

# A Comprehensive Study on Green Solvents for Environmental Assessment

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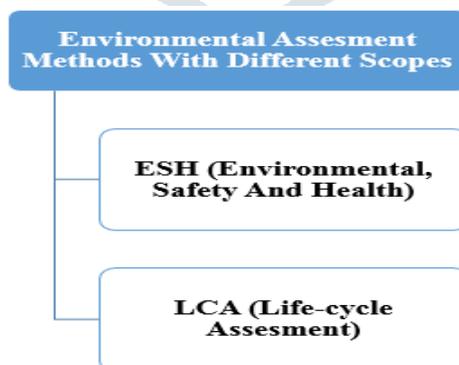
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**ABSTRACT:** Solvents are widely used in industrial and manufacturing settings for a various purpose, it including the product development, washing and degreasing equipment and structures, dealing with materials such as coatings and paints, and promoting chemical processes. Chemical compounds interfere with daylight in the atmosphere, creating a pollutant known as "pavement ozone." The health of humans, animals, and plants is harmed by high levels of pavement ozone. They can have a negative impact on construction materials, trees, and crops. The concept of "green" solvents reflect the need to reduce the environmental effect of solvent use in chemical processing. The current research recommends a systematic study on green solvents, including environmental impact study techniques and hazard assessments for particular substances. The study concludes that basic alcohols or alkanes are preferable solvents for the atmosphere, whereas dioxane, acetonitrile, acids, formaldehyde, and tetrahydrofuran are not. In addition, by replacing hazardous solvents with bio-based solvents derived from natural materials, scientists are trying to use a wider range of solvents. Extension of emerging tools to modern solvent developments, such as ionic fluids or supercritical liquids needs further testing. The fabrication of membrane by green solvents is a recent development in the pharmaceutical sector by employing green chemistry. Using water, as a casting solvent this method has a great potential in future.

**KEYWORDS:** Biodiesel, Environmental, Polymer, Solvents, Waste.

## INTRODUCTION

The disposal of toxic chemicals into the atmosphere is a significant source of concern in terms of biodiversity. Green chemistry has the potential to make a big difference in this field. Solvents, for example, are widely used in academic, commercial, and government research labs[1]. Green chemistry has been proposed by the US Environmental Protection Agency (EPA) for advanced methods that minimize hazardous, unwanted waste, and environmental effects. As a result, green chemistry is gaining traction as an open door to a vast research field[2]. Solvents are found in large amounts in the pharmaceutical sector today. Huge volumes are used per mass of finished products in fine-chemical and medication processing, in particular. As a result, solvents play a very important role in a process's environmental efficiency, as well as its expense, protection, and safety concerns. The concept of "green" solvents refers to the intention of reducing the environmental effects of solvent use in chemical manufacturing. The current research suggests a methodology for solvent environmental evaluation that takes into account significant aspects of solvent sustainability in chemical processing, as well as safety and health concerns. This framework entails the use of two separate environmental monitoring approaches of varying scopes (Figure 1).



**Figure 1: Ecological Assessment Approaches with Different Possibilities[3].**

The EHS evaluation tool is the first method, and it is a screening method that wishes to detect possible chemical threats. The next process, life-cycle assessment (LCA), can be used to evaluate pollution to the atmosphere as well as resource usage over the course of a solvent's whole life cycle, including processing,

use, future recycle, and dispose. The findings of the two evaluation processes are merged to determine the environmentally best performing solvent or solvent blend.

## 1. Methods:

### 1.1. Ecological, Protection, and Health Method for Detecting Potential Substance Hazards:

Chemical solvents are potentially flammable and volatile, as well as poisonous and long-lasting. The EHS evaluation system is a screening procedure for detecting potential chemical product hazards during the early stages of chemical production processes. The EHS approach is highly reliant on the existence of data on the substances' chemical and physical properties, poisonousness, ecological, and security dimensions. Recently, a streamlined Excel tool was developed that only takes into account some factors and criteria for the various impact types. Till now, the latest EHS evaluation method has included about 100 compounds, mostly organic solvents. Substances are classified into nine impact groups using the simpler EHS system. Each impact component is assigned a score between zero and one, giving a total score for each chemical ranging from zero to nine.

### 1.2. Life-Cycle Evaluation Approach for Pollution and Resource Quantitative analysis:

The organic solvent life-cycle considered in this study includes petroleum refining, utilized as reaction medium in a synthetic manufacturing operation, and following discarded solvent disposal. Solvents are both reused by decontamination procedures or processed in a toxic leftover burning plant during waste-solvent handling. The Eco-solvent software process was used to quantify the environmental effect of a given solvent or solvent mixture. This tool incorporates life-cycle stocks of 45 organic solvents' petrochemical processing and disposal, either by fermentation or in a waste disposal anaerobic digestion facility. Life-cycle inventory (LCI) models are used to describe these developments, and they are all founded on market data. Solvent specific ecological effects, such as pollution flows, ancillary applications, and commodity generations, were measured using these projections[3].

Many chemical compounds are hazardous, poisonous, and environmentally harmful. As a result, their use endangers human health as well as the climate. Recognizing solvent characteristics is essential for long-term growth, many such solvents are being rated according to their ecological, protection, and health (ESH) features. Solvents collection manuals, the majority of which are provided by pharmaceutical firms including GSK, AstraZeneca, Pfizer, and Sanofi, as well as specialist organizations like the Innovative Medicines Initiative (IMI)-CHEM21, and ACS Green Chemistry Institute Pharmaceutical Roundtable (GCI-PR) are based on these lists[4].

A variety of factors must be considered when determining how green a solvent is. Consolidating the EHS methodology with the LCA method will result in a multi-criteria assessment. The three stages that make up this job are given below (Figure 2)[3].

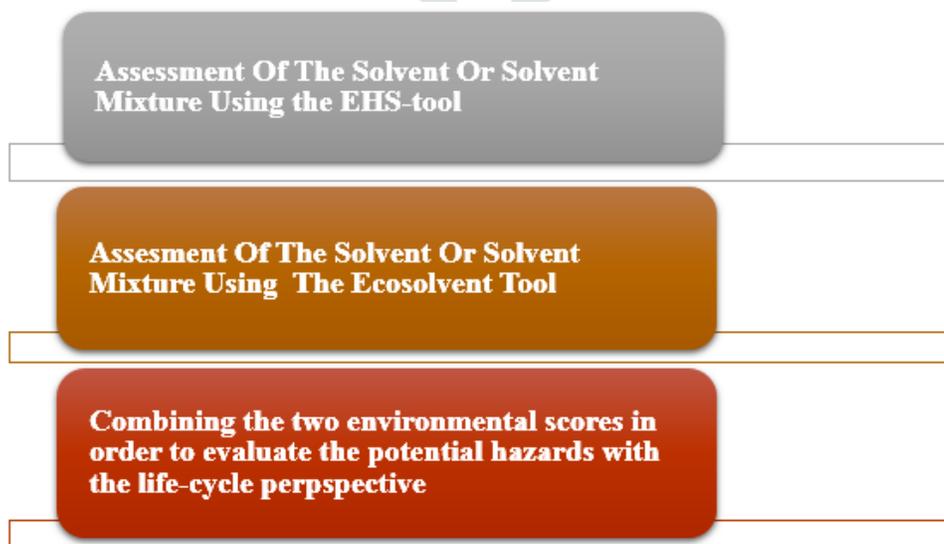


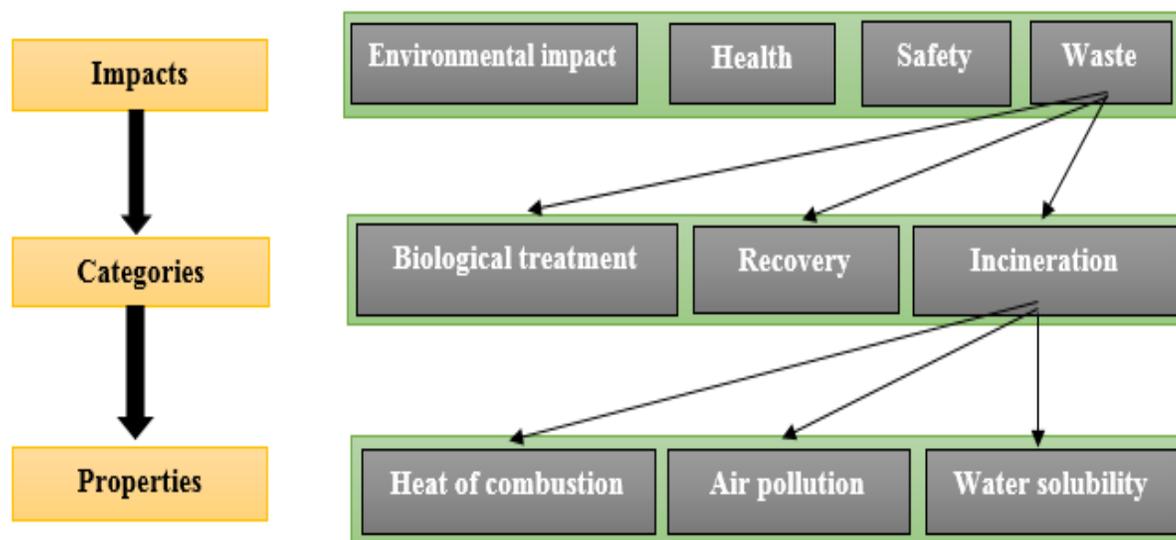
Figure 2: Steps for The Assessment of the Solvent's Greenness[3].

Among the chemical industry, the basic idea of generating ratings of solvent greenness has chosen a better turn. Since the discovery that the solvent is the most essential element of a standard reaction in the manufacturing of a drug product, the healthcare industry has been eager to create its own organizational structures of solvent greenness. As a result, process solvents comprise the most of energy utilization, pollution, and carbon secretions. This makes reducing solvent usage and substituting green alternatives a focus, and it's a common goal of green chemistry programmes. While solvent-free chemistry has long piqued the attention of green chemists, it is not often used in the manufacture of medicines and other industrial products. The dissolvent may have a significant impact on response rates and material specificity, and the advantages of using solvents in processes in particular could not be underestimated. Solvents serve as a temperature sink and heat controller, lowering combination consistency and improving mass transmission, as well as allowing for specific extraction method and separations. Simple visual aids can be used to pick substitute solvents with low toxicity, reduced safety risks, and no environmental effects. Solvent collection manuals for clinical industry small-scale chemistry laboratories are usually lists of solvents grouped as per company use policies.

The color scheme is a widely used "traffic signal" scheme, with of solvent's statement tailored to the company's requirements. Thus, where Pfizer considers a solvent to be "available," GSK (GlaxoSmithKline) says it have "few problems," and Sanofi says "replacement is recommended". Pfizer was the first to make their color-coded, structured solvent collection guide available to therapeutic agents. The method consists of a basic paper that categorizes solvents as 'favored,' 'accessible,' or 'unwanted'. If only to inspire chemists to use it, Pfizer prioritized customer when creating this solvent collection document. As a consequence, this tool can seem to be restricted and unimaginative, but by encouraging minor improvements that few would find detrimental to their jobs, a significant advantage may be realized corporation. At the moment the Pfizer clinical development tool was released, GSK was already developing solvent collection manuals for process chemists. The only noticeable difference in solvent greenness ratings between Pfizer and GSK is for methyl ethyl ketone (MEK), which Pfizer prefers but which GSK considers to have significant problems. Sanofi has also released an analogous solvents collection guide. The tool emerged after a primary form of the organization's corporate solvent collection chart, which classified solvent into two categories: suggested and substitute. Sanofi's solvent collection guide has far more solvents than Pfizer and GSK's pharmaceutical chemistry resources.

## 2. Rating Solvent for Green Chemistry

The three tiered and color-coded system for categorizing solvent in pharmacology has the advantage of being simple to grasp. Since the method is designed for large-scale production, any worries about EHS matters are exaggerated when modelling larger-scale reactions; more information for each solvent is needed. In GlaxoSmithKline's (GSK) original introduction, each of the 35 presented solvent's was given a comparative scoring from 1 (ungreen) to 10 (green) in four groupings: pollution, ecological impacts, wellbeing, and care. For example, Composting, chemical recycling, and organic waste disposal are also used in the waste division. The combustion of the solvent, the probability of HCl or dioxin formation or NOX and SOX pollutants, and its dissolving ability in water are all factors that influence reprocessing (Figure 3).



**Figure 3: Some of the properties used in the GSK solvent collection guides to determine the waste score of solvents[5].**

The American Chemical Society (ACS) Green Chemistry Institute (GCI) Pharmacological Roundtable was established in the year 2005 with the aim of uniting 14 member organizations to set mutual goals and recommendations in relation to green chemical activities. They worked together on a solvents cosmetic protocol that was based on the GSK solvents collection guide and an undisclosed AstraZeneca equivalent that used the same numeric scoring and color coding. There are three environmental standards and one wellbeing and care division in the ACS GCI solvents assortment guide. The levels that classify the various color-coded points are set as per the guide's designers' preferences, and they may or may not be compatible across resources or applicable to regulation. This is addressed in a much recent effort at a solvents assortment guideline that places a better prominence on controlling constraints. This instrument was developed as part of a cooperative study scheme including researchers from Pfizer, Sanofi, GSK, the University of York, and Charnwood advisors.

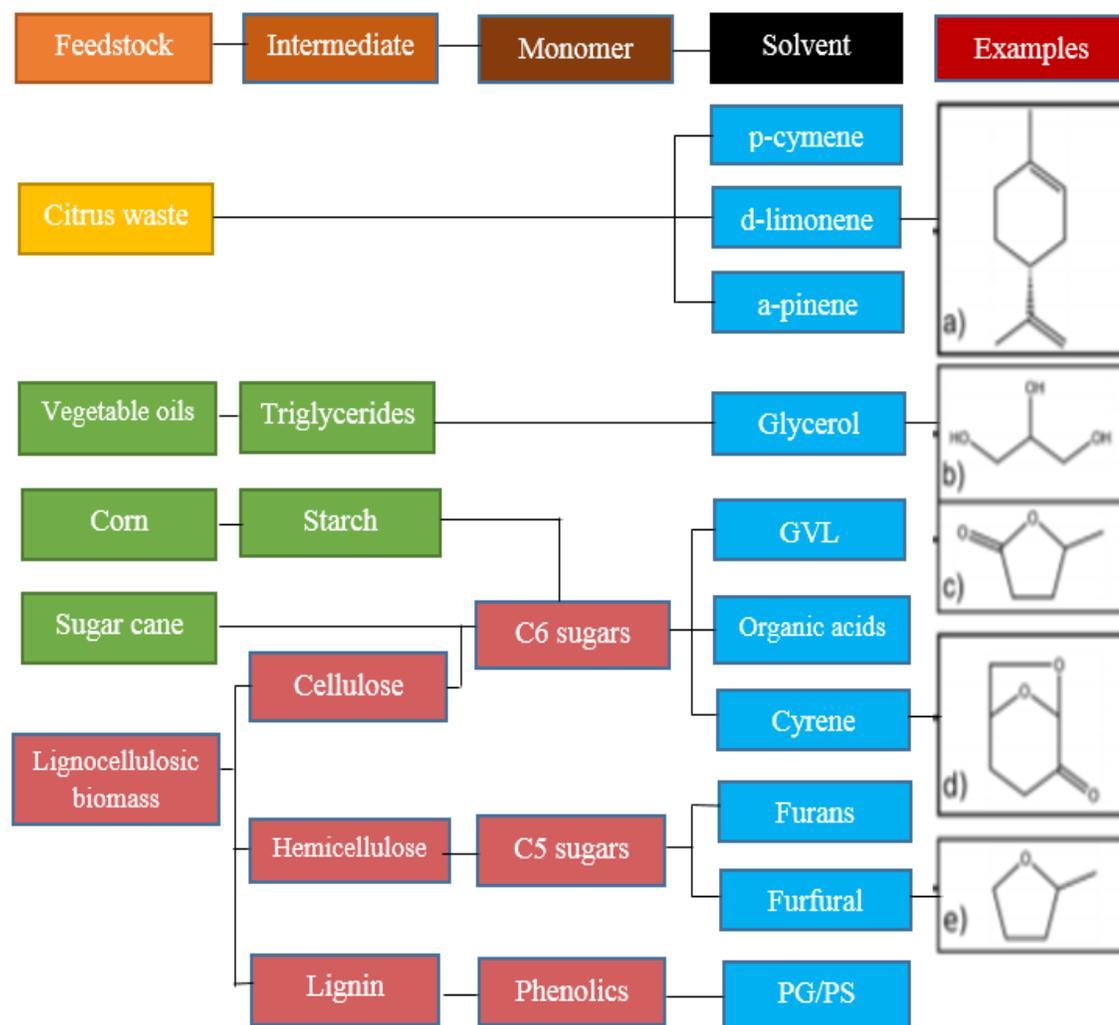
### 3. Foundations of Solvent:

Solvent collection guides have been an important part of the movement to make the fine chemical industry more environmentally friendly, but few efforts have been made to emphasize the renewability of diluents or only to provide solvents with a biologically grounded basis in these resources. Since the large proportion of solvents is derived from natural gas, any advancement in green solvent production would be limited until sustainable solvents are given equal consideration. Biomethanol (or synthetic gas), bio-isobutanol (or bio-isobutene), bio-acetic acid, bio-ethanol (or bio-ethylene), bio-1-butanol, and bio-acetone (which can too be used as a predecessor to isopropanol) are all solvents that can be made from biomass. Many of these bio-based alternatives are delivering sustainable drop-in replacements for conventional solvent supply chains. Protic solvents, as well as esters, ketones, and ethers, are readily available bio-based solvents. Green and renewable hydrocarbon solvents, particularly dipolar aprotic solvents, are required for this. The use of chemometrics to cluster and rate solvents has shown that such solvents are inherently undesirable. As a result, selecting a solvent based on a direct 'like-for-like' replacement is limited. It is impossible to have a green solvent replacement widely accessible for any application if one relies solely on the current catalogue of mostly traditional solvents. Since green solvent's seem to be identical (e.g., alcohol and ester), some areas of solvent use have a surplus of green solvent alternatives, while others have a dire requirement[5].

### 4. Commercial Consideration:

The cost of solvents has a major effect on process performance. The feasibility of using a solvent in a given application is governed by a variety of performance factors. Equally application precise technological (like performances) and method definite monetary variables are included (like solvent cost). Despite the fact that the bulk of the literature and scientific study has focused on efficiency metrics (such as yield), industrial use is usually motivated by the financial feasibility of expending the solvent in the device, as well as further

overall deliberations like obtainability, scale, and safe dumping, along with concerns about deterioration, thermal steadiness, and poisonousness. Renewable energy sources and the commercialization of wastes are also being seen as key sources of recycled solvents by the chemical sector. Recycling commodities is expected to save the circular economy over \$340 billion in material prices, with a further \$520 billion in annual savings expected with the implementation of renewable energy methods in the EU. By 2024, the demand for bio-based goods is projected to expand from \$203.3 billion in 2015. Researchers have developed a number of solvents from renewable materials, some of which are straightforward substitutes for non-renewable solvents and others with new compositions, properties, and formulations. A study found that limonene extracted from citrus residue can be used to substitute poisonous solvents including toluene in the waste management industry. Figure 4 shows examples of biologically derived solvents, as well as their intermediates and feedstock's [4].



**Figure 4: Production of Sustainable Solvent from Plant's Bio-mass. Structural Examples Show (A) D-Limonene, (B) Glycerine, (C)  $\Gamma$ -Valerolactone, (D) Cyrene, and (E) 2- Methf[4].**

### LITERATURE REVIEW

Shaoqing Zhang et al. in their research looked at the creation of green solvent produceable organic photovoltaics (OPVs) in terms of construction parameters, substrate use, and solvent selection, as well as two solvent specific expertise and material design strategies for light absorption surfaces. Combination of these two techniques could lead to a breakthrough in output in green-solvent-processable OPVs. Solution-processable OPV has long been regarded as a leading renewable power making machinery due to its cost effective production and high energy/mass proportion. A rational structure for processing environmentally sustainable solvent and vigorous material for larger and ecologically responsive OPVs will be one of the solutions outlined in this report. Precisely, the most current green solvents processable OPVs with efficiency improvements of over 9% are highlighted[6].

Sameer P. Nalawade et al. studied several polymer melts' solubility and viscosity experimentally and hypothetically. When CO<sub>2</sub> comes into contact with a rubber, it mostly serves as a plastic resin or solvent. The sorption of CO<sub>2</sub> can be measured or estimated using a variety of experimental techniques and state equations. The viscosity of polymer matrix is significantly decreased as CO<sub>2</sub> is dissolved, which a crucial condition for the applications is listed above. However only uncommon polymer is solvable in supercritical CO<sub>2</sub>, it is pretty solvable in several melted polymer. CO<sub>2</sub> breakdown in polymers has also remained described substantially, but FT-IR (Fourier Transform Infrared Spectroscopy) experiments point to a poor association among acid and alkaline areas as an interpretation. The vast variety of applications shows that CO<sub>2</sub> aided polymer processing has a promising future, but it too demonstrates the necessity for a better understanding of the underlying associations in polymer CO<sub>2</sub> systems[7].

Yanlong Gu et al. summarizes the benefits, drawbacks and possible usages of glycerin as a green solvable liquid for catalytic process, carbon-based production, partings and constituent's interaction. Glycerol, a byproduct of the biofuel production, has lately been suggested as a beneficial renewable solvent. The author demonstrated that glycerol's can conglomerate the attributes of water (non - poisonousness, cheap cost, broad supply, and recyclability) and inorganic anions by a series of examples (low vapor pressure, high breaking point, less dissolvable in scCO<sub>2</sub>). According to the findings of this study, using glycerol as a solvent effectively introduces additional resources in the search for novel methods for the gradual substitution of synthetic chemistry with eco - friendly alternatives. Quite broadly, a new topic helps to expand the spectrum of viable green solvents, or to the best of understanding, glycerol's has been the single renewable solvents comparable to water that can balance a lower cost with fewer side effects[8].

Jianbo Hu et al. studied the solvent power of biodiesels as new green solvent. The kauri-butanol worth was used to determine the solvents influence of processed methyl, ethyl, propyl, 1-butyl, and 2-butyl biofuels, along with raw methyl biodiesel comprising glycerols. Analyzing the kauri-butanol qualities of biofuels with various fatty-acids outlines and alcohols type yielded some thought-provoking outcomes. Unadulterated methyl esters have higher kauri-butanol levels than glycerols. Unsaturated fatty-acids ester has higher kauri-butanol value than substituted fatty-acids ester, and the amount of the dual bond in free fatty acids has slight influence on the assessment. The carbon chain of the fatty acid or alcohol group is shorter in biodiesel with a higher kauri-butanol content. Biodiesel's with a straight chain has more kauri-butanol than biodiesel with a bifurcated chains[9].

Santiago Aparicio et al. reported a broad scope study on ethanol lactate (EL) arrangement and properties spending a collective experimental/theoretical tactic. The pressure–viscosity–temperature and pressure–volume–temperature activities are described in this paper, along with several derived properties that are crucial for material selection. Density Functional Theory and classic computer simulations models are used to examine the liquid's composition at the microscopic level. The intermolecular interaction frequencies calculated reveal strongly organized fluids with low molecular movement and short self-diffusion correlations. According to the thermophysical properties, the liquid is dense and has a mild viscosity, allowing it a candidate for use in a wide range of industrial fields. The prognostic potential of the protective shield utilized in molecular fluctuations is evaluated, with favorable aspects for the majority of the project specification[10].

## DISCUSSION

Green chemistry is being used in a growing number of studies and industries. The explanation for this is that the world's resources are finite, so consumption must be done with caution. Solvents play an important role in the chemical industry's environmental success, as well as cost, regulation, and health concerns. Green solvents, nanocatalysts, and biocatalysts open up a slew of new possibilities for environmentally friendly processes. To achieve near-total "greenness" of chemical reactions, any element of the chemical process must be considered. The current thesis covers a simple description of green solvents as well as environmental evaluation methods with various scopes and instruments. Biocatalysts are recyclable, disposable, renewable, more effective, and stereo specific, which means they are more atom economical than traditional methods, according to the article. They are more powerful instruments for green technology in this regard. Seeing the

potential application of green solvents, it is projected that the ultimatum for bio-based solvents will increase from \$203.3 billion in 2015 by 2024.

## CONCLUSION

Solvents are the most significant category of chemicals in the chemical industry owing to the vast quantities used per year. As a result, solvents play an important role in a process's environmental success as well as protection and health concerns. However, in the chemical sector, solvent sourcing for chemical reactions and waste-solvent disposal are primarily driven by fiscal, environmental, and practical concerns. Environmental issues are often dismissed by decision-makers, owing to a shortage of adequate tools or resources. The present work has presented an easily implementable method for a systematic environmental impact assessment of solvent usage, which includes both environmental sustainability of diluents in chemical processing along with safety and health concerns. The use of this structure in the solvents and leftover management with an ecological unit makes decision-making easier.

Environmental impacts resulting from factory processing, transportation and reuse practices, as well as EHS features, must all be considered when determining how green a solvent is. Since these measurement approaches supplement one another, integrating the EHS approach with the LCA method results in a multi-criteria test. While the EHS approach emphasizes on the potential risks of diluents, the LCA manner quantifies a general power consumption associated with solvent processing and waste-solvent disposal. The architecture discussed in this work is built on two free automatic computing tools that have dissimilar scopes. Both methods were created in close cooperation with the chemical sector and thus have findings that are useful in the real world. Until now, the model has only been used to evaluate organic solvents. Extension of available technologies to emerging solvent applications, such as ionic fluids or supercritical solutions, would need further testing.

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