Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Quantitative Sustainable Design (QSD) for the Prioritization of Research, Development, and Deployment of Technologies: A Tutorial and Review

Yalin Li, John T. Trimmer, Steven Hand, Xinyi Zhang, Katherine G. Chambers, Hannah A.C. Lohman, Rui Shi, Diana M. Byrne, Sherri M. Cook, Jeremy S. Guest

Table S1. Additional literature examples illustrating concepts, steps, and applications of QSD.

	Example 1	Example 2	Example 3	Example 4
Title	A Unified Modeling Framework to Advance Biofuel Production from Microalgae [1]	Health and Climate Impacts from Long-Haul Truck Electrification [2]	Life Cycle Assessment of The End-of-Life Phase of a Residential Building [3]	Prioritization of Bioethanol Production Pathways in China Based on Life Cycle Sustainability Assessment and Multicriteria Decision-Making [4]
QSD objectives	Inform potential research and development priorities; Provide recommendations for different microalgae processing technologies to leverage specific biomass components to improve the economic viability of the overall system	Account for the climate and health impacts of a potential large-scale transition to truck electrification	Assess the environmental performance of the overall end-of-life stage of a specific residential building, particularly focusing on the management of the generated demolition waste	Determine the most sustainable scenario for bioethanol production for a particular region
Step 1. Define Problem Space				
System boundary	Microalgae cultivation and downstream biorefinery conversion	Truck manufacturing and freight transportation	Building deconstruction/demolition, waste collection, pre-sorting, transportation, recycling, and disposal	Crop production, bioethanol production, and transportation (crop to biorefinery and biorefinery to market)
Life cycle stages	Construction, operations, maintenance	Construction, operations, maintenance	End-of-life	Not reported
Decision variables*	Microalgae species; microalgae cultivation retention time; downstream conversion technologies	Truck type; grid scenario	Demolition (selective vs. non-selective) and waste management (recycle all valuable materials vs. all but inert vs. only recycle steel and copper) methods	Crop type for bioethanol production
Technological parameters*	Subset of stoichiometric (e.g., maximum achievable ratio of stored carbohydrates to functional cells) and kinetic (e.g., specific maintenance rate) parameters for microalgae growth; Natural gas consumption for in-house hydrogen production	Battery specific energy, capacity, and charging power; truck energy efficiency, charging power, refueling time, payload	Material (glass, copper, steel, plastics, and combustibles) recovery and generated waste during sorting	Not included
Contextual parameters*	Capital cost index; equipment costs; unit costs of chemicals and utilities	Electricity mix for the contiguous United States; marginal damages for local air pollutants	Climate conditions (wind, rain, moisture)	Not included
Step 2. Establish Simulation Algorithms				
Algorithm types and levels of complexity*	**Theoretical values:** theoretical methane yield in anaerobic digestion for chemicals with no data in literature **Existing design & data:** product yields from fermentation, catalytic hydrothermal gasification, and hydrotreating **Design heuristics; empirical models:** reactor design; product yields from hydrothermal liquefaction **Mechanistic models:** microalgae cultivation	**Theoretical values:** CO2/SO2 emissions (from mass balance) **Existing design & data:** freight demand from highway assignment database **Design heuristics; empirical models:** truck dispatch model **Mechanistic models:** vehicle energy consumption	**Existing design & data:** use material flow analysis with site visit and literature data to quantify waste based on the bill of quantity for the building materials **Design heuristics; empirical models:** calculation of the amount of dust generated during various demolition activities (mechanical dismemberment, debris loading, onsite lorry traffic and bulldozer pushing) **Mechanistic models:** calculation of the amount of needed sand during demolition	**Existing design & data:** values for economic and environmental indicators (from literature)
Step 3. Characterize System Sustainability				
Sustainability dimensions	Economic	Environmental; human health	Environmental	Economic; environmental; social
Characterization techniques	Techno-economic analysis	Life cycle assessment; monetization of human health damages	Life cycle assessment	Life cycle costing; life cycle assessment; stakeholder survey
Sustainability indicators	Minimum biomass/diesel/fuel selling price	Monetized climate and human health (primary and secondary fine particulate matter from NOx, SO2, and NH3) damages	Carcinogens, non-carcinogens, respiratory inorganics, respiratory organics, ionizing radiation, ozone layer depletion, aquatic ecotoxicity, terrestrial ecotoxicity, terrestrial acidification/nutrification, aquatic acidification, aquatic eutrophication, land occupation, global warming, non-renewable energy, and mineral extraction	**Economic:** production cost **Environmental:** climate change, human toxicity, terrestrial acidification, and particulate matter formation **Social:** social benefits, contribution to economic development, food security
Execution and Applications				
Execution tools*	MATLAB; Microsoft Excel	GREET	SimaPro	Not reported
Analyses*	**Uncertainty analyses:** Figures 3, S1-S5 **Sensitivity analyses:** Figures S6, S7 **Scenario analyses:** Figures 3, S3-S5	**Scenario analyses:** Figure 3	**Scenario analyses:** Figures 7-10	**Scenario analyses:** Tables 3, 4, 6

*Non-exhaustive list in the example paper.

References

[1] Leow et al., *Environ. Sci. Technol.* **2018**, *52* (22), 13591–13599
[2] Tong et al., *Environ. Sci. Technol.* **2021**, *55* (13), 8514−8523
[3] Vitale et al., *Waste Management* **2017**, *60*, 311–321
[4] Ren et al., *Int J Life Cycle Assess.* **2015**, *20* (6), 842–853