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INNOVATIVE RESEARCH FOR A SUSTAINABLE FUTURE

GREENSCOPE: Sustainable Process Modeling

Background

The chemical industry is fundamental in the U.S. This sector accounts for five percent of the U.S. nominal gross domestic product and six percent of the total U.S. energy consumption, directly employs approximately 800,000 people nationwide, and is the source for 11% of all U.S. patents granted annually.

The chemical industry faces environmental and health challenges that are common across business sectors. From the use of nonrenewable feedstocks, to the cost and handling of waste disposal and workers' exposure to toxic substances, the industry must overcome complex hurdles to secure a more sustainable future.

Overview

EPA researchers are responding to the problems outlined above by incorporating sustainability into process design and evaluation. EPA researchers are developing a tool that allows users to assess modifications to existing and new chemical processes to determine whether changes in critical sub-processes or substances will make the overall process more or less sustainable.

The GREENSCOPE (Gauging Reaction Effectiveness for Environmental Sustainability of Chemistries with a multi-Objective Process Evaluator) research project focuses on developing a systematic methodology and software tool that can assist researchers from industry, academia, and government agencies in developing more sustainable processes. In the project, the sustainability of a process is measured in terms of Environmental, Efficiency, Energy and Economic indicators (the 4 E's), with each indicator being mathematically defined. The indicators express diverse aspects of performance in a format that is easily understood, supporting realistic usage. The indicators enable and demonstrate the effectiveness of the application of green chemistry and green engineering principles in the sustainability context.

Sustainability Indicators

To evaluate the environmental aspects of alternative chemistries or technologies, GREENSCOPE employs the Waste Reduction (WAR) algorithm (Young and Cabezas, 1999). The WAR algorithm determines the potential environmental impacts of releases from a process in eight impact categories: human toxicity by ingestion and dermal/inhalation routes, aquatic toxicity, terrestrial toxicity, acidification, photo-chemical oxidation, global warming and ozone depletion. While these potential impacts are defined as mid-point indicators (as opposed to end-point indicators), the measures for the categories are well defined, which is a substantial improvement over arbitrary environmental or mass-based scores.

Efficiencies for chemical reactions are reflected in values such as conversion and selectivity, which track yields, product distributions, and recycle flows needed to make a desired amount of product. Another measure of how green a reaction is can be obtained from the atom economy (i.e., how many atoms from the feed are in the product). These measures, which are well known in green chemistry, are related to environmental impacts since the product distribution defines what chemicals (and amounts) may leave a process. These efficiencies represent a bridge between the lab-scale experiments of a chemist and further engineering calculations.

Energy is a basic component of chemical processes. Its use depletes resources and creates potential environmental impacts. Connecting to yet another sustainability indicator, a less efficient process can be expected to use more energy.

Without a positive economic performance, no industrial process is sustainable. The economics of processes are measured according to their costs. For economists, this is an oversimplified view of markets, but for engineering calculations, the annualized costs are significant measures. The costs are tied into the process through efficiencies, energy, and environmental impacts.

Another novel aspect of the GREENSCOPE methodology and tool is that each indicator is placed on a sustainability scale enclosed by scenarios representing the best target (100% of sustainability) and the worst case (0% of sustainability). This sustainability scale allows the transformation of any indicator score

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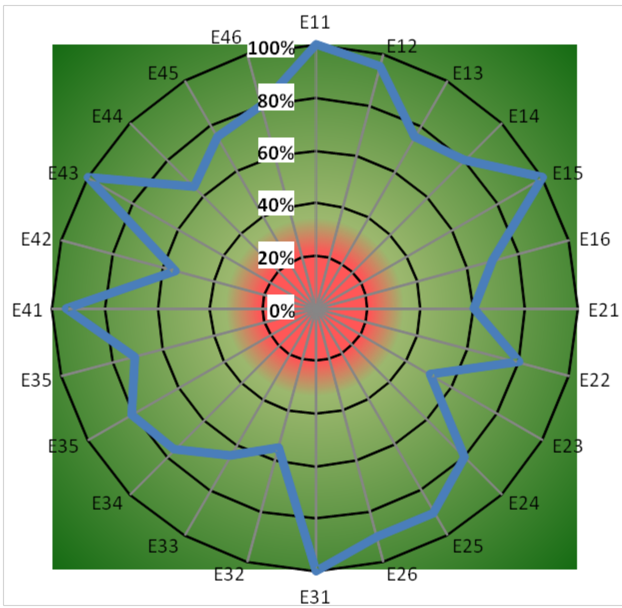
to a dimensionless form using the worst and best scenarios.

A process that is better in environmental, efficiency, energy, and economic terms will most likely be sustainable, although one can expect that tradeoffs will need to be made.

Below, the indicators for a hypothetical process illustrate measures (in blue) that fall between 0 and 100% of sustainability.



Data Needs

GREENSCOPE requires diverse data. These data can be obtained from experimental work, process modeling, physical and thermodynamic multi/pure component properties, product and process design specifications, life cycle inventory, physical and thermodynamic commercial databases, and emissions, discharge, and consumption data from agencies such as EPA, the U.S. Department of Energy, the U.S. Department of Agriculture, and non-governmental organizations such as the World Resources Institute and the Carbon Disclosure Project.

Results

Development of the methodology has centered around three focal points. The first is a taxonomy that describes the indicators and provides absolute scales for their evaluation. The use of best and worst limits (100 and 0% of sustainability, respectively) for each indicator allows the user to know the status of the process under study in relation to understood values and to strive towards realizable targets.

A second area is advancing definitions of data needs for the many indicators. Each indicator has specific data that are necessary for its calculation. Values needed and data sources have been identified. These needs can be mapped according to the information source (e.g., input stream, output stream, external data, etc.). The user can visualize data-indicator relationships before choosing indicators for evaluation.

The third focus is on case studies. Example calculations were performed on an alternative catalyst for the oxidation of cyclohexane. The results indicate how beneficial the new catalyst technology could be. For this and future studies, once one knows what success would mean, the decision to pursue research can be made on a firmer basis.

In addition, the scalability of GREENSCOPE results was addressed to ensure that optimized sustainable designs, as well as experimental studies at the lab scale, would be reflected at the process scale.

Current and Future Research

The methodology is being applied to the production of biodiesel. Analyses identify where biodiesel processes can be made more sustainable based on environmental, economic, efficiency, and energy measures. Process improvements can be suggested or those that were made can be evaluated.

Future work will incorporate models and experiments in an iterative process using a GREENSCOPE software tool to support sustainable chemical process synthesis. An integrated computational tool for multi-objective chemical simulation software will be developed.

References

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