10% higher than that of the current state. Scenario 2, which maximizes mechanical recycling, has 25% and 11% lower GHG emissions than those of Scenarios 3 and 4, respectively, which incorporated chemical recycling. Therefore, from a GHG perspective, the use of mechanical recycling is more beneficial, as it has the lowest GHG emissions of all the PET production pathways (0.48 kg CO_2 e/kg PET resin), as shown in Figure 15. If upcycling is included (Scenario 5), the GHG emissions can be reduced by 1% compared to Scenario 2. Overall, all scenarios, with the exception of Scenario 3, show lower GHG emissions than the current state. Chemical recycling is very water intensive, so the water consumption in the system is considerably increased when chemical recycling is included, as seen in the results of Scenarios 3, 4, and 6, which show values 50%, 17%, and 11% higher, respectively, than the current state.

The evaluation of the circularity metrics (see Figure 18) shows that virgin material consumption and solid waste generation decrease with the integration of the different recycling technologies. Virgin material use decreases by 31% compared to the current state when the recycling rate is maximized to 90% (Scenario 2). However, the use of virgin material is decreased by 56% compared to the current state if chemical recycling and upcycling are incorporated (Scenario 6). This result is due to the increased contribution of other feedstock materials to PET resin production. The solid waste generation also decreases with increasing recycling rates (by 36% compared to the current state) and inclusion of the different recycling technologies (by 69% compared to the current state). In Scenarios 5, 6, and 7, which include upcycling, an additional credit for solid waste generation is considered, because the waste PET fibers used as raw materials were usually sent to landfill disposal. For Scenario 7, this factor actually results in the conservation of material within the system.

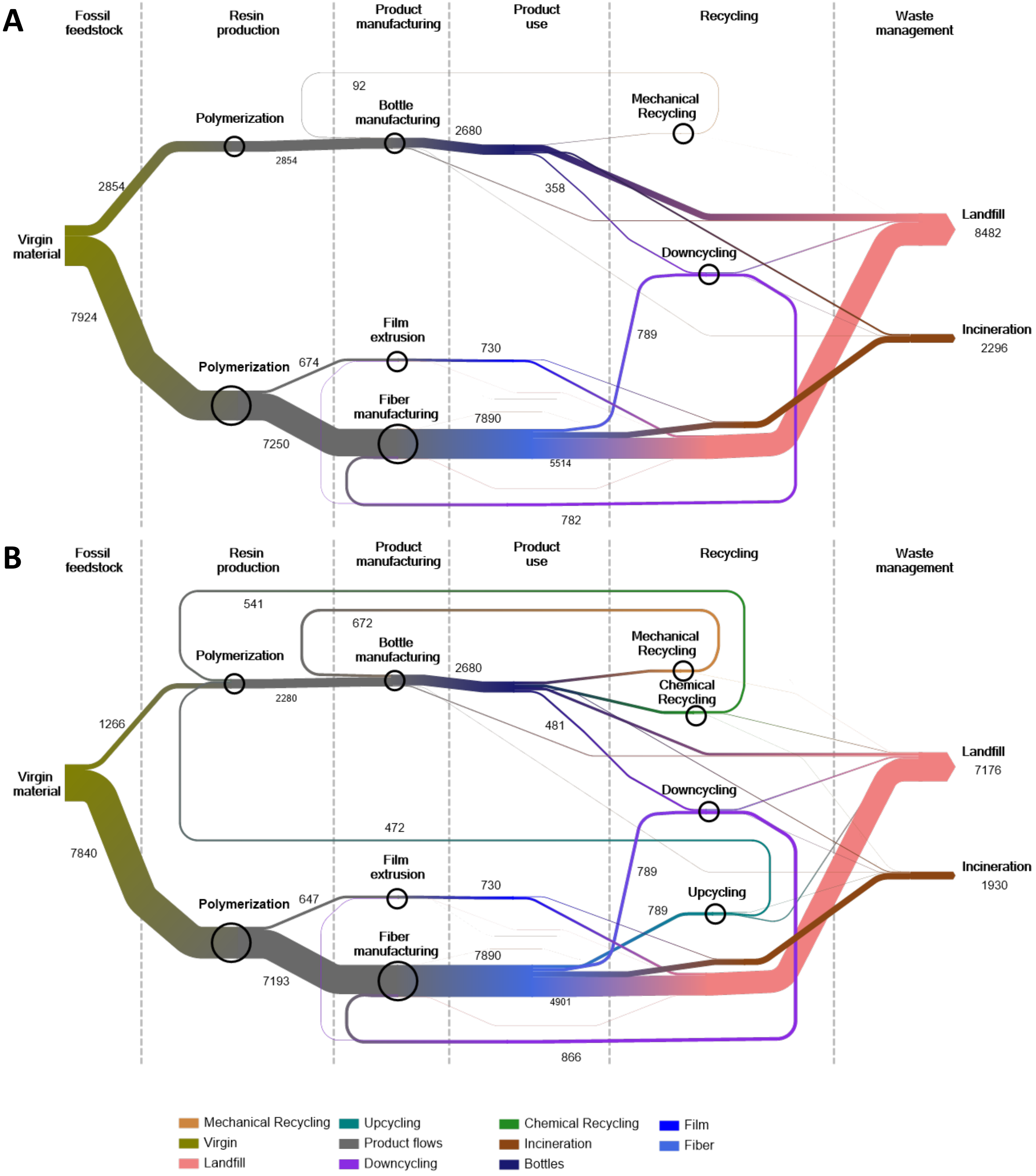

Figure 17. Sankey diagrams from the MFA: (A) Current state (Scenario 1) and (B) mechanical recycling, chemical recycling, and upcycling (Scenario 6)

Numbers in the diagrams indicate thousands of tonnes.

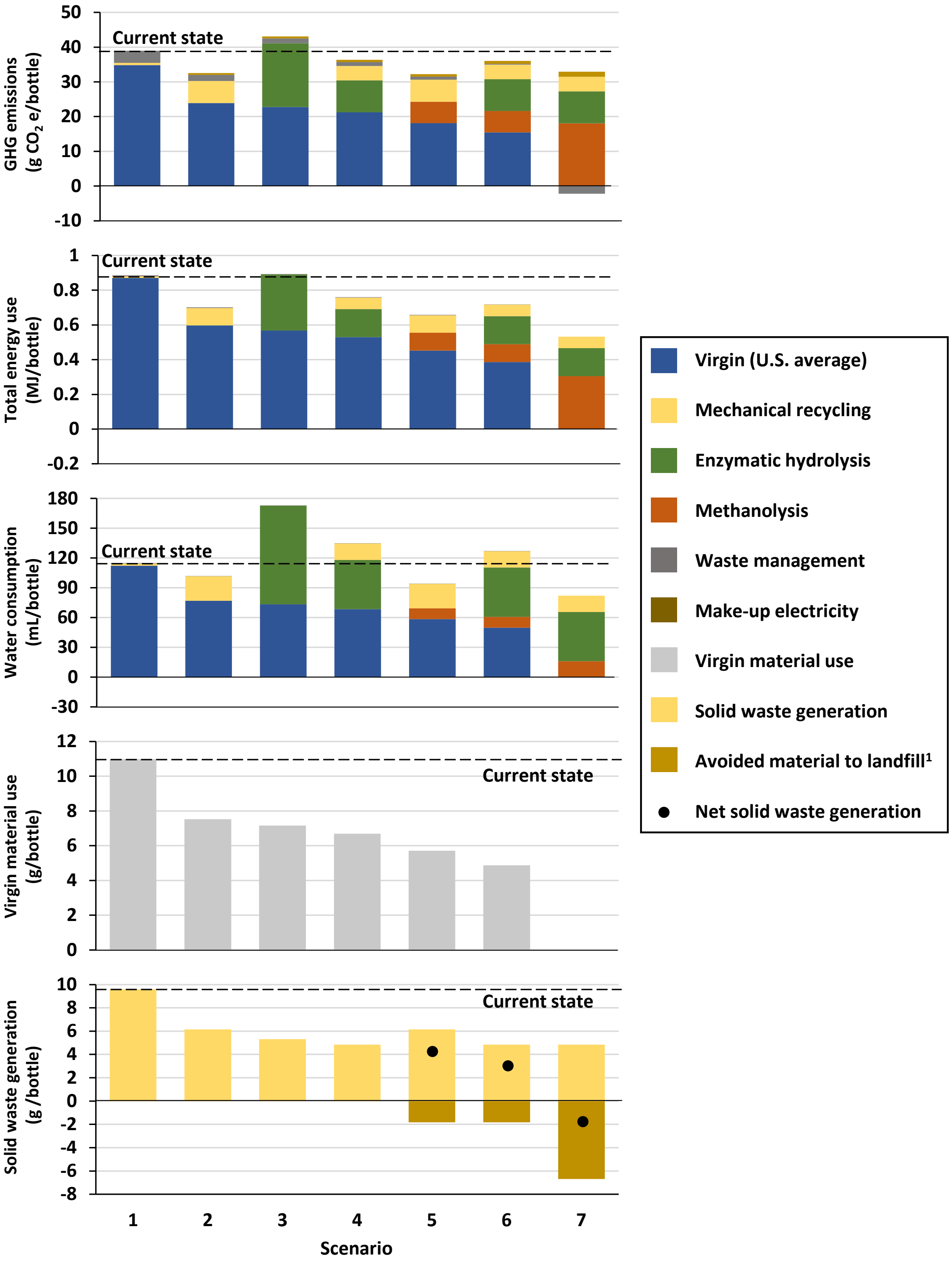

Figure 18. Comparison of the results of the LCA and circularity metrics of the different scenarios of CE strategies (Walzberg, et al. 2021)

In Scenario 7, upcycled resin is substituted for virgin material.
[1] Avoided material to landfill is due to upcycling.

6 Discussion

The case studies indicate that the CE sustainability analysis framework presented in this study can serve as a useful tool to inform sustainable industry development, identify key barriers and opportunities, and guide technology development. Results for PET recycling reveal that a successful CE depends on the coordination and performance of all key stages along the PET recycling supply chain. So far, much of the attention in the research community has been paid to various chemical recycling technologies (Chaudhari, et al. 2021, Horodytska, Kiritsis and Fullana 2020). However, our analysis indicates key factors like waste collection rate, efficiency of material recovery facility operation and resin reclaiming, and limitations on recycled content use in the final product could also affect the performance of PET recycling. These factors affect not only the circularity metrics (virgin material use and solid waste generation) but also the environmental impacts of the system. Lower efficiencies and collection rates imply larger amounts of feedstock materials processed, which increase the requirements for material and energy resources.

One contribution made by the study is to provide economy- and system-level modeling capabilities through the integration of LCA and MFA. Because the modeling framework leverages the extensive plastics-related databases and LCA capabilities in GREET, is well suited to comparing energy use and carbon intensities of novel and emerging technologies at the resin or product level. It is helpful to compare alternative technologies on an apples-to-apples basis. Evaluating the full life cycle of PET recycling, from used products collection to waste management, is critical for reliable and accurate benchmarking and environmental impact assessments. When scaling up novel technologies like enzymatic hydrolysis to the economy level, a relevant and interesting question would be what are the magnitudes of material, energy, and emission savings achievable through the addition of chemical recycling technologies (e.g., hydrolysis). Addition of MFA to the modeling framework helps to address this question.

In this study, several scale-up scenarios were assessed, including mechanical-recycling-oriented and chemical-recycling-oriented analysis. The results illustrate, at the system or economy level, the presence of trade-offs between the environmental impacts and the circularity metrics of the technologies. For example, chemical recycling increases the amount of recovered material but has greater environmental impacts than mechanical recycling. Thus, the combination of chemical and mechanical recycling increases the amount of recovered material while reducing the environmental impacts of the system as compared to current production practices. As observed, different technologies can be complementary to each other, making their combination more beneficial than relying on a single technology. Multisector interactions also influence the results, as demonstrated by the inclusion of upcycling. Technologies processing alternative waste materials provide benefits to the circularity metrics because they divert the flows of materials traditionally sent to EOL management for recycling. Moreover, the development of technologies to process alternative waste materials can improve the overall production yield of recycled resins and reduce the energy use in the system.

The results also reveal opportunities in a circularity strategy to reduce environmental impacts and to guide research and development efforts. Increasing the yield of chemical recycling, reclaiming, and sorting operations is one of the alternatives with potential reduction of the use of material and energy resources. Inclusion of separation, purification, and cleaning processes with more-efficient use of energy is an option that provides simultaneous reductions of energy use and GHG emissions. Making the transition to cleaner energy sources, by using electric grid mixes with high contributions of renewable sources or by generating heat with renewable natural gas, reduces the carbon footprint of the recycling technologies and processes involved. Through the framework described, it is also possible to understand that increasing recycling rates has an impact on material retention, but this strategy cannot be considered as the only driver to reach a full circular economy, as there are material losses involved in other processes (i.e., sorting at the material recovery facility).

The analysis of a complex system including production of virgin and recycled resins and circularity assessment requires the use of extensive data that can model the process stages from the extraction of fossil resources (i.e., crude oil and natural gas) to the manufacturing of bottles. The integration of such a large amount of data would not be possible without the use of the energy and material inventories available in GREET. Reliance on the GREET database resulted in focused efforts to update and disaggregate the information for virgin PET production and to incorporate the inventory data for new recycling technologies (mechanical recycling, chemical recycling, and upcycling) and values of the material factors used for the MFA. Similarly, the new data included in GREET to implement this case study will aid in performing other analyses involving PET production and recycling. Moreover, the framework structure can enable the simultaneous circularity and sustainability analysis of other plastic resins and products just by adding the inventory data and adapting the values of the material factors. The framework might also provide for the circularity analyses of other materials, which may need to consider the definitions of other factors.

Data acquisition for this study relied on publicly available information from government agencies, reports from recycling organizations, and peer-reviewed papers, and the data were continuously reviewed and evaluated to ensure their accuracy and consistency. The implementation of data included the processing of the different data sets to ensure their correspondence to the format used in GREET and accurate modeling. These activities ensured a fair and transparent comparison of the technologies included in the case study. Partnerships with industries were important in that aspect of the framework development: industry partners provided a point for quality assurance and judgment of the data and results of the analysis, suggested sources for data acquisition, and provided values of material factors employed in the MFA and operational data for the analysis of upcycling. Furthermore, the background supply chain information and energy data sets of GREET are updated annually, ensuring the inclusion of recent conditions and values of the electric grid mix and energy use of industrial processes.

Having a framework capable of accepting detailed parameter data—and connecting it to a combined LCA-MFA framework—is important to ensure accurate results and precise identification of the hotspots that will guide the implementation of CE strategies. Also, a clear focus on the objectives of the analysis, and an understanding of the capabilities of the available tools and data acquisition requirements, will enable the development of analysis frameworks that that can provide insightful and targeted results for circularity strategies.

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Appendix A. Research Questions EERE Tools are Designed to Answer, and CE Research Questions They Could Potentially Answer

Appendix Table 1. Summary of Research Questions EERE Tools are Designed to Answer, and CE Research Questions They Could Potentially Answer

Tool	Research Questions the Tool Answers	CE Research Questions the Tool Might Answer
Additive Manufacturing Energy Impacts Assessment Tool (AM)	n/a	n/a
Available Water Remaining in United States (AWARE-US)	What are the spatial-temporal water-stress impacts of water consumption scenarios?	What are the spatial-temporal water-stress impacts of ReX strategies?
Behavior, Energy, Autonomy, and Mobility (BEAM)	What are the mobility patterns and energy demand (fossil fuel and electricity) from adopting CE strategies in use of light duty vehicles?	What are detailed transportation energy consumption and mobility patterns under different future technology and behavioral scenarios?
Bio-based circular carbon economy Environmentally-extended Input-Output Model (BEIOM)	What are the socioeconomic and environmental trade-offs and benefits of plastics upcycling (versus virgin plastics)? What are the net socioeconomic and environmental trade-offs and benefits for different bioeconomy expansion scenarios? How do these effects vary across supply chain tiers (regional impacts)? What are the main contributing sectors of the economy or commodities that drive the results for specific metrics? How do the impacts change over time?	What is the U.S. national-level net impact (benefits and trade-offs across sustainability dimensions) of transitioning to a different CE paradigm? What are the resulting environmental and social justice implications (geographical and demographical trade-offs and benefits across sustainability dimensions)?
Bioeconomy Air emissions, Greenhouse gas emissions, and Energy use model (BioAGE)	What are the energy and environmental effects of bioeconomy at scale under different technology development and adoption scenarios?	What are the effects of scenarios for the implementation of ReX strategies on system-wide energy and environmental metrics?
Bioenergy Sustainability Tradeoffs Assessment Resource (BioSTAR)	n/a	n/a
BioVEST	How much cellulosic feedstock leads to significant improvements in water quality and carbon sequestration?	n/a

Tool	**Research Questions the Tool Answers**	**CE Research Questions the Tool Might Answer**
Circular Economy Agent-based model (CE ABM)	None (CE-focused tool)	What are the technical, economic, and market conditions that maximize value retention and minimize raw material inputs when applying CE strategies to energy-generating and energy-consuming technologies?
Circular Economy Capacity Expansion model (CECE)	What is the optimal geographic and temporal deployment of CE technologies that will enable the United States to reach a given CE goal?	What is the optimal geographic and temporal deployment of CE technologies that will enable the United States to reach a given CE goal?
Circular Economy Life cycle Assessment and Visualization Framework (CELAVI)	What are the environmental and economic impacts of transitioning to a CE for energy materials?	What are the environmental and economic impacts of transitioning to a CE for energy materials?
ComStock	How does commercial building stock use energy and how technologies and demand-side management strategies can improve that energy use pattern in the future?	What are the energy use and GHG emissions associated with different energy conservation measures or technology subsidization?
System Dynamics Model for Assessing **D**ynamic **R**are **E**arth Production, D**EM**and and U.S. Wind Energy Demand (DREEM)	Could the U.S. and Chinese supply could conceivably provide all the rare earth elements needed to satisfy demand from U.S. wind energy and other global NdFeB applications (e.g., electric vehicles, electronics)?	What are the circularity impacts on light rare earth elements, including Lanthanum, Cerium, Praseodymium, and Neodymium?
EverBatt (EBatt)	What are the cost and environmental impacts at each stage of a battery's life, from manufacture to recycle and back to manufacture with recycled materials?	How can enabling circularity of lithium-ion batteries by closed-loop recycling help reduce their cost and environmental impacts?
GeoSpatial Roadmap (GSR)	Where and how can environmental credits make biomass for energy profitable?	What is the magnitude of water quality improvement that is possible from animal waste digestion?
Global Critical Materials agent-based model (GCMat)	How to model decision-making at the individual market participant level which allows greater insight into how the decision rules used within each segment of the supply chain affect the overall critical materials market?	How do access to, and adoption of, technologies based on CE strategies by key players in the critical materials SC affect the CE transition of critical materials? How could reduced use of critical materials contribute to better resilience in the face of disruptions and less volatile prices? How could recycling pathways differ depending on whether a technology is being newly adopted, more mature, or even declining?

Tool	Research Questions the Tool Answers	CE Research Questions the Tool Might Answer
Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET)	What are the environmental impacts (life-cycle energy use by type, GHG emission, criteria air pollutant emissions, and water consumption) of various energy systems pathways?	n/a
Iron & Steel CE Model (ISCEM)	n/a	n/a
Life cycle Analysis Integration into Scalable Open-source Numerical models (LiAISON)	How can the systematic incorporation of integrated, i.e., interdependent energy and material system futures in the LCA of the technologies in focus can highlight the impacts of potential sectoral or upstream transitions/shifts (e.g., breakthrough technologies or consumption pattern changes) over time.	What are the spatiotemporally explicit impacts and trade-offs of transitioning to technological and systemic adoption of CE strategies over time?
Life cycle Industry GreenHouse gas, Technology and Energy through the Use Phase (LIGHTEnUP)	What are the material use, energy consumption, and CO_2 emission implications of adopting technologies within the U.S. manufacturing sector and the U.S. economy?	What are the material use, energy consumption, and CO_2 emission implications of adopting ReX strategies R0 through R9 within the U.S. manufacturing sector and the U.S. economy?
Lithium-ion Battery Resources Analysis model (LIBRA)	What are the supply chain risks and synergies? Scenario development an	How does battery chemistry affect the economics of battery recycling over time?
Market Acceptance of Advanced Automotive Technologies (MA3T)	What are the demand scenarios for various automotive powertrain technologies in response to changes in technologies, infrastructure, energy prices, consumer preferences, and policies?	n/a
Materials Flow through Industry (MFI)	What are the energy use and GHG emissions associated with a certain level of production of a commodity in the United States?	What are the energy use and GHG emissions associated with products and or technologies resulting from implementing CE strategies in industry?
Non-Light Duty Energy and GHG Emissions Accounting Tool (NEAT)	What are the energy and environmental impacts (full-fuel cycle energy use by type, GHG emission) at the regional and national levels of (1) adoption of alternative fuels and technologies in freight, (2) mode shifts (e.g., from truck to rail), and (3) use of mobility technologies in freight (e.g., platooning)? The model could be customized to consider the technology survival function, consider mode shifts for selected	What are the energy and emission impacts of extending life span of fuel technologies in freight?

Tool	Research Questions the Tool Answers	CE Research Questions the Tool Might Answer
	commodities and freight routes, and quantify the resulting energy and emission impacts.	
ParaChoice (PChoice)	For light-duty vehicles, what are (1) the potential for alternative fuel vehicles to penetrate the market, reduce light-duty vehicle emissions and petroleum consumption, and impact energy use and (2) the factors that influence alternative energy vehicle deployment and impact, the path to cleaner vehicles, tipping points for impactful penetration, and sensitivities? Heavy-Duty Vehicle Analysis goal: Mirror light-duty vehicle analysis capability to evaluate what is the potential for alternative fuel vehicles to increase freight hauling efficiency and reduce pollution?	What is the fleet level impact of increased alternative fuel vehicle use on emissions and equivalent fuel efficiency? What is the impact of increased fueling infrastructure utilization from shared light-duty heavy-duty vehicle usage on adoption? What are the adoption rates of alternative fuel vehicles in replacing incumbent technologies to meet transportation demand?
Photovoltaics in the Circular Economy (PViCE)	How to quantify and assign a value framework to efforts on redesign, reduction, replacement, reuse, recycling, and lifetime and reliability increases in the photovoltaics value chain?	How to implement circularity metrics, quantify, and assign a value framework to efforts on re-design, reduction, replacement, reusage, recycling, and lifetime and reliability increases of photovoltaics. Use the quantification of dynamic material flows to evaluate tradeoffs and prioritize CE strategies for energy technologies?
Planning and Operations Language for Agent-based Regional Integrated Simulation (POLARIS)	What are the transportation system management strategies involving emerging vehicle and information technologies?	How can we maximize people and goods movement with minimum cost, energy, life cycle impacts?
Plant Water Profiler Tool (PWater)	n/a	n/a
Regional Electric Vehicle Infrastructure Strategic Evolution (REVISE)	Where and when should charging stations be opened? How much capacity (number of plugs) should there be for each station? Who will use the systems, and who will not? What are the energy and environmental impacts of the answers to these questions?	n/a
Scalable Integrated Infrastructure Planning (SIIP)	How should infrastructure systems be schedule and operated under different conditions?	What are the operational values of different ReX strategies?

Tool	**Research Questions the Tool Answers**	**CE Research Questions the Tool Might Answer**
Scalable Linked Dynamic Equilibrium (SLiDE)	What are the net employment impacts of a high renewable energy future? How is trade impacted by low solar costs?	With further development, how does plastic recycling impact the petroleum sector?
UrbanOpt Advanced Analytics Platform (UrbanOpt)	n/a	n/a
VISION	What are the energy and environmental impacts (full-fuel cycle energy use by type, GHG emission) at regional and national level of (1) market penetration of different vehicle powertrain technologies, (2) use of various mobility technologies, and (3) adoption of alternative fuels? The model could be customized to consider the technology survival function, vehicle usage (e.g., vehicle miles traveled) per year or lifetime, elasticity to fuel price, and to quantify the resulting energy and emission impacts.	What are the energy and emission impacts of extending the life span of vehicle and fuel technologies, such as vehicle survival functions and annual vehicle miles?
Water Analysis Tool for Energy Resource (WATER)	What are the energy and water resource demand and availability for a specific region based on a water footprint methodology, including freshwater, and reclaimed municipal water resources?	What is the reuse potential of wastewater to produce goods and services?
Water Technoeconomic Assessment Pipe-Parity Platform (Water-TAP3)	What are the costs, energy and LCA analysis for water treatment and reuse opportunities?	What are the potential applications of recover, recycle, treatment and reuse strategies for waste and stranded water sources?

Appendix B. EERE Tools Reviewed for Modeling the CE

Appendix Table 2. EERE Tools Reviewed for Modeling the CE

Tool	Technology Areas	Hyperlink	Description
Additive Manufacturing Energy Impacts Assessment Tool (AM)	Additive manufacturing	https://energyefficiency.ornl.gov/wp-content/uploads/2018/09/AM-Energy-Impacts-Assessment-Tool-and-Case-Studies-Guidebook-FINAL-02262015.pdf	The Additive Manufacturing Energy Impacts Assessment tool, developed by ORNL, assesses the life cycle energy of an additively manufactured product by considering energy used in the material, manufacture, freight and distribution, use, and the disposal phases.
Available Water Remaining for the United States (AWARE-US)	Energy, food, and manufacturing systems that use a significant amount of water resource	https://greet.es.anl.gov/aware	Analysis of the environmental, social, or economics effects of bioenergy and bioproduct technologies across their entire life cycle.
Behavior, Energy, Autonomy, and Mobility (BEAM)	Transportation	https://github.com/LBNL-UCB-STI/beam	BEAM enables detailed analysis of the energy impacts of changing mobility trends as well as the potential impacts of electric vehicle adoption and the benefits of managing charging to support grid reliability and access emerging markets for grid flexibility services.
Bio-based circular carbon economy **E**nvironmentally-extended **I**nput-**O**utput **M**odel (BEIOM)	Biofuels, bioproducts, and plastics upcycling	https://bioenergymodels.nrel.gov/models/42/	BEIOM quantifies the net socio-economic and environmental effects of transitioning from the present U.S. economy to a new paradigm at national and regional levels. It is presently used to assess the net system effects across 18 different sustainability dimensions outlining the trade-offs and benefits between the present U.S. economy (baseline) and future bioeconomy scenarios consisting of near-commercial technology portfolios or individual emerging and/or breakthrough technologies at industrial scale. It is presently expanded to perform more detailed prospective analyses, accounting for cross-sectoral production and consumption shifts, as well as international or trade effects. The team is also scoping increased domestic specificity to detail potential geographic and demographic benefits and trade-offs (environmental and social equity questions).

Tool	Technology Areas	Hyperlink	Description
Bioeconomy AGE (BioAGE)	Biofuels, bioproducts, biopower, light-duty vehicles and heavy-duty vehicles of various fuel and powertrain technologies	https://bioenergymodels.nrel.gov/models/10/	Integrative scenario assessment of sector-wide energy and environmental effects of bioeconomy at scale.
Bioenergy Sustainability Tradeoffs Assessment Resource (BioSTAR)	Biofuels	https://bioenergykdf.net/content/biostar	Tool to quantify the costs and benefits of integrating cellulosic biomass production into U.S. landscapes. BioSTAR walks users through the evaluation of a suite of environmental and socioeconomic indicators that can be tailored to local conditions and stakeholder priorities. Progress toward individual sustainability indicator targets and potential tradeoffs between sustainability indicators can then be visualized across a set of feedstock production scenarios evaluated at the scale of the biomass supply shed.
BioVEST	Ecosystem services valuation, geospatial analysis	https://www.energy.gov/sites/prod/files/2019/04/f61/Visualizing%20Ecosystem%20Service%20Portfolios%20of%20Agricultural%20and%20Forestry%20Biomass_NL0022890.pdf	BioVEST includes data and spatial modeling tools needed to assign value to ecosystem services. The model creates value supply curves showing how much of supply has combined value from ecosystem services to be profitable if payments were available.
Circular economy agent-based model (CE ABM)	Photovoltaics, wind, and hard disk drives	https://github.com/NREL/ABSiCE	CE ABM is an agent-based modeling approach for studying circular economy strategies, starting with understanding which factors behind the relationships and decisions of system actors will help lead to increased circularity of product systems.
Circular Economy Capacity Expansion model (CECE)	Polymers (Industry)	Not yet publicly released	Seed laboratory directed R&D project with the goal of conceptualizing an economic model of CE material flow and quantifying the impact of expanding CE infrastructure on both conventional (fossil) and alternative material markets.
Circular Economy Life cycle Assessment and	Wind, but can be applied to many other systems	https://github.com/NREL/celavi	CELAVI hybridizes existing methods to meet the demands of modeling circularity transitions and associated impacts.

Tool	**Technology Areas**	**Hyperlink**	**Description**
Visualization Framework (CELAVI)			
ComStock	Industry, buildings	https://comstock.nrel.gov/	ComStock is a model that provides a high-fidelity building stock representation of U.S. commercial building stock with a realistic diversity of building characteristics.
System Dynamics Model for Assessing **D**ynamic **R**are **E**arth Production, D**EM**and and U.S. Wind Energy Demand (DREEM)	Rare earth elements, supply chain, wind, magnets, phosphors, catalysts, metallurgy, glass, ceramics, and polishing	https://github.com/IdahoLabResearch/DREEM	DREEM model estimates U.S. and Chinese rare earth element (REE) availability that could support U.S. direct-drive and other REE demand.
EverBatt (EBatt)	Batteries, but can be adapted to model other products	https://www.anl.gov/egs/everbatt	EverBatt is an Excel-based model that evaluates cost and environmental impacts for the various life cycle stages of a lithium-ion battery. It can be used to compare impacts of virgin batteries to those with recycled content, to compare processes, and to identify sensitivities to various parameters.
GeoSpatial Roadmap (GSR)	Geospatial	Not yet publicly released publicly	This web-based screening tool will host demand-side data with the goal of identifying promising watersheds for production of perennial feedstocks and/or biogas production from animal wastes. It will include geospatial user interface and prioritization algorithm.
Global Critical Materials agent-based model (GCMat)	Critical materials	https://doi.org/10.2172/1631454	GCMat provides capabilities to explore supply chain dynamics and uncertainty under scenarios of demand growth or shrinkage, technology adoption, supply disruptions, and trade policies and mitigation strategies of new supply sources, product substitution, consumer thrifting, and stockpiling. Supply chain participants from rare earth mining through final demand are modeled as interacting agents who make market decisions independently as time progresses. Two separate projects, one funded by AMO that focuses on recovery of RE materials from NiMH batteries, and one funded internally by Argonne focused on modeling of Li, Co and Ni use in Li-ion batteries, including recycling

Tool	Technology Areas	Hyperlink	Description
Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET)	Transportation, petroleum, natural gas, hydrogen, electricity, biofuels, waste-to-energy, e-fuels, agriculture, chemicals, vehicles, vehicle materials (e.g., metals, plastics, and fluids), battery, building materials/components/technologies (e.g., insulation, cement/concrete, steel, aluminum, walls, and lumber products), whole buildings	https://greet.es.anl.gov/	The GREET model is a publicly available life cycle analysis tool for consistently examining life cycle energy and environmental effects of a wide range of technologies in transportation, power, and material (vehicles, building, and others) products. It takes a holistic approach to model energy and environmental effects over the entire supply chain of a technology with process-level granularity. GREET currently has two models: the Fuel-Cycle Model focusing on transportation fuels and vehicle operation, and the Vehicle-Cycle Model focusing on vehicle materials, manufacturing, and recycling. GREET is available in two platforms: the Excel and the .net GREET model. It currently has over 40,000 registered users, and has been widely used by government agencies, industry, and academia for technology evaluation and policy making. GREET is an integral part of the transportation and bioenergy technology evaluation. High-quality, consistent, and peer-reviewed analyses and publications using GREET play a valuable role in identifying opportunities to improve sustainability of technologies, promoting clean and efficient vehicle and fuel technologies, and informing policies.
Iron & Steel CE Model (ISCEM)	Iron and steel	https://www.nrel.gov/docs/fy18osti/70609.pdf	Hybrid Input-Output model for exploring potential energy and material impacts of CE strategies for iron and steel sector
Life cycle Analysis Integration into Scalable Open-source Numerical models (LiAISON)	Industry, biofuels, renewable energy, and crosscutting technologies	Not yet publicly released	LiAISON computes temporally explicit life cycle impacts and resource uses for selected technologies (foreground) in a dynamic system context (background) out to 2100. This reproducible and open-source coded framework can show potential environmental tradeoffs over an extended time horizon, which is important specifically for new and emerging technologies whose large-scale impacts will take shape only in the distant future. The systematic incorporation of integrated, i.e., interdependent energy and material system futures in the LCA of the technologies in focus can highlight the impacts of potential sectoral or upstream transitions or shifts (e.g., breakthrough technologies or consumption pattern changes) over time. At present, the integrated futures or background scenarios are derived from integrated assessment models (IAM) in the shared-socioeconomic pathways (SSP) and representative concentration pathways (RCP) matrix. Future versions of LiAISON are planned to be able to use

Tool	Technology Areas	Hyperlink	Description
			scenarios from other models as well. LiAISON is a complementary capability to single point-in-time technology LCAs, utilizing process-based life cycle inventories (LCIs) and putting them in a dynamic system context for informed decision support. It leverages peer-reviewed methods and code and aims to eventually utilize open source LCI databases of the Federal LCA Commons.
Life cycle Industry Greenhouse Gas, Technology and Energy through the Use Phase (LIGHTEnUP)	Industry	https://doi.org/10.2172/1345200	Life cycle Industry GreenHouse gas Technology and Energy through the Use Phase (LIGHTEnUP) model is used to forecast both the manufacturing sector and product life cycle energy consumption implications of manufactured products across the U.S. economy.
Lithium-ion Battery Resources Analysis model (LIBRA)	Batteries, energy storage	https://www.nrel.gov/transportation/libra.html	LIBRA is a system dynamics model that evaluates the macro-economic viability of the battery manufacturing, reuse, and recycling industries across the global supply chain under differing dynamic conditions
Market Acceptance of Advanced Automotive Technologies (MA3T)	Vehicles	https://teem.ornl.gov/ma3t.shtml	MA3T simulates how the market for advanced vehicle technologies could potentially change depending on several technological, behavioral, and economic variables, including technological learning by doing, range anxiety, access to recharging points, daily driving patterns, and willingness to accept new technologies
Materials Flow through Industry (MFI)	Industry	https://www.nrel.gov/manufacturing/mfi-modeling-tool.html	The MFI tool is a linear network model of the U.S. industrial sector that tracks the material and energy demands from manufacturing supply chains.
Non-light duty Energy and GHG Emissions Accounting Tool (NEAT)	Freight	https://www.anl.gov/es/neat-tool-download	NEAT provides estimates of the potential end-use energy consumption, upstream energy consumption, and GHG emissions impacts through 2050 of a Base Case and user defined alternative case(s) relating to five domestic freight carrying modes and their use of alternative fuels. The five modes are: (1) Intercity freight-carrying Trucks, (2) Freight Rail, (3) Domestic Freight Marine, (4) Domestic Freight Aviation, and (5) Pipeline. The tool consists of a Microsoft Excel© workbook that contains Base Case estimates of U.S. freight mode energy use and carbon emissions to 2050. This file can be modified to reflect alternative assumptions about commodity ton-mile changes, mode share changes, modal energy intensity changes,

Tool	Technology Areas	Hyperlink	Description
			alternative fuel market penetration, and electricity generation mix for pipeline compressors. Base Case which is calibrated to match Energy Information Administration's Annual Energy Outlook.
ParaChoice (PChoice)	Vehicles	https://prod-ng.sandia.gov/techlib-noauth/access-control.cgi/2017/1713263r.pdf	Objective is to provide system-level analysis of the dynamics among the light and heavy-duty vehicle (LDV and HDV) fleets, fuels, infrastructure mix, and emissions
Photovoltaics in the Circular Economy (PViCE)	Photovoltaics, energy storage systems	https://github.com/NREL/PV_ICE	PViCE estimates the impact of re-design, reduce, replace, reuse, recycle, and lifetime and reliability extension of PV systems. It can also quantify the material and energy impacts of PV system designs, lifetime, reliability, and disposal.
Planning and Operations Language for Agent-based Regional Integrated Simulation (POLARIS)	Transportation, electric vehicle supply equipment, and grid demand for plug-in electric vehicles	https://www.anl.gov/es/polaris-transportation-system-simulation-tool	POLARIS is a high-performance, open-source agent-based modeling framework designed for simulating large-scale transportation systems. As an integrated network-demand model, all aspects of travel decisions (departure time, destination choice, planning and rescheduling as well as route choices) and travel execution (traffic flow, transit simulation, fleet movements) are modeled simultaneously to estimate the energy impact of vehicle technologies and mobility services at a range of scales (neighborhood to metropolitan region). POLARIS is integrated with powertrain simulator Autonomie to perform regional energy use analysis and GREET for LCA.
Plant Water Profiler Tool (PWater)	Industry	https://www.energy.gov/eere/amo/plant-water-profiler-tool-excel-version-10-pwpex-v10	The Plant Water Profiler Tool helps an organization understand how water is being procured and consumed at its plant and identifies potential water and cost savings. The PWP Tool helps break down the water intake, water consumption, and true cost of all water-using systems in a plant. It quantifies potential water savings that can be achieved from minimizing water loss and increasing water recirculation
Regional Electric Vehicle Infrastructure Strategic Evolution (REVISE)	Vehicles, charging Infrastructure	https://github.com/xiefei0117/REVISE-national-charging-infrastructure-model	A long-term multiyear inter-city corridor public charging infrastructure planning optimization framework. It provides scenario analysis on infrastructure requirement (station layouts) and effectiveness (travelers' usage) based on VTO technology, social, and economic assumptions

Tool	Technology Areas	Hyperlink	Description
Scalable Integrated Infrastructure Planning (SIIP)	Power systems (main), other infrastructure systems (less mature)	https://github.com/NREL-SIIP	Modular, interoperable, modeling components that define infrastructure modeling problems informed by system data.
Scalable Linked Dynamic Equilibrium (SLiDE)	Economic market systems	https://github.com/nrel/slide	SLiDE is a computational general equilibrium model capable of producing defensible net employment, trade, welfare, and wage estimates.
UrbanOpt Advanced Analytics Platform (UrbanOpt)	Buildings, infrastructure	https://www.nrel.gov/buildings/urbanopt.html	URBANopt is composed of several modules that can be customized to integrate with other tools and generate new workflows to perform urban environmental design tasks, such as capturing interactions between individual buildings, district energy systems, distributed energy resources, and the electric distribution grid.
VISION	Vehicles	https://www.anl.gov/es/vision-model	VISION provides estimates of the potential energy use, oil use and GHG emissions of advanced light- and heavy-duty vehicle technologies and alternative fuels through the year 2050 for scenario analysis. The major inputs are vehicle market penetration, vehicle efficiency, vehicle miles traveled, and vehicle survival rates, etc., while the major outputs are full-fuel cycle energy consumption by fuel type, vehicle class and vehicle powertrain type. The tool consists of a Microsoft Excel© workbook that contains base Case which is calibrated to match Energy Information Administration’s Annual Energy Outlook.
Water Analysis Tool for Energy Resources (WATER)	Biofuels	https://water.es.anl.gov/	WATER simulates geospatial-explicit water footprint for production pathways and regional scenarios at county, state, and region levels for the United States in an online platform; estimates impact of water use on regional water availability to other economic sectors by using a water availability index
Water Technoeconomic Assessment Pipe-Parity Platform (Water-TAP3)	Industry	https://github.com/NREL/WaterTAP3	NAWI is developing Water-TAP3 to facilitate consistent technoeconomic assessments of desalination treatment trains. Water-TAP3 is intended to be an analytically robust platform to evaluate water technology cost, energy, environmental, and resiliency tradeoffs across different water sources, sectors, and scales.