

Integrating Safety Metrics and Regulatory Compliance for Green Solvent Selection in Sustainable Chemistry

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ABSTRACT: The shift toward sustainable practices in chemical manufacturing necessitates the replacement of traditional solvents with safer, environmentally benign alternatives. This study proposes a dual-criteria evaluation framework that integrates Safety, Health, and Environmental (SHE) scores with REACH regulatory compliance to support green solvent selection. Using a curated dataset of solvents characterized by physical and operational risk metrics, the methodology identifies high-performing green solvents suitable for sustainable process design. Quantitative assessments were performed based on SHE scores (scale 1–10), flash point, boiling point, and regulatory status. Correlation analysis revealed key relationships between solvent physical properties and SHE risk indicators. Recommended solvents were further evaluated for practical applications in extraction, synthesis, and purification processes. Solvents such as ethanol, water, and propylene carbonate demonstrated favorable SHE profiles and full REACH compliance. Results confirmed the utility of simple scoring systems in streamlining solvent substitution while ensuring safety and regulatory alignment. The framework offers a transparent, efficient method for solvent screening, serving as a foundation for broader sustainability tools like Process Mass Intensity (PMI), E-Factor, and Life Cycle Assessment (LCA). This model enhances industrial decision-making by enabling safer and more sustainable solvent use. Its adaptability supports both laboratory-scale and industrial applications, promoting compliance and long-term environmental stewardship.

Keywords: Green Solvents, SHE Scores, REACH Compliance, Solvent Selection, Sustainability, Chemical Safety, Regulatory Screening



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INTRODUCTION

The chemical manufacturing industry is undergoing a critical transformation driven by mounting environmental regulations, societal expectations, and the need to improve safety standards. One

of the most pressing challenges faced by this sector lies in the widespread use of traditional organic solvents, which are essential in various chemical processes but are also major contributors to environmental pollution and occupational hazards. Conventional solvents such as benzene, toluene, and chlorinated hydrocarbons are widely recognized for their adverse ecological impacts, including toxicity, persistence, and potential for air and water contamination (Meringolo et al., 2018; Sharma et al., 2025). In industrial contexts, these solvents contribute significantly to operational risks, exposing workers to health hazards that can lead to both acute and chronic illnesses (Sharma et al., 2025; Meringolo et al., 2018).

In response to these concerns, green chemistry has emerged as a guiding framework for redesigning chemical products and processes to reduce or eliminate hazardous substances. A key area of innovation within this field is the development and adoption of green solvents. Green solvents are broadly defined as substances that maintain performance efficiency in chemical transformations while minimizing environmental and health-related risks. Among the prominent classes of green solvents are deep eutectic solvents (DESs) and natural deep eutectic solvents (NADES), which have gained attention for their low toxicity, high biodegradability, and economic viability (Owczarek et al., 2016). These solvents represent a new generation of sustainable materials aligned with the principles of green chemistry, which prioritize safety, efficiency, and ecological stewardship (Hansen et al., 2020).

The challenge, however, lies not only in identifying green solvents but also in establishing practical, data-driven methods for evaluating and selecting them. In industrial chemistry, solvent sustainability is commonly assessed through various criteria including toxicity to human health and ecosystems, chemical durability, persistence in the environment, and the overall environmental impact as measured by life cycle assessments (Byrne et al., 2016; Sheldon, 2017). These parameters are crucial in determining the long-term implications of solvent use and in guiding companies toward safer alternatives. Moreover, sustainability metrics such as Process Mass Intensity (PMI) and Reaction Mass Efficiency (RME) provide quantitative insights into material utilization and environmental burden (Kar et al., 2021).

Despite the availability of sustainability criteria and metrics, the solvent selection process in both academic and industrial settings often remains inconsistent. Green chemistry practices typically rely on solvent selection guides and integrated sustainability frameworks that assess toxicity, environmental persistence, regulatory status, and cost-effectiveness. Foundational principles such as the “twelve principles of green chemistry” offer theoretical guidance, while digital tools and solvent selection software increasingly support informed decision-making (Rapinel et al., 2020). Nonetheless, the absence of a unified evaluation system that balances operational safety, environmental performance, and regulatory compliance continues to impede efficient solvent substitution.

One of the most influential regulatory frameworks shaping solvent use is the European Union’s REACH (Registration, Evaluation, Authorisation, and Restriction of Chemicals) regulation. REACH mandates comprehensive safety evaluations of chemical substances and compels manufacturers to demonstrate that their chemicals do not pose unacceptable risks to human health

or the environment (Santos et al., 2025). Its scope encompasses the use of solvents, placing restrictions on hazardous substances and promoting transparency and responsibility among producers. Comparable regulations are emerging globally, imposing tighter controls on solvent use and pushing the industry toward greener alternatives (Sportiello, 2024). The alignment of solvent selection with regulatory standards thus becomes a key determinant of compliance and long-term sustainability.

Beyond compliance, the risks associated with conventional solvents have tangible implications for the overall sustainability of chemical operations. The continued use of high-risk solvents results in elevated waste generation, heightened accident potential, and exposure to legal liabilities. These risks often translate into increased operational costs, reputational damage, and delayed innovation efforts (Lawrenson et al., 2017; Warokar et al., 2025). Furthermore, the environmental remediation efforts necessitated by solvent contamination place additional strain on resources that could otherwise support proactive sustainability programs. By transitioning to green solvents, organizations can significantly reduce these liabilities, enhance workplace safety, and fulfill sustainability goals outlined by both internal policy and external regulation (Valderrama et al., 2023).

In light of these considerations, this study introduces a practical and transparent evaluation framework for green solvent selection. The framework is grounded in the integration of two critical decision-making tools: SHE (Safety, Health, and Environment) scoring systems and REACH regulatory compliance status. SHE scores offer a simple yet robust mechanism for quantifying operational risks associated with solvent use, employing a numeric scale where lower values indicate superior performance. REACH status, in turn, provides an institutionalized filter to identify substances that are legally acceptable and aligned with sustainability objectives. Together, these tools form a dual-criteria assessment model that can be readily implemented in chemical laboratories, research and development (R&D) pipelines, and manufacturing environments.

The novelty of this approach lies in its operational simplicity and wide applicability. Unlike traditional solvent assessment models that require extensive data processing or advanced life cycle analysis tools, the SHE–REACH framework is designed for rapid application and scalability. It bridges the gap between theoretical green chemistry guidelines and practical industry needs, offering a middle ground that facilitates informed, timely, and compliant solvent substitution. The current study applies this framework to a curated dataset of solvents, analyzing key physical and regulatory variables, and highlighting green candidates based on SHE performance and REACH status. Through this analysis, we aim to demonstrate the value of integrated solvent evaluation in advancing sustainable chemical processes and promoting the broader adoption of green chemistry principles.

METHOD

The methodology employed in this study integrates multiple dimensions of solvent assessment to support the selection of green solvents within a sustainability framework. It focuses on three

principal components: quantification of solvent risk through Safety, Health, and Environmental (SHE) scores; verification of REACH regulatory compliance; and application of analytical tools to identify correlations among solvent properties. These components are supported by literature-driven approaches including multi-criteria decision models, compliance evaluation protocols, and advanced analytical techniques such as correlation and risk ranking.

Quantification of SHE Risks

Quantifying the safety, health, and environmental risks associated with solvents is foundational in assessing their suitability for green chemistry applications. A variety of scoring models have been developed to provide a systematic evaluation of solvent risk profiles. In this study, each solvent is assigned a SHE score on a scale from 1 (least concern) to 10 (most concern) for each dimension safety, health, and environment.

Notably, multi-criteria decision analysis (MCDA) has been highlighted as a reliable method for consolidating diverse environmental risk parameters into a unified ranking system. Tobiszewski et al. (2017) demonstrated how an MCDA framework, combined with a multimedia environmental fate model, can be employed to rank solvents based on their toxicity and environmental persistence. Such integrated methods allow for more nuanced comparisons between solvents beyond individual risk dimensions.

Artificial intelligence-based tools such as SUSSOL have also been developed to automate and enhance the scoring process. These platforms utilize algorithmic logic to evaluate solvent attributes across multiple sustainability criteria, thereby expediting solvent screening and selection (Sels et al., 2020). The adoption of such tools reflects a broader trend toward data-driven solvent evaluation in line with digital chemical process design.

Evaluation of REACH Regulatory Compliance

Complementing the SHE scores, regulatory compliance status particularly with the European Union's REACH regulation is a key determinant in sustainable solvent selection. Under REACH (Registration, Evaluation, Authorisation, and Restriction of Chemicals), manufacturers and importers are required to register substances and provide detailed data regarding their safe use, physicochemical properties, and associated hazards.

The REACH compliance status used in this study was sourced from established chemical safety databases. These databases contain up-to-date records of chemical registration and regulatory assessments, and they classify solvents as either "Compliant" or "Not Listed" based on their fulfillment of REACH requirements (Wang, 2025). The process involves not only verifying a substance's legal status but also understanding the broader implications of its hazard profile on environmental and occupational safety.

Rajappa et al. (2025) emphasize that ongoing updates to compliance databases are vital for ensuring that industry practices reflect current regulatory landscapes. The ability to rapidly verify compliance

status through integrated systems supports proactive solvent substitution and minimizes risk associated with using outdated or restricted substances.

Analytical Techniques for Property Assessment and Correlation

To interpret and extract insights from solvent property data, analytical techniques such as correlation analysis and risk ranking were employed. Correlation analysis enables the identification of statistically significant relationships between solvent physical properties (e.g., boiling point, flash point) and SHE scores. This helps in understanding which physicochemical properties are predictive of higher risk and can thus be targeted for optimization or avoidance.

Murugan et al. (2021) discuss how correlation analysis supports solvent safety assessments by clarifying how specific properties impact overall hazard levels. For example, a strong inverse correlation between flash point and safety score would suggest that lower flash points are generally associated with greater safety concerns.

Risk ranking systems complement correlation analysis by providing a multi-factorial assessment framework. Subramaniam et al. (2016) describe a method that ranks solvents by aggregating scores across toxicity, volatility, and biodegradability dimensions. Such an approach ensures that solvents are not only evaluated for individual risks but also for their comprehensive sustainability performance.

Integration of Life Cycle Assessment Tools

Although not the primary focus of this study, the methodology acknowledges the importance of Life Cycle Assessment (LCA) in advanced solvent evaluations. LCA tools provide a broader environmental perspective by quantifying impacts across a solvent's life cycle from raw material acquisition to disposal.

Recent developments in LCA methodologies have made it possible to identify environmental “hot spots” in solvent production and use (Zhang et al., 2020). Purkait et al. (2022) highlight how integrating LCA with solvent selection processes allows for better-informed decisions that account for cumulative environmental burdens. In future applications, the SHE–REACH framework presented here may be extended to include LCA data for a more holistic solvent sustainability evaluation.

Dataset Overview and Filtering Criteria

The dataset analyzed in this study consists of a range of organic solvents categorized into functional classes such as alcohols, esters, ethers, polar protics, and carbonates. Each solvent entry includes values for:

- Boiling point (°C)
- Flash point (°C)
- Safety score (1–10)
- Health score (1–10)

- Environment score (1–10)
- Recommendation status (Recommended, Problematic, Hazardous)
- REACH compliance (Compliant / Not Listed)

Solvents were filtered for further analysis if they met the following criteria:

1. Safety, Health, and Environment scores each below 5 (low to moderate risk).
2. Classification as "Recommended" or "Problematic" (excluding "Hazardous").
3. Confirmed REACH compliance.

This filtering process enabled the identification of high-potential green solvents for further comparative analysis.

Summary of Methodological Framework

The methodological framework established in this chapter provides a structured approach to solvent selection based on risk assessment, regulatory compliance, and statistical analysis. It draws on validated literature models and tools to ensure both scientific robustness and practical applicability. By integrating SHE scores with REACH data and applying advanced correlation techniques, the study offers a pragmatic tool for rapid and transparent green solvent evaluation.

RESULT AND DISCUSSION

This chapter presents the results of the solvent assessment framework applied to a curated dataset. The findings are structured into three main sub-sections: (1) solvent category profiles, (2) correlation insights between physical and risk-based properties, and (3) comparative analysis of selected green solvent candidates. Each section integrates empirical data analysis with supporting literature.

Solvent Category Profiles

Frequent Solvent Categories in Sustainable Processes

Among sustainable chemical applications, solvent categories such as bio-based solvents, deep eutectic solvents (DESs), and ionic liquids are frequently prioritized. Ethanol and ethyl acetate are particularly favored due to their low toxicity and high biodegradability, facilitating widespread use in synthesis and extraction processes. DESs also offer strong solvation properties while maintaining eco-compatibility (Ahmad et al., 2023).

Variation in Physical Properties

Boiling and flash points vary significantly across solvent families, influencing their applicability and operational risk. For example, ethanol and ethyl acetate exhibit relatively low flash points (around

13 °C and 25 °C, respectively), increasing their flammability risk despite favorable environmental traits. In contrast, solvents like DMSO exhibit high boiling points (~189 °C), reducing volatility and potential for atmospheric release (Lee et al., 2016).

Empirical Patterns and Safety Trends

Empirical data suggest distinct patterns linking solvent categories to safety performance. Polar protic solvents, while effective in solvation, often pose higher toxicity and flammability risks (Ahmad et al., 2023). Solvents with high boiling points typically present lower volatility, reducing flammability hazards and contributing to safer operational profiles (Bonhomme et al., 2022).

SHE Score Benchmarks

SHE scoring benchmarks rely on quantitative assessment of toxicity, persistence, and biodegradability. Lower SHE scores indicate more favorable performance. Ethanol and ethyl acetate routinely score better than traditional solvents such as dichloromethane or toluene (Ravivarman et al., 2023), reflecting their suitability for green chemistry applications.

Correlation Insights

Predictive Value of Physical Properties

Analysis confirmed that physical properties like flash point, boiling point, and vapor pressure are predictive of solvent risks. Higher volatility correlates with increased inhalation hazards and environmental dispersion. For instance, acetone's high volatility underscores its inhalation risk despite widespread use (Brox et al., 2016).

Use of Statistical Correlation Tools

Statistical tools such as Pearson correlation and multi-dimensional scaling were used to map relationships among solvent attributes. Regression analyses revealed strong inverse correlations between flash point and safety scores: lower flash points consistently aligned with higher SHE risk indicators (Yen & Quoc, 2021).

Flash Point vs Environmental Trade-Offs

Case analyses confirmed trade-offs between flammability and environmental performance. Ethanol's favorable biodegradability contrasts with its low flash point, requiring enhanced operational precautions (Yen & Quoc, 2021). Meanwhile, high-boiling-point solvents may be safer in terms of flammability but risk persistence in ecological systems.

Limitations of Correlation Approaches

While useful, correlations are limited in fully capturing the multifactorial nature of solvent risks. Ahmad et al. (2023) emphasize that relying solely on simplified indicators may obscure the interactive effects of concentration, temperature, and application context. Hence, SHE score interpretation must be embedded within a broader evaluation strategy.

Green Solvent Comparison

Validation of Ethanol, Ethyl Acetate, and Water

Data analysis and literature confirm ethanol, ethyl acetate, and water as benchmark green solvents. These solvents demonstrate superior SHE scores, high biodegradability, and versatility across chemical applications (Yen & Quoc, 2021). Ethanol, in particular, stands out for its favorable regulatory profile and compatibility with both polar and nonpolar systems.

SHE Score Validation Methods

SHE scores were validated using empirical safety data and regulatory compliance reports. The process involved assessing human toxicity, environmental persistence, and risk exposure. Tools such as life cycle inventory databases and regulatory frameworks (e.g., REACH) helped support these validations (Bellasi et al., 2020).

2-MeTHF and Propylene Carbonate: Case Analysis

2-MeTHF offers improved flash point characteristics compared to traditional ethers like THF, while maintaining similar reactivity profiles in synthesis applications. Propylene carbonate, a non-flammable, bio-derived solvent, excels in environmental performance but may introduce operational limitations due to high viscosity and reduced volatility (Ghatta et al., 2021).

Comparison to Conventional Solvents

When compared with conventional petroleum-based solvents, green alternatives consistently perform better in health and environmental categories. Water-based extractions are particularly advantageous for their safety and low ecological impact. Moreover, 2-MeTHF has demonstrated improved safety compared to legacy ether solvents while retaining functional performance (Lee et al., 2016).

These findings affirm the value of integrating empirical property data with regulatory and SHE risk assessments to identify solvents that align with the principles of green chemistry.

The findings of this study reinforce the importance of structured, quantitative frameworks for solvent evaluation, particularly within the context of sustainable chemical manufacturing. By

integrating SHE (Safety, Health, and Environmental) scoring systems with REACH regulatory compliance data, this work presents a streamlined methodology for identifying suitable green solvents. This discussion addresses the strengths and limitations of SHE scores in guiding practical solvent substitution, the value of regulatory integration in sustainability assessments, and the potential for expanding solvent evaluation frameworks through additional metrics such as Process Mass Intensity (PMI), E-Factor, and Life Cycle Assessment (LCA).

SHE scoring systems have emerged as practical tools for solvent screening, particularly in early-stage assessments. They allow for the quantification of complex safety and environmental risks using a simple 1–10 scale, which enhances transparency and accessibility for both researchers and industry practitioners (Maranghi et al., 2019). This numerical approach facilitates comparison between solvents based on factors such as flammability, toxicity, and biodegradability. In this study, the SHE scores proved effective in distinguishing low-risk solvents like ethanol and water from more hazardous alternatives.

However, while SHE scores offer valuable first-line insights, they do not encompass all critical factors affecting solvent utility in industrial applications. Kosnik et al. (2022) argue that considerations such as cost, process compatibility, and reaction specificity are often overlooked in such scoring systems. For example, a solvent may receive a favorable SHE score yet prove unsuitable for a reaction requiring high polarity or specific temperature conditions. Thus, although SHE scores streamline initial decision-making, they should be complemented with contextual and application-specific evaluations to avoid oversimplification.

The integration of regulatory compliance frameworks, such as REACH, adds a crucial dimension to sustainability assessments. REACH mandates the registration and hazard evaluation of chemical substances, ensuring that manufacturers meet safety and environmental protection standards. By incorporating REACH status into solvent assessments, companies can align their sustainability efforts with current regulatory expectations, thereby reducing liability and enhancing market acceptability (Costa et al., 2025; Müller et al., 2016). Moreover, REACH integration supports credibility in environmental claims and fosters stakeholder trust by providing a verifiable compliance benchmark.

This study's dual-criteria approach combining SHE scoring and REACH status offers a transparent and defensible framework for solvent substitution. The ability to rapidly filter solvents based on both operational risk and legal compliance provides a significant advantage in time-sensitive or resource-constrained contexts. As noted by Maranghi et al. (2019), embedding regulatory filters within sustainability frameworks facilitates anticipatory compliance, allowing firms to stay ahead of evolving regulatory landscapes.

Despite these benefits, the use of SHE scores in industrial practice must be critically evaluated. Esposito et al. (2021) emphasize that such scores improve communication among interdisciplinary teams by translating complex solvent characteristics into easily interpretable metrics. This enhances decision-making agility, particularly during solvent screening and substitution phases. Yet, as Rong et al. (2018) point out, the simplicity of SHE scores may lead to an underappreciation of nuanced risks, such as reaction-specific hazards or long-term ecological effects. Therefore, while the

method is useful for general screening, it is not a substitute for comprehensive environmental and process-specific evaluations.

To address the inherent limitations of SHE scores and enhance the robustness of solvent selection, integration with additional sustainability tools is recommended. One such tool is Process Mass Intensity (PMI), which measures the total mass of inputs relative to the mass of the desired product. As Calvo-Serrano et al. (2018) explain, PMI provides insights into resource efficiency and material optimization, enabling solvent choices that contribute to waste reduction and cost control.

Another key metric is the E-Factor, which quantifies the mass of waste generated per unit of product. This measure is particularly relevant in green chemistry, where minimizing waste is a core objective. Incorporating E-Factor assessments can support solvent selection that aligns with broader waste reduction goals (Maranghi et al., 2019).

Finally, Life Cycle Assessment (LCA) tools offer a comprehensive environmental profile by evaluating solvent impacts across their entire life span from raw material extraction to disposal. LCA enables the identification of environmental “hot spots” that might not be visible through SHE scores alone. Studies by Costa et al. (2025) confirm that LCA integration improves the reliability of sustainability evaluations by capturing cradle-to-grave impacts.

In conclusion, while SHE scoring and REACH compliance form a solid foundation for green solvent evaluation, their effectiveness is enhanced when combined with broader assessment tools such as PMI, E-Factor, and LCA. This multi-dimensional framework not only supports safer and more sustainable solvent selection but also aligns chemical manufacturing practices with current regulatory and environmental standards. Future research should continue refining this approach to ensure that it accommodates emerging solvent technologies, sector-specific requirements, and evolving sustainability benchmarks.

CONCLUSION

This study introduced and validated a dual-criteria framework for evaluating green solvents, integrating Safety, Health, and Environmental (SHE) scores with REACH regulatory compliance. The research addressed a pressing need within the chemical industry for simplified, transparent, and actionable methods to support solvent substitution in line with sustainability goals.

Key findings demonstrate that SHE scores are effective tools for identifying solvents with lower toxicity, flammability, and ecological impact. Solvents such as ethanol, ethyl acetate, water, 2-MeTHF, and propylene carbonate were identified as high-performing candidates due to their favorable SHE profiles and REACH compliance. The study's correlation analysis revealed important insights into the relationships between solvent physical properties such as boiling and flash points and associated operational risks, helping clarify trade-offs between safety and environmental performance.

The integration of REACH status further enhances the credibility and regulatory alignment of solvent selection. This compliance check acts as a critical filter to ensure solvent viability in both

current and future industrial applications. Combining these tools results in a robust framework capable of guiding solvent substitution at various stages of chemical process design, from laboratory experiments to full-scale production.

The scientific contribution of this study lies in its pragmatic approach to solvent evaluation. Unlike many complex sustainability models, the proposed framework is easy to implement and interpret. It bridges the gap between regulatory compliance and sustainability metrics, supporting chemists, process engineers, and regulatory professionals in making informed decisions.

This study also emphasizes the importance of expanding solvent selection methodologies. Future research should explore how SHE–REACH frameworks can be integrated with advanced sustainability tools such as Process Mass Intensity (PMI), E-Factor, and Life Cycle Assessment (LCA). These tools provide additional layers of insight into resource efficiency, waste generation, and cradle-to-grave environmental impacts.

In summary, the adoption of simplified yet comprehensive solvent evaluation models can accelerate the shift toward safer and more sustainable chemical processes. By embedding regulatory and risk considerations into the core of solvent selection, this research contributes to both operational efficiency and environmental stewardship within the broader goals of green chemistry.

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