DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

Biobased and Biobenign, an Environmental Reference Framework for Product Design: RIPE *(**R**esponsible **I**nnovation for bio**P**lastics in the **E**nvironment)*

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Technology Area Session

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This presentation does not contain any proprietary, confidential, or otherwise restricted information

PROJECT OVERVIEW

- ***Problem***: Most used plastics are discarded, many “leak” to environment
  - Scale: US generates most waste *(~50M t/yr in 2016*), ranks 3rd in coastal litter
  - Concerns: Persistence, ecological & health implications, resource linearity
  - Need: Environmentally benign plastics

- ***Our goal***: Provide environmental reference framework to enable developers at the bench to consider post-use fate at the outset, as part of bioplastics design
  - ➢ Toward new bioplastics that excel in use *and* post-use performance, advancing the EERE/BETO bioeconomy initiative, plastics innovation challenge, analysis & sustainability platform

- ***Current situation***: Product design largely focuses on use, key data are limited & scattered
  - Lack systematic approach for considering polymer after-life up front

- ***Importance***: Advance the bioeconomy and circular economy, improve recyclability-upcyclability & reduce future environmental liabilities, strengthen bioproduct adoption and industry competitiveness

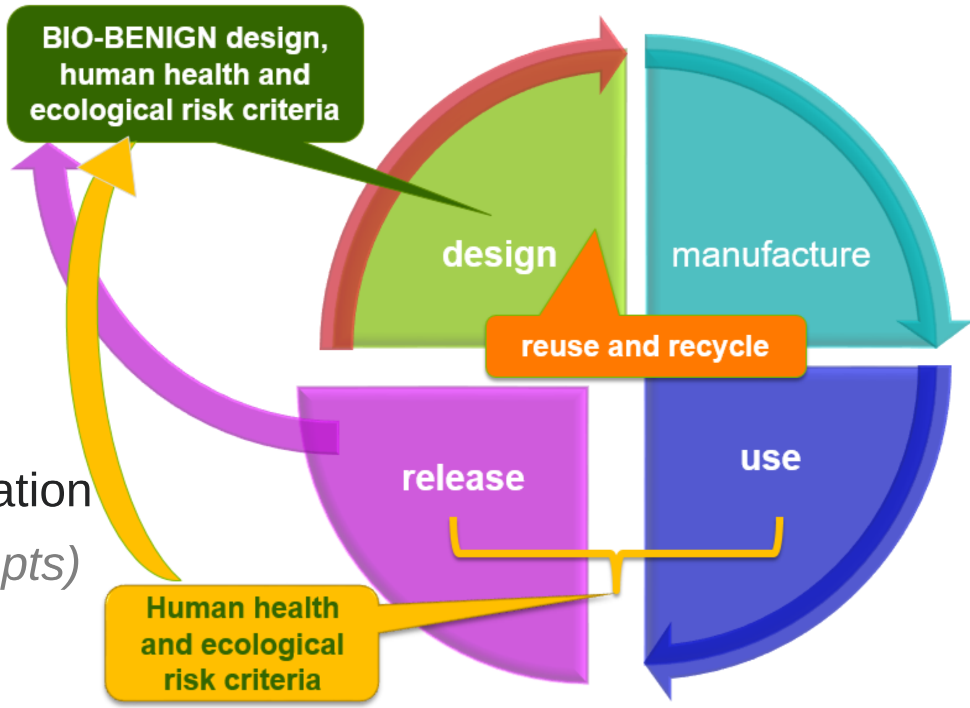
RESPONSIBLE INNOVATION FOR bioPLASTICS IN THE ENVIRONMENT

Environmental reference framework

- *Why?* Enable environmentally responsible design
  - Reduce environmental footprint, avoid future liability *(bisphenol A, per/polyfluoroalkyl substances)*
  - Strengthen bioproduct adoption & industry competitiveness
- *How?* Apply predictive environmental understanding to propel innovation
  - Incorporate human & eco risk in performance criteria at design phase

Elements

- **Disposition**
  - *What?* End-of-life path *(source of releases)*
- **Environmental fate**
  - *What?* Polymer composition, setting characteristics
  - *Where?* Transport, mobility
  - *When?* Persistence / degradation / phys-chem-bio transformation
- **Risk:** Eco & human health *(mixtures, cumulative risk concepts)*
  - *How?* Exposures, bioaccumulation
  - *How bad?* Effects, toxicity



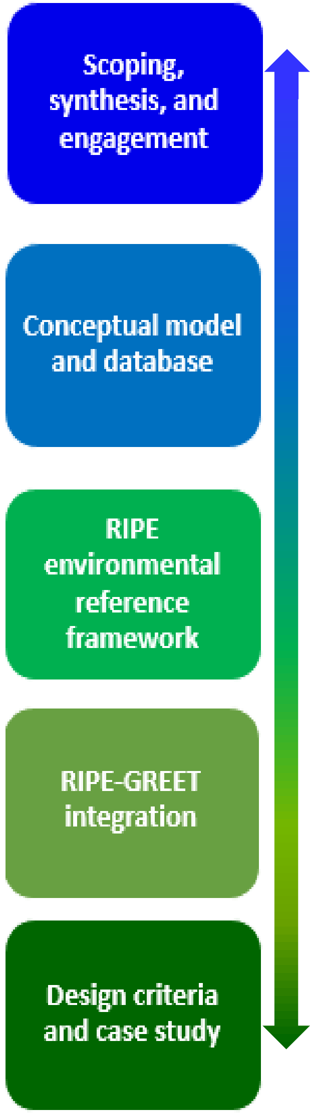
1 – MANAGEMENT

- **Critical success factors**
  - Incorporating stakeholder inputs to address needs
  - Synthesizing information from multiple sources to build framework
  - ➢ *Helping specific part of bioeconomy: bioproducts-bioplastics*

- **Progress measurement**
  - Tracking milestones, reporting monthly progress, team & collaborator meetings
  - Go/no go decision, redirect if indicated
- **Communication and collaboration**
  - Projects: *BETO competitive awards*: ResIn/Northwestern, BOTTLE/NREL; *AMO*: food waste to film
  - Stakeholders: Agencies, industry, universities, non-governmental organizations
- **Project risks and approach to mitigate**
  - Stakeholder engagement: Provide opportunities for regular input *(workshop & follow-on interactions)*
  - Data availability: If lacking, pursue analogues & develop surrogates
- **Project team structure**
  - Principal investigator (PI): M. Cristina Negri — overall project direction
  - Co-PI: Margaret MacDonell — day-to-day operations, technical approach
  - Framework modeler: Minh Vo — structure framework
  - Database: Chris Rademacher, Khanh Nguyen+ — extract & integrate data

2 – APPROACH

- **Technical approach for achieving goals**
  - Implementation: Phased & iterative *(5 tasks)*
  - Collaboration: Practical context via insights & leveraging *(e.g., databases, toxicity testing)*
  - Demonstration: Testing to refine components, linkages
  - Application: Illustrate practical case, in coordination with BETO-stakeholders
- **Top potential challenges**
  - Data availability: Missing, limited (proprietary), scattered, discordant
  - Buy-in: Stakeholder tradeoffs, adaptable to needs *(e.g., weightings, multiple indices)*
- **Go/No-Go decision point**
  - *Go*: Have 10% of data needed to test conceptual model
- **Technical metrics used to measure progress**
  - Extent of data & information sources tapped, thematic coverage of conceptual model
  - Variety of stakeholders engaged, range of inputs received
  - Type of application case enabled



3 – IMPACT

- **Anticipated impact on the state of technology and/or industry**

  - Bioproduct developers (& broader community interested in environmentally friendly bioplastics) will have a tool to consider *post-use fate* during design

- **Disseminating results**

  - Engaging stakeholders to inform project deliverables

    - Discussed early concepts with 50 stakeholders in highly interactive virtual workshop, valuable suggestions are being incorporated into framework development

  - Sharing progress with scientific & technical community

    - 2 international conferences: 12 presentations & 5 proceedings papers
      - – Environmental Informatics (Sep 2020)
      - – Society for Risk Analysis (Dec 2020)

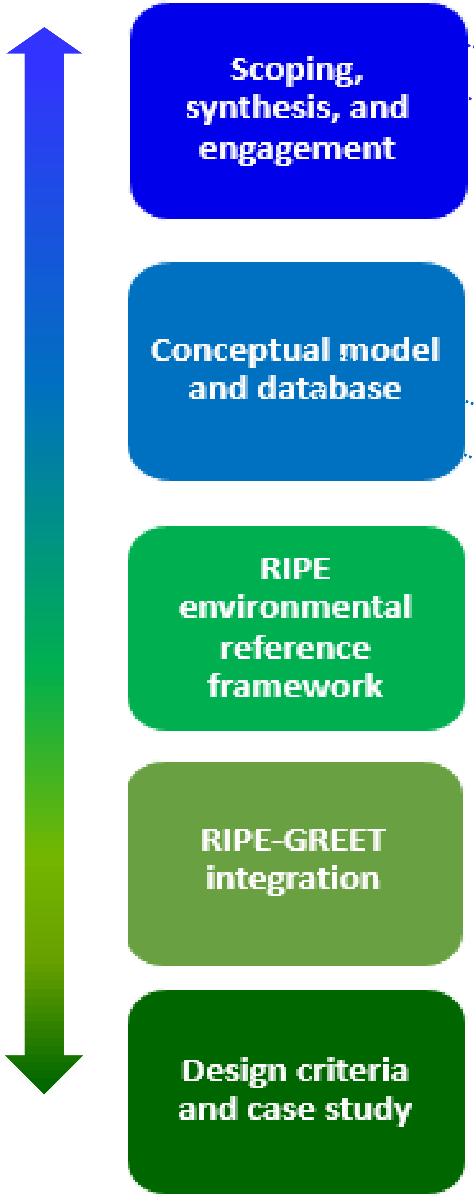
enviroinfo

(Cyprus, virtual)

SRA 2020 Risk Science for Sustainability December 13 - 17

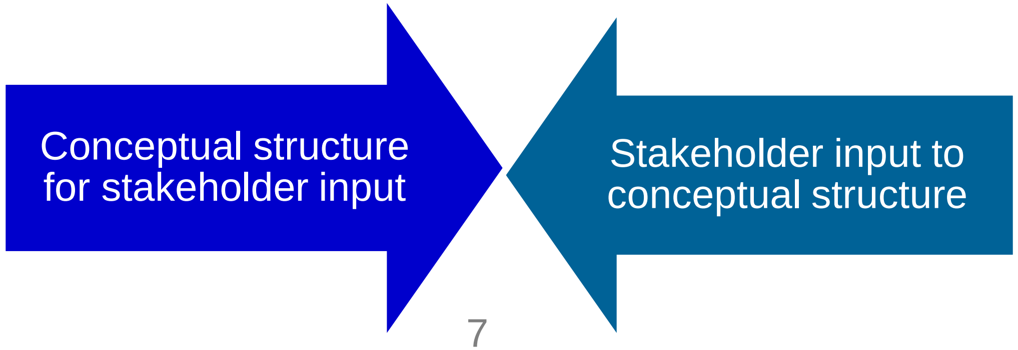
(Washington DC, virtual)

4 – PROGRESS AND OUTCOMES



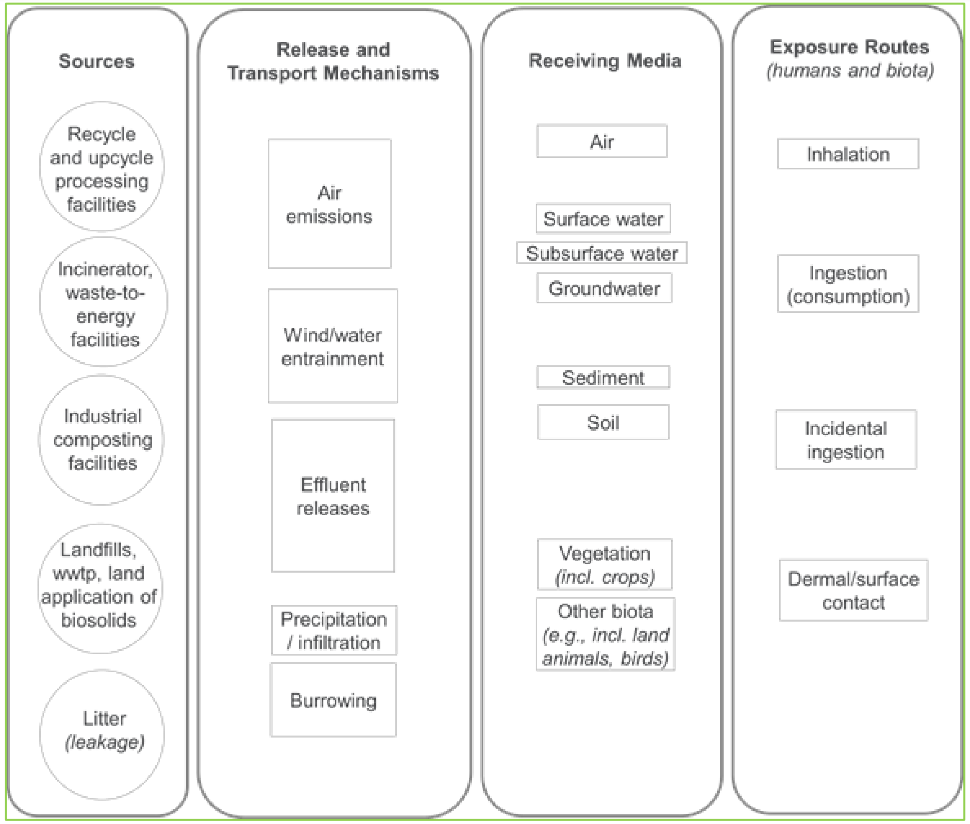
Focus on two tasks in 2020

- **Task 1**
  - literature search & synthesis
  - RIPE stakeholder workshop
- **Task 2**
  - conceptual exposure model for post-use plastics
  - data schema to guide database plan
- *Need to build both at same time*:



4 – PROGRESS AND OUTCOMES

- Progress on schedule, no risk mitigation needed to date
- Accomplishments, including key milestones:
  - Conceptual exposure model: *Organizing themes for database*
  - Data schema: *Informing database structure*
  - Stakeholder workshop: *Gaining insights & buy-in*
  - Initial synthesis of state of knowledge: *Framing the framework*

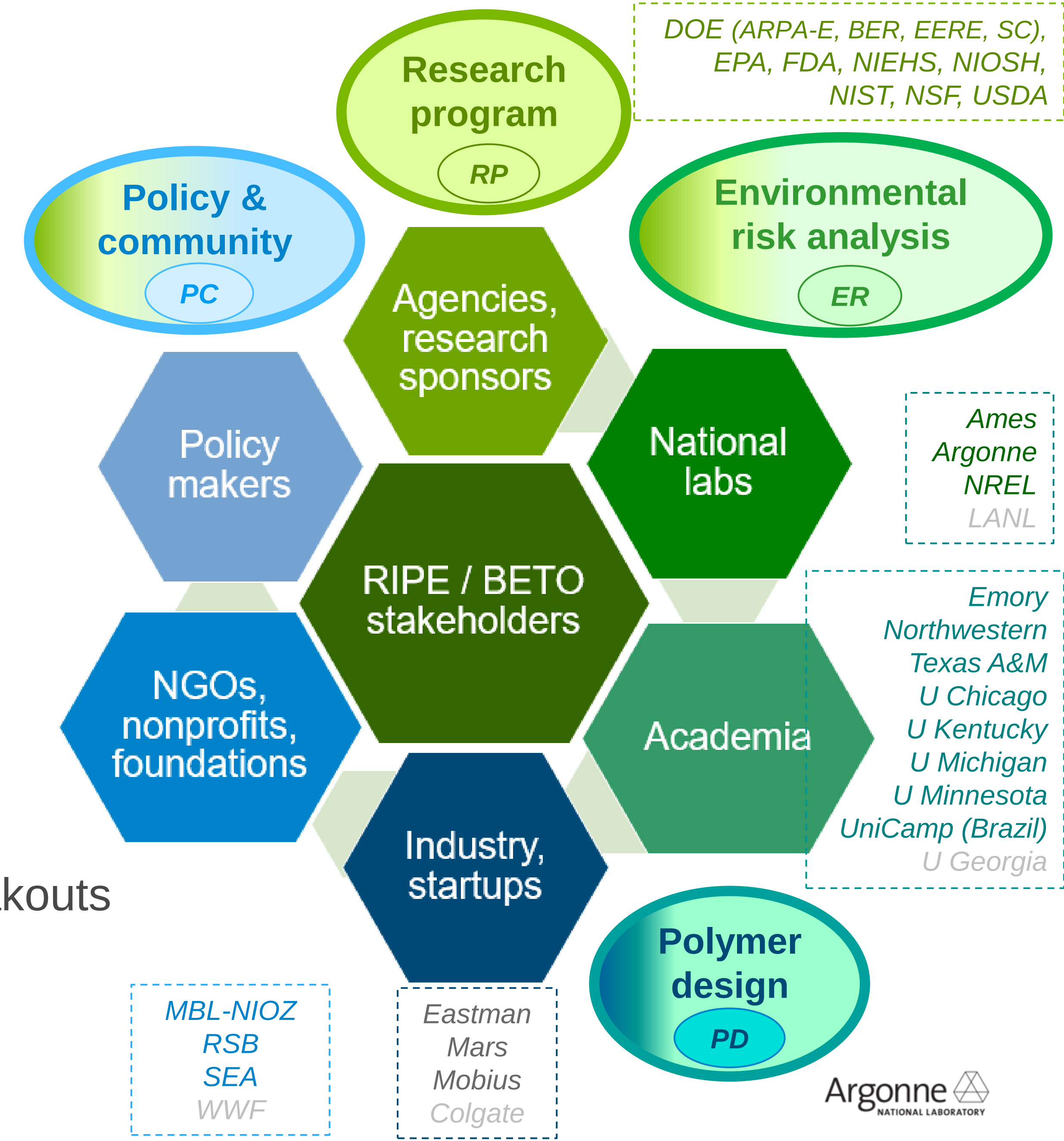


- Tasks leading to technical accomplishments:
  - Extensive planning for stakeholder workshop, collaborator network
    - ➢ User needs & approach options: refined framework concept
  - Literature & database syntheses inform conceptual model & data schema
    - ➢ Foundation for environmental reference framework & database

RIPE STAKEHOLDER WORKSHOP

- **Objectives**
  - Dialogue with those interested in this tool: range of sectors, perspectives, needs
  - Share what we're building & how can help; benefit of data-driven choice for downstream
  - Get input into needed functions of RIPE
  - Create connections to progress together

- **Planning & implementation**
  - 50 experts, 4 perspectives
  - 2 panels *(framing & agencies),* interactive breakouts
  - facilitated by Community@Work

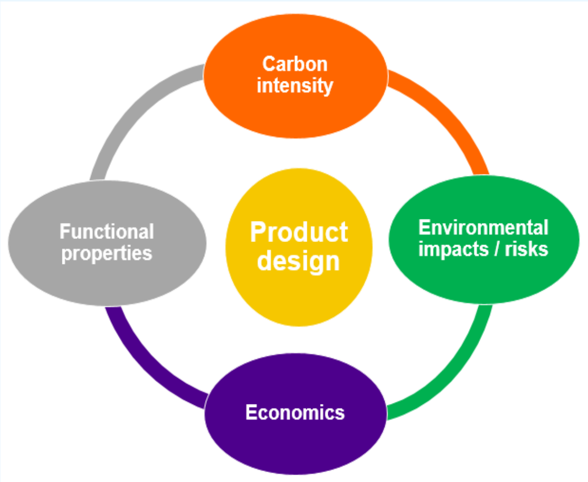


EXAMPLE: MULTIPLE STAKEHOLDERS & PROCESS STAGES

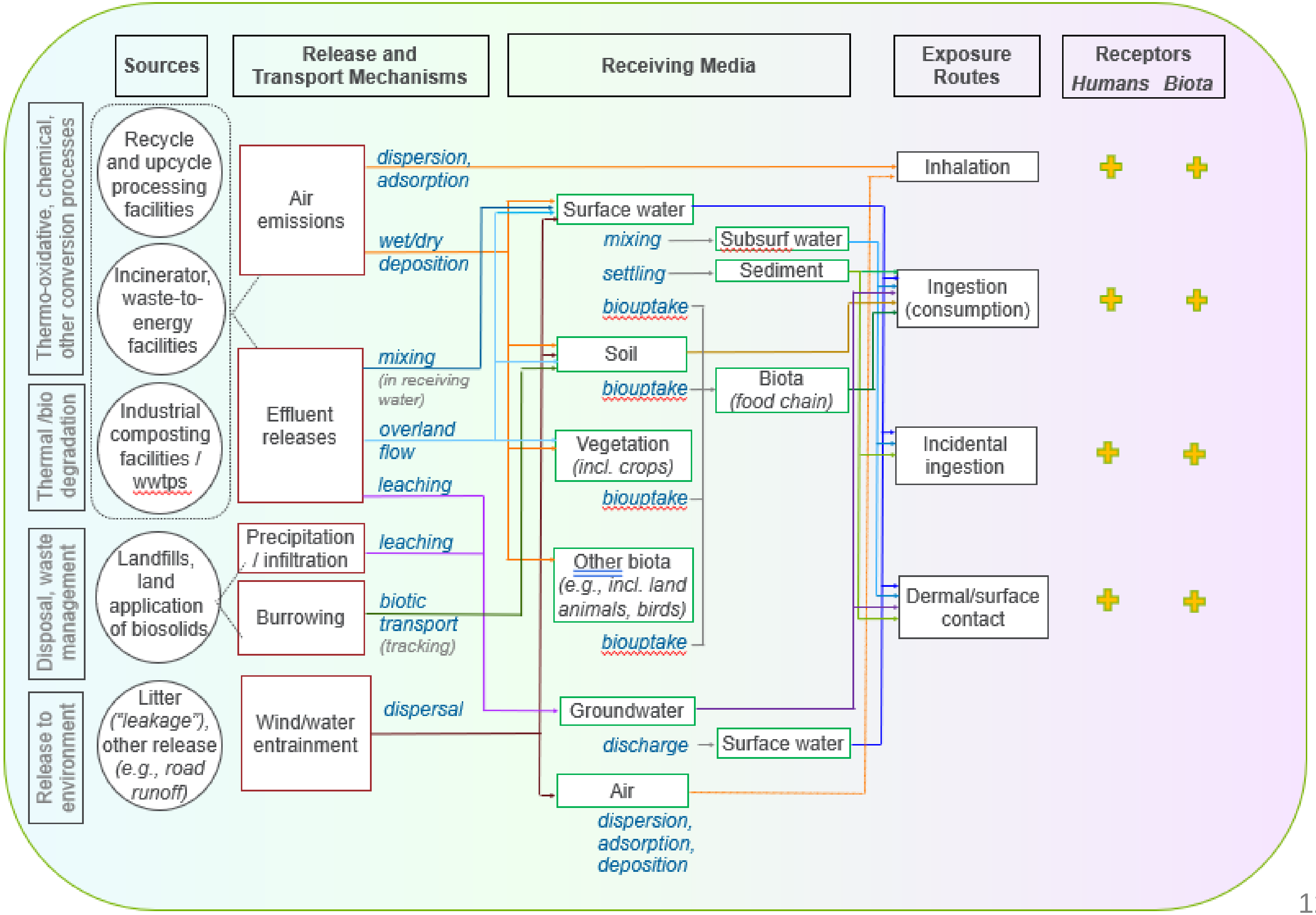
What answers do you need from this tool?	**Intended Application/ Anticipated Product Use**	**Exploration**	**Screening & Design**	**Testing & Validation**	**Sourcing & Production**	**Disposition & Afterlife**
	Policy & Community PC	***Polymer Design*** PD	***Polymer Design*** PD	***Research Programming*** RP	***Policy & Community*** PC	***Environmental Risk Analysis*** ER
Examples from different perspectives:	What polymer composition could be more "biofriendly" for a new single-use plastic?	What kinds of uses are best suited for a new polymer with low crystallinity and high melting point?	What polymer/ additive combination will provide sufficiently high heat resistance for use in making an innovative tire?	Could a compostability certification metric for large-scale production be downscaled to serve as a screening indicator for small amounts at the bench scale?	What byproducts could be anticipated from the manufacturing process for this new polymer, and could they be hazardous?	Will this new polymer naturally degrade? in what setting? *(e.g., inland surface water, silty soil, ocean floor?)* -- how? how much, over how long? to what fate products? could those cause harm? to what organism/system? at what exposure level?

STAKEHOLDER INPUTS INFORM RIPE OBJECTIVES

Themes	RIPE Objectives	Stakeholder Inputs
Circularity of man-made & natural systems	RI paradigm: end of life *(EOL)* at design stage	Pursue system-level analysis
	Address multiple circularities: use **+** post-use performance	Needs vertically integrated basic research *(from feedstock sourcing to conversion, use, & post-use)*
	Enable design of biofriendly plastics, improve re/upcycling	Biodegradability as fail-safe option
Tradeoffs *through* EOL	Arm developers with way to reduce future environmental liabilities	Better understand disposition-fate paths to develop optimal choices, minimize unfavorable tradeoffs
	Enhance bioproduct adoption & industry competitiveness	Varied community; good / bad differs *(pulling one lever can harm another)*
		Collaboration key! define terms, cases



STRUCTURED APPROACH: CONCEPTUAL EXPOSURE MODEL



RISK ANALYSIS CONTEXT: EXPOSURES & EFFECTS

Intake

$$\textit{Risk} = \text{Concentration} \times \frac{(IR \sim ET \times EF \times ED)}{BW \times AT} \ {*}/ \ \text{Tox Value}$$

cancer risk, noncancer hazard index current / future

Risk Characterization

chemical concentration from measurements and modeling (over time)

Data Collection and Evaluation

scenario-specific **intake parameters**

Exposure Assessment

toxicity value: chemical-specific and medium/route-specific (slope factor or unit risk; reference dose or concentration)

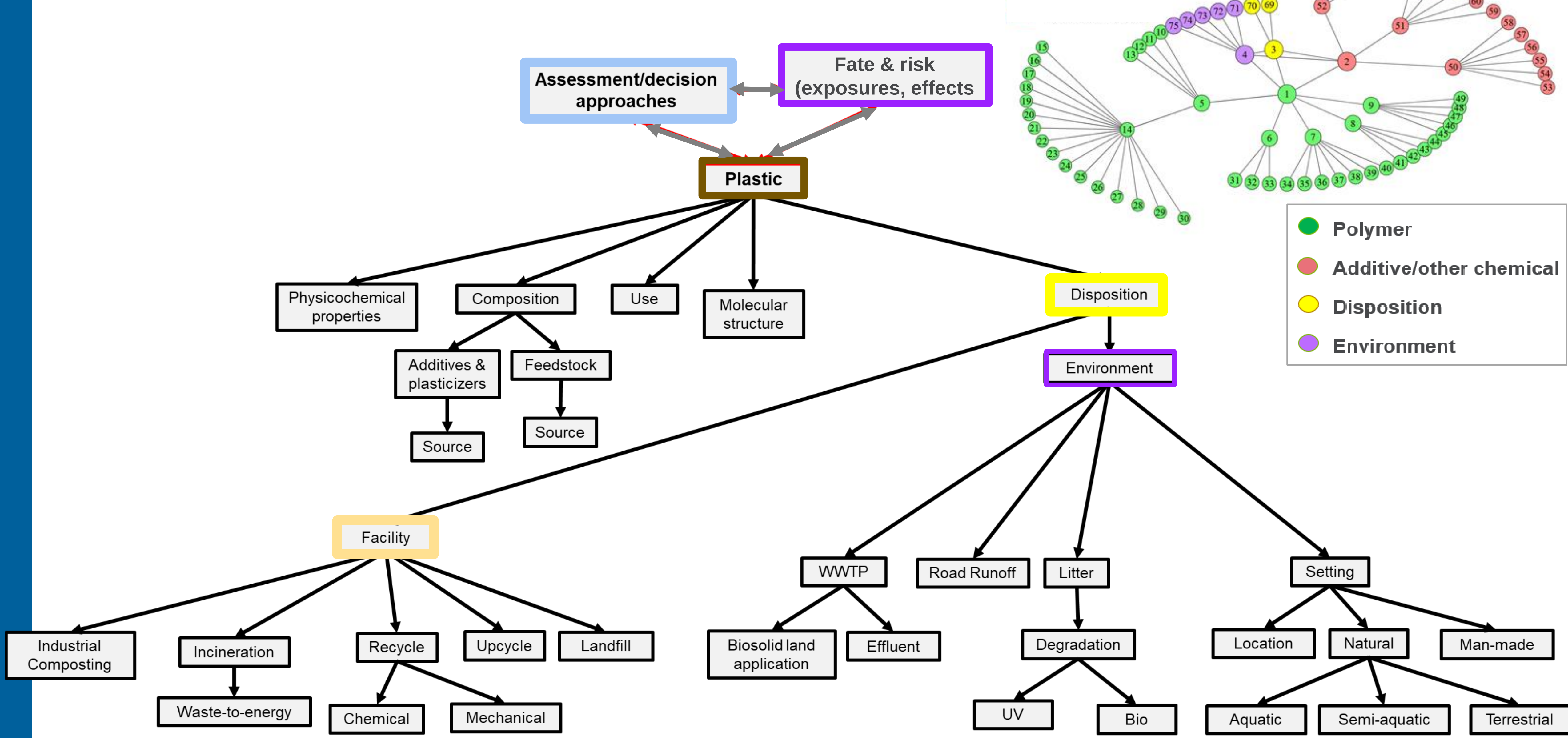
Toxicity Assessment

IR = intake rate

ET = exposure time *(e.g., hours/day)*
EF = exposure frequency *(e.g., days/year)*
ED = exposure duration *(e.g., years)*

BW = body weight *(kg)*
AT = averaging time *(days)*

DATA SCHEMA CONCEPT



DATABASE CONCEPT

Publications, databases, atlases, tools-models *(e.g., NIST MALDI, CHiMaD, PPDB, materiom.org; USEtox; EPA IRIS, CompTox, TRACI, EcoScale)*

Polymer

Composition
Chain length, MW
Structure, properties
Degree of crystallinity
Aging metrics

Environmental fate *(from disposition)*

Salinity, DO, temp *(profile)*
Soil texture, CEC
Moisture content, f_{oc}
Partition coefficients
Microbial composition
Fate mechanisms & products

Computational data

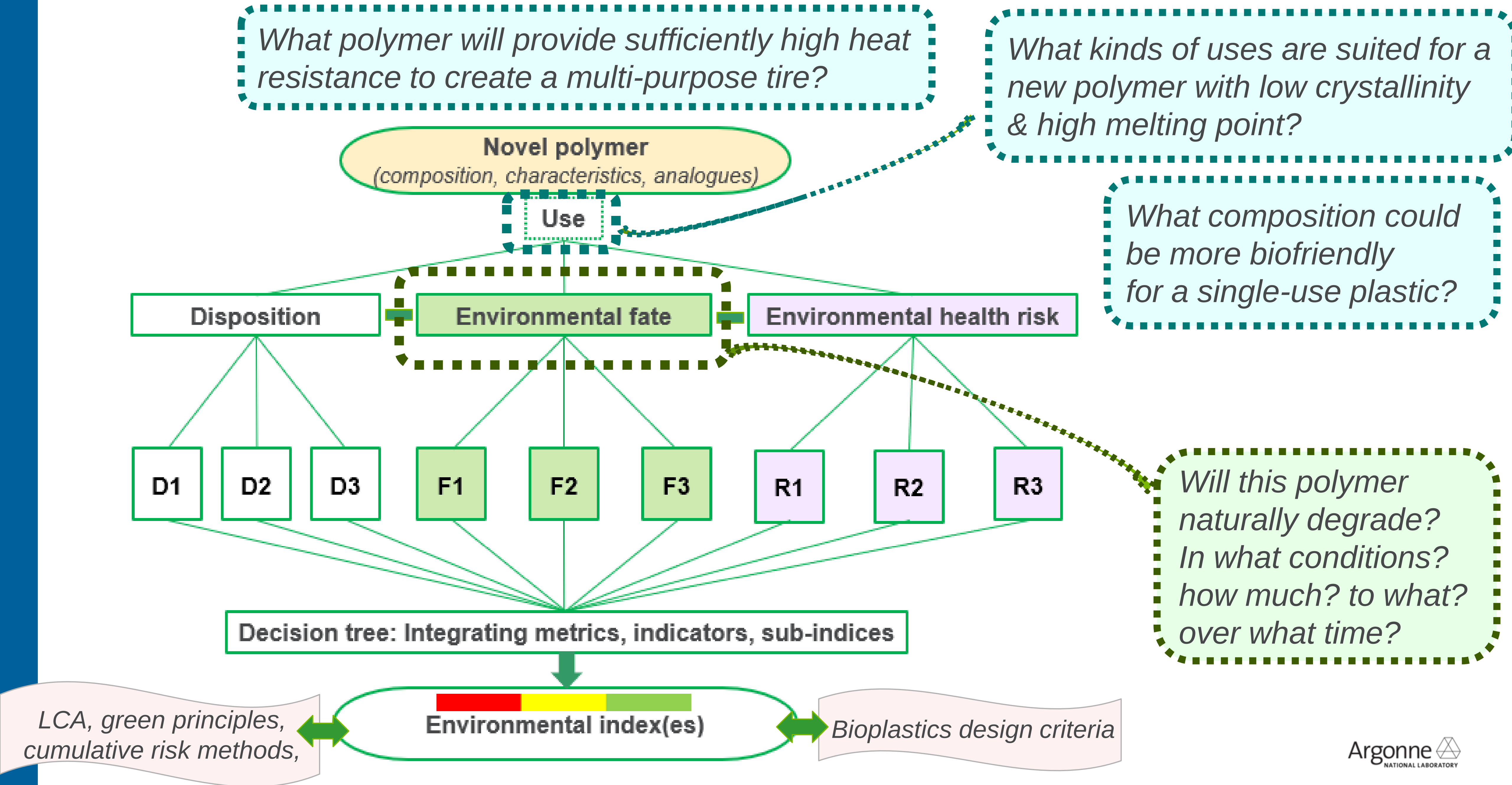
Analogues, surrogates *(QSAR, QSPR, HTS, read-across, index chemicals, whole mixture & component approaches)*

Environmental health risk *(exposures + effects)*

Exposure pathway/routes, amounts
Endpoints, impact types
Effect, timing, level/severity
Exposure-response arrays
TK-TD, adverse outcome pways

CEC = cation exchange capacity
CHiMaD = Center for Hierarchical Materials Design (NIST/NU)
DO = dissolved oxygen
f_{oc} = fraction organic carbon
HTS = high-throughput screening
IRIS = Integrated Risk Information System (EPA)
MALDI = matrix-assisted laser desorption ionization
MW = molecular weight
NIST = National Institute of Standards and Technology
PPPD = Polymer Property Predictor and Database (NIST/UC, ChiMaD)
QSAR = quantitative structure-activity relationship
QSPR = quantitative structure-property relationship
TD = toxicodynamics
TK = toxicokinetics
TRACI = Tool for Reduction and Assessment of Chemicals and other environmental Impacts

GUIDING THE RIPE FRAMEWORK: EXAMPLE QUESTIONS



DEVELOPING PERSISTENCE, FATE & TOXICITY INDICATORS

Ethylene glycol

CAS RN 107-21-1

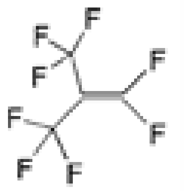
$C_2H_6O_2$ *(MW 62.1)*

Water	Days to weeks *(biodegradation)*
Air	Hours to days *(hydroxyl radical oxidation and deposition)*

Perfluoroisobutylene (PFIB)

CAS RN 382-21-8

C_4F_8 *(MW 200.0)*

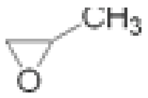


Water	Hours to days *(dissolution and reaction)*
Air	Days *(deposition)*

Propylene oxide

CAS RN 75-56-9

C_3H_6O *(MW 58.1)*



Water	Days *(volatilization and hydrolysis)*
Air	Days to weeks *(hydroxyl radical oxidation and deposition)*

Chemical Name	CAS RN	Formula or Symbol	Molecular Weight *(g/mole)*	Water			Air		
				General Persistence Estimate	Key Fate Process	Toxicity Indicator	General Persistence Estimate	Key Fate Process	Toxicity Indicator
Ethylene glycol	107-21-1	$C_2H_6O_2$	62.1	Days to weeks	*Biodegradation*		Hours to days	*Hydroxyl radical oxidation and deposition*	
Perfluoroisobutylene (PFIB)	382-21-8	C_4F_8	200.0	Hours to days	*Dissolution and reaction*		Days	*Deposition*	*i*
Propylene oxide	75-56-9	C_3H_6O	58.1	Days	*Volatilization and hydrolysis*		Days to weeks	*Hydroxyl radical oxidation and deposition*	

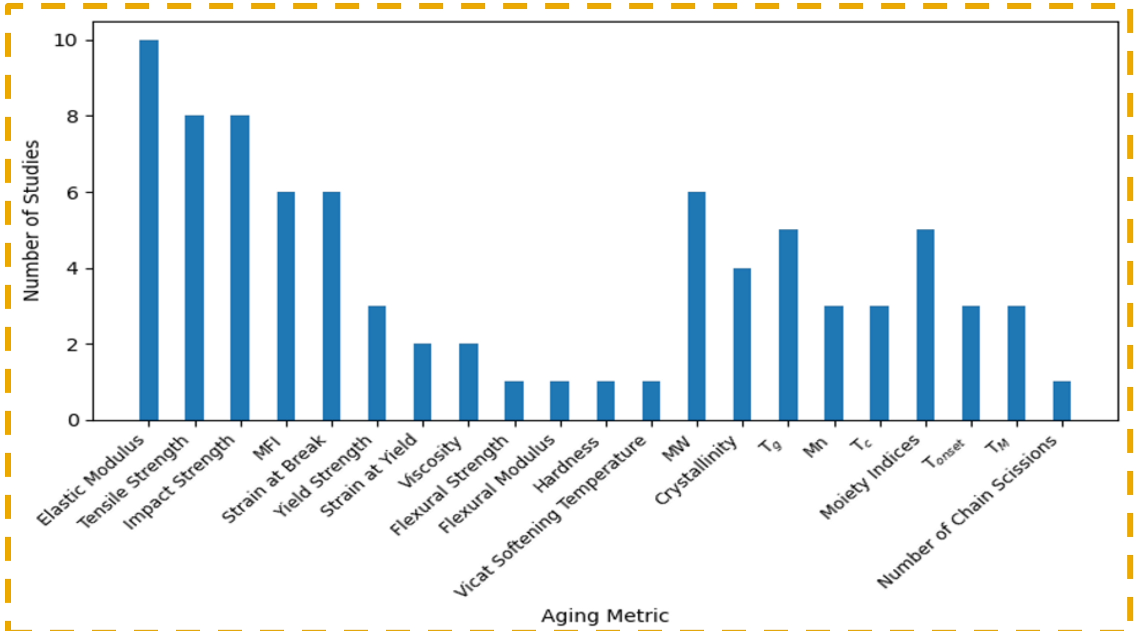
EXAMPLE: DATA CHALLENGES & OPPORTUNITIES

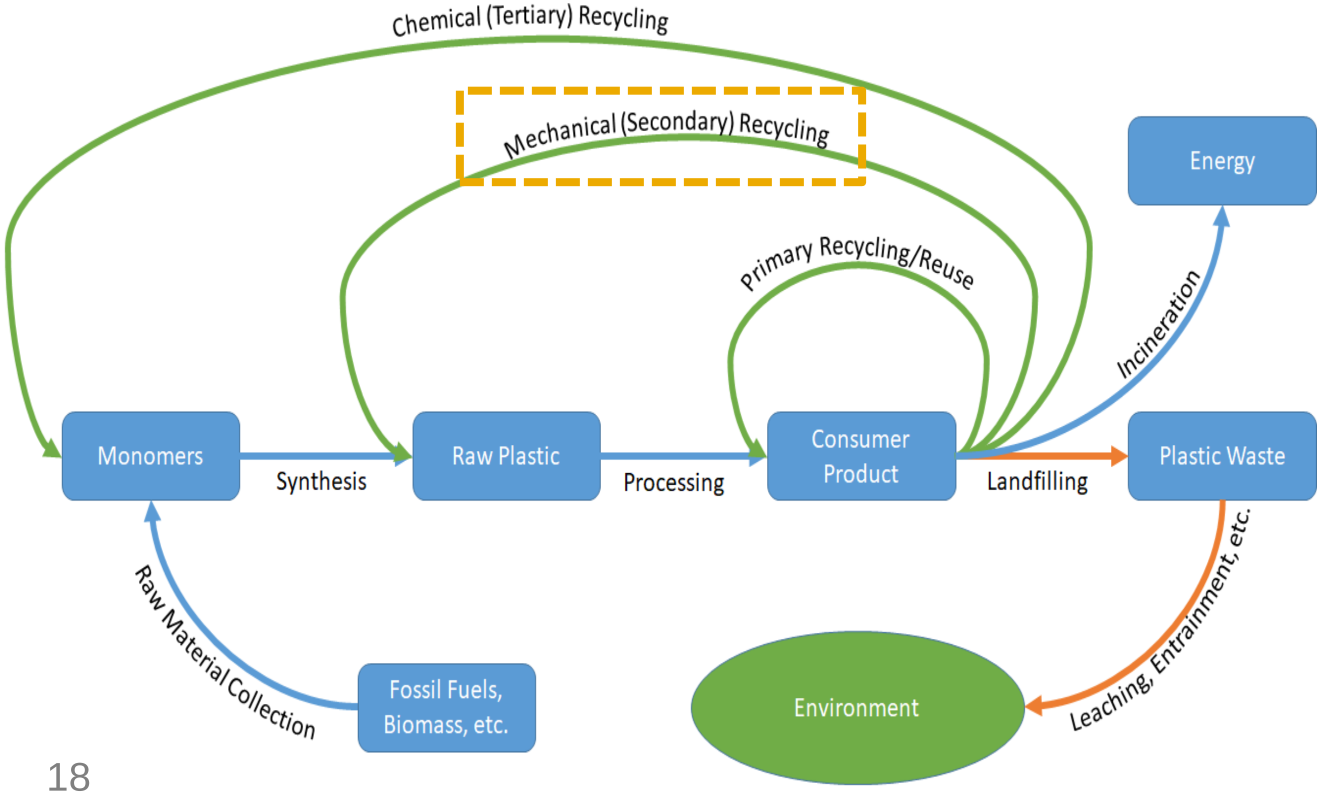
- Relevant data & standards: lacking or limited, varied, inconsistent, hard to extrapolate
  - Biodegradation measure: weight loss – no context *(e.g., if/how much amorphous crystalline regions changed)*
  - Toxicity measure: same – same lack of context

- Discordant metrics

- Promise lies ahead
  - Expanding research & standardization efforts

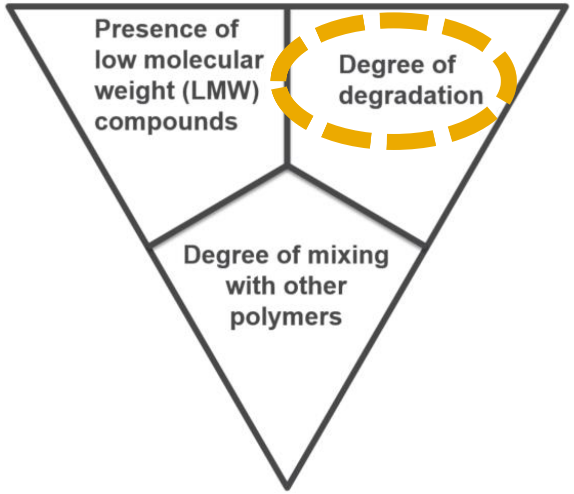
Recycle example illustrated at workshop





RECYCLING EXAMPLE: OUTCOME / IMPACT OPPORTUNITIES

3 factors are key to performance of mechanically recycled polymers, 21 metrics



1. **Degree of degradation** ~depends on material properties, *not* particulars of recycle program
   - PD ➢ Make data available for widely used polymers to guide replacements w/similar properties
2. **Aging effects**: quantify degradation so can predict properties of recycled plastic
   - PD ➢ Could suggest alternate uses for recycled plastics rendered unsuitable for original use
3. Most data: mechanical changes, ~few on **chemical & structural changes** *(no standard)*
   - RP
   - ➢ Targeted research program could generate data to fill both gaps
   - ➢ Make these data available to inform design of new materials more suited for recycling
4. **Additives** used to improve recycling performance
   - ER ➢ Apply RIPE to assess environmental implications, to inform candidate downselect
5. **Social-behavioral** aspect
   - PC
   - ➢ Combining data on recycle performance and stream compositions & quantities to illuminate improvement areas for recycling industry
   - ➢ If good performers were found to be under-represented in recycling streams, could target awareness-engagement campaigns to increase recycling of *these* materials

SUMMARY: RIPE

Responsible innovation:

Taking care of the future through collective stewardship of science & innovation in the present *

** Stilgoe, Owen, &MacNaghten. 2013. Research Policy.*

- Framework concept: Apply **new paradigm** for bioplastics
- Conceptual model: Scope "environment"
- State of knowledge: Anchor environmental reference framework
- Stakeholder input: Inform objectives, approaches, interactions

Illustration: iStockphoto

➢ Toward a *practical tool* for **bench scientists** & beyond
  – Design to strengthen post-use performance
  – Reduce environmental footprint, future liability
  – Propel R&D strategies for bioplastics
  – Enhance bioproduct adoption, industry competitiveness

After-life up front: *design from the start* to enhance our natural capital & human well being

QUAD CHART OVERVIEW

Timeline

- Project start date: January 2, 2020
- Project end date: September 30, 2022

	FY20	Active Project
DOE Funding	10/01/2019 – 9/30/2020	$250K

Barriers addressed

Strategic analysis and cross-cutting sustainability

At-A. Analysis to Inform Strategic Direction: Better understand factors influencing growth and development of bioenergy and bioproducts industries, identify impactful R&D strategies, define BETO goals, and inform BETO strategic direction.

At-B. Analytical Tools and Capabilities for System-Level Analysis: Models need to be developed and refined to reflect new knowledge, scientific breakthroughs, and enable informed decision-making. Improvements in model components and linkages are needed to improve utility, consistency, and reliability.

Project Goal

Design, develop, and demonstrate an environmental reference framework that enables polymer developers to account for the potential post-use fate of a plastic during its design, with an emphasis on new bioplastics

End of Project Milestone

Case study completed, illustrating design criteria for a novel bioproduct, including benchmarks to achieve target objectives identified in coordination with BETO and stakeholder inputs; RIPE toolset available online for BETO community and the public (environmental reference framework decision tree and environmental index, conceptual model, supporting database)

Funding Mechanism

National Laboratory Annual Operating Plan (AOP)

THANK YOU!

QUESTIONS?

ADDITIONAL SLIDES

PUBLICATIONS *(conference proceedings)* **AND PRESENTATIONS:**
Environmental Informatics Annual Meeting (Sep 2020)

enviroinfo

International conference
(Cyprus, virtual)

1. Mechanical Recycling Considerations for Responsible Plastic Innovation
   James Drayton, Justice Wright, Minh Vo

2. Engineering for a Circular Economy: Key Factors for the Design of Biodegradable Plastics and Plastic-Degrading Enzymes
   Mary Rommer, Margaret MacDonell

3. Developing a Preliminary Data Structure to Assess Plastics in Freshwater Environments
   Sneha Nachimuthu, Jennifer Cronin, Margaret MacDonell

4. Database Development and Special Considerations for Storing Polymer Fate Information
   Christopher Rademacher, Marina Slijepcevic, Tanden Hovey, Margaret MacDonell

5. A Database on the Health Risks of Plastics
   Marina Slijepcevic, L'Nazia Edwards, Aijalon Kilpatrick, Phuong Khanh Tran Nguyen, Margaret MacDonell

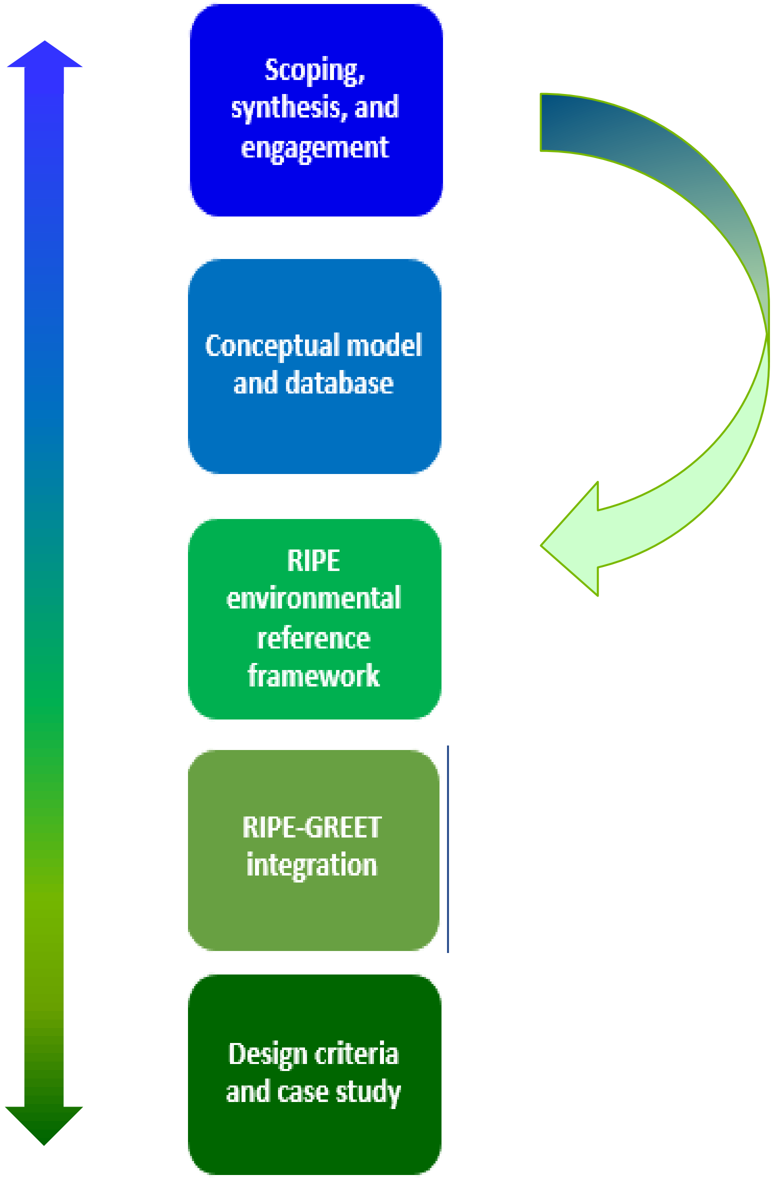
PRESENTATIONS:
Society for Risk Analysis Annual Meeting (Dec 2020)

SRA 2020
Risk Science for Sustainability
December 13 - 17

International conference
(Washington DC, virtual)

1. Exploring the Interactions of Microplastics and Nanoplastics in the Environment
   Tanden Hovey, Margaret MacDonell
2. Exploring the Potential for Exposure to Microplastics in Groundwater
   Sneha Nachimuthu, Jennifer Cronin, Margaret MacDonell
3. Assessing the Susceptibility of Organisms to Adverse Impacts from Environmental Plastics
   Mary Rommer, Margaret MacDonell
4. Assessing Ecological Risks of Microplastics in Terrestrial Ecosystems
   Jennifer Cronin, Margaret MacDonell
5. Informing Performance Tradeoffs for Responsible Plastics Innovation
   Cristina Negri, Margaret MacDonell, Minh Vo, Christopher Rademacher, Kurt Picel, Bruce Biwer, Rao Kotamarthi, Andres Tapia
6. Computational Approaches to Inform Engineering Options for Recycling Plastics
   Minh Vo, Aijalon Kilpatrick
7. Combining Polymer and Environmental Data to Inform Responsible Innovation for Plastics
   Christopher Rademacher, James Drayton, Minh Vo, Margaret MacDonell

FRAMEWORK DEVELOPMENT & LINKAGES AHEAD *(FY21-22)*



- **Environmental reference framework**
  - decision tree
  - environmental index approach
- **LCA linking**
  - existing life cycle analysis tool/s (GREET)
  - ResIn, BOTTLE, & more
- **Demonstration**