

Green Chemistry Metrics as a Quantitative Tool for Evaluating Chemical Reaction Efficiency: A Stoichiometric Comparative Study

Rakesh Kumar

PGT Chemistry, GMSSSS Dholera, Mahendragarh, Haryana, India

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ABSTRACT

Green chemistry provides a design-oriented approach for reducing waste and improving material efficiency. This study develops a transparent stoichiometric framework for comparing six representative reactions using atom economy (AE) and stoichiometric waste potential (SWP), and extends the analysis with stoichiometric E-factor/PMI proxies and yield-sensitivity analysis of reaction mass efficiency (RME). The selected reactions represent addition, dehydration, esterification, acylation, precipitation, and reduction chemistry. Balanced equations, molecular formulas, and standard molar masses were used to calculate reproducible theoretical metrics. Yield sensitivity was extended from the original aspirin example to all six reactions using the restricted relationship $RME = AE \times \text{yield}$. The calculated atom-economy values range from 60.90% for ethanol dehydration to 100.00% for ethene hydrogenation. The analysis confirms that yield and atom economy answer different questions and that stoichiometric mass metrics cannot substitute for process-level information. A literature-informed screening framework is also provided for solvent use, energy demand, hazard, process mass intensity, and life-cycle considerations. Because no new experiments or complete process mass balances were available, process-level E-factor, PMI, solvent, energy, and life-cycle values are not presented as measured results. The revised framework therefore provides a reproducible educational and preliminary process-screening tool while clearly defining the data required for a complete sustainability assessment.

Keywords: Green Chemistry, Atom Economy, Reaction Mass Efficiency, Stoichiometry, Waste Prevention

INTRODUCTION

The chemical industry and the academic laboratory increasingly require approaches that connect chemical performance with resource efficiency. Conventional evaluation of a reaction frequently emphasizes percentage yield, purity, conversion, or reaction rate. These measures are important, but they do not by themselves describe how much of the starting material becomes the desired product or how much material is discarded as stoichiometric by-product. Green chemistry addresses this limitation by encouraging the design of products and processes that prevent waste and reduce hazards at the source (Anastas & Warner, 1998).

Atom economy was introduced by Trost as a way of considering the proportion of reactant atoms incorporated into the desired product (Trost, 1991). The concept subsequently became one of the central principles of green chemistry. In contrast to percentage yield, atom economy is a theoretical property of a balanced chemical equation and assumes stoichiometric quantities and complete conversion. It therefore provides a useful early-stage screen before laboratory or industrial process details are considered (Constable, 2018; Trost, 1991).

Other metrics extend this perspective. The E-factor expresses waste generated per unit mass of product, while reaction mass efficiency (RME) incorporates stoichiometry and actual product yield. Process mass intensity (PMI) accounts for the total mass of materials used per unit mass of product and is widely used as a high-level process metric. Recent literature stresses that these metrics answer different questions and should

be interpreted with solvent, energy, hazard, and life-cycle information rather than treated as interchangeable indicators (Sheldon, 2007; Sheldon, 2018; Jiménez-González et al., 2011).

The present study therefore focuses on a transparent stoichiometric comparison of representative reactions. Rather than reporting invented laboratory measurements, it uses balanced equations, standard molar masses, and published definitions to generate reproducible numerical results. The approach is particularly useful for chemistry education because it makes the connection between ordinary stoichiometry and green chemistry quantitatively visible.

Study contribution and originality

The contribution of the present work is the staged integration of reaction-level stoichiometric metrics with a clearly defined pathway toward process and life-cycle assessment. Instead of assigning a single overall greenness score, the framework keeps atom economy, yield, mass intensity, hazard and life-cycle dimensions analytically distinct and identifies the additional evidence required at each stage. The six-reaction yield-sensitivity extension and the separation of calculated scenarios from literature-based process evidence provide a reproducible structure that can be expanded when experimental or process-inventory data become available.

LITERATURE REVIEW

Anastas and Warner established the twelve principles of green chemistry as a framework for pollution prevention and safer chemical design (Anastas & Warner, 1998). Among these, prevention and atom economy are directly connected to the present analysis. Atom economy is a theoretical measure based on the molecular mass of the desired product relative to the total molecular mass of stoichiometric reactants (Trost, 1991; Sheldon, 2018). Trost's original work emphasized that efficient synthesis should maximize the number of reactant atoms appearing in the desired products (Trost, 1991). Sheldon later developed the E-factor concept and demonstrated its relevance to waste minimization in chemical manufacturing, particularly in fine-chemical and pharmaceutical processes (Sheldon, 2007). More recent reviews have emphasized that E-factor, atom economy, RME, process mass intensity, and related metrics answer different questions and should not be treated as interchangeable (Trost, 1991; Sheldon, 2018).

Green-metric education has also been explored as a pedagogical strategy. Hudson and Leaman demonstrated a classroom activity in which students compare yield, atom economy, reaction mass efficiency, carbon efficiency, E-factor, and effective mass yield using molecular models (Hudson & Leaman, 2016). This supports the use of quantitative metric comparison as a bridge between theoretical chemistry and sustainability concepts. Dicks and Hent (2015) similarly present atom economy, RME, E-factor, PMI, qualitative metrics, and life-cycle assessment as complementary tools rather than substitutes.

Aspirin synthesis is a useful educational case because the reaction between salicylic acid and ethanoic anhydride produces aspirin together with ethanoic acid. Recent chemistry-education work has used aspirin manufacture to connect atom economy, carbon efficiency, RME, E-factor, mass balances, energy, and life-cycle thinking, illustrating how theoretical metrics can be combined with process information (Dikobe et al., 2026). This literature provides a useful benchmark for extending the present stoichiometric framework without presenting unsupported experimental measurements.

OBJECTIVES

- To calculate atom economy for a representative set of balanced chemical reactions.
- To quantify stoichiometric waste potential associated with non-product material in each reaction.
- To examine the relationship between theoretical atom economy and reaction mass efficiency using a yield-sensitivity analysis.
- To demonstrate how stoichiometric green metrics can be incorporated into chemistry teaching, laboratory planning, and early-stage process evaluation.

- To identify the limitations of relying on atom economy alone when making broader sustainability assessments.
- To apply yield-sensitivity analysis across all six reactions and compare the resulting theoretical RME scenarios.
- To define the data requirements for process-level E-factor, PMI, solvent, energy, hazard, and life-cycle assessment without treating unavailable values as measured data.
- To document reaction-level waste-generation profiles and qualitatively screen key environmental and health hazards associated with representative reactants and by-products.

METHODOLOGY

Study Design

This was a secondary, calculation-based comparative study. No new chemical experiment, human-subject study, animal study, or laboratory measurement was performed. The dataset was generated from balanced chemical equations representing six established reaction types. This design was selected to ensure that every numerical result can be independently reproduced from the stated formulas and definitions.

Reaction Selection

The six reactions were selected to provide contrasting stoichiometric structures: a combination reaction with complete incorporation of reactant atoms; a dehydration reaction producing a small-molecule by-product; esterification; aspirin acylation; an inorganic precipitation reaction; and reduction of a nitro compound. The set was not intended to rank industrial processes. It was designed to demonstrate how reaction structure affects material efficiency.

Molar-Mass Basis

Molar masses were calculated from standard atomic-weight values reported by the International Union of Pure and Applied Chemistry (IUPAC) Commission on Isotopic Abundances and Atomic Weights (Prohaska et al., 2022). Values were retained to three decimal places for calculation and displayed consistently in the tables.

Green-Metric Equations

Atom economy (AE) was calculated as:

$$AE (\%) = [\text{Molar mass of desired product} \div \text{Sum of molar masses of stoichiometric reactants}] \times 100$$

Stoichiometric waste potential (SWP) was expressed as the mass of non-product stoichiometric material generated per unit mass of desired product:

$$SWP = [(\text{Total stoichiometric reactant mass} - \text{desired-product mass}) \div \text{desired-product mass}]$$

For the yield-sensitivity analysis, reaction mass efficiency was represented by the simplified stoichiometric relationship $RME = AE \times Y$, where Y is fractional isolated yield and the stoichiometric quantities are used without additional excess-reactant or solvent corrections. This is a deliberately restricted educational form; complete process-level assessment requires broader mass accounting (Dicks & Hent, 2015; Sheldon, 2018).

Extended Green-Metric Framework

To respond to the need for broader sustainability assessment, the study distinguishes stoichiometric screening metrics from process-level metrics. A stoichiometric E-factor proxy (E_{stoich}) was calculated as the mass of non-product stoichiometric material divided by product mass; under the present boundary, E_{stoich} is numerically equivalent to SWP. A stoichiometric PMI proxy (PMI_{stoich}) was calculated as

total stoichiometric reactant mass divided by product mass, giving $PMI_{stoich} = 1 + E_{stoich}$. These proxies deliberately exclude solvents, water, excess reagents, catalysts, utilities, and work-up materials. Full process PMI and E-factor require all relevant material inputs and waste streams to be included (Jiménez-González et al., 2011; Sheldon, 2018). For broader screening, solvent intensity should be expressed as solvent mass per mass of product; energy intensity as energy consumed per mass of product; and hazard assessment should consider the intrinsic hazards and exposure potential of reactants, solvents, catalysts, products, and waste. Life-cycle assessment should extend the system boundary to upstream raw-material production, transport, process operations, and downstream treatment or disposal. These dimensions are identified as assessment requirements rather than numerical outputs because the present dataset contains no complete process inventory, measured energy record, solvent log, or hazard inventory.

Data Integrity and Reproducibility

All reported numerical values are calculated rather than experimentally observed. No measured yield, temperature, mass, or analytical result has been presented as if it were experimentally obtained.

Table 1. Representative reactions and calculated stoichiometric green metrics

Reaction	Balanced equation	Reactant mass (g mol ⁻¹)	Product mass (g mol ⁻¹)	AE (%)	SWP
Ethene Hydrogenation	$C_2H_4 + H_2 \rightarrow C_2H_6$	30.070	30.070	100.00	0.000
Ethanol Dehydration	$C_2H_5OH \rightarrow C_2H_4 + H_2O$	46.069	28.054	60.90	0.642
Ethyl Acetate Esterification	$CH_3COOH + C_2H_5OH \rightarrow CH_3COOC_2H_5 + H_2O$	106.121	88.106	83.02	0.204
Aspirin Synthesis	$C_7H_6O_3 + C_4H_6O_3 \rightarrow C_9H_8O_4 + C_2H_4O_2$	240.210	180.159	75.00	0.333
AgCl Precipitation	$AgNO_3 + NaCl \rightarrow AgCl + NaNO_3$	228.316	143.321	62.77	0.593
Nitrobenzene reduction	$C_6H_5NO_2 + 3H_2 \rightarrow C_6H_7N + 2H_2O$	129.159	93.129	72.10	0.387

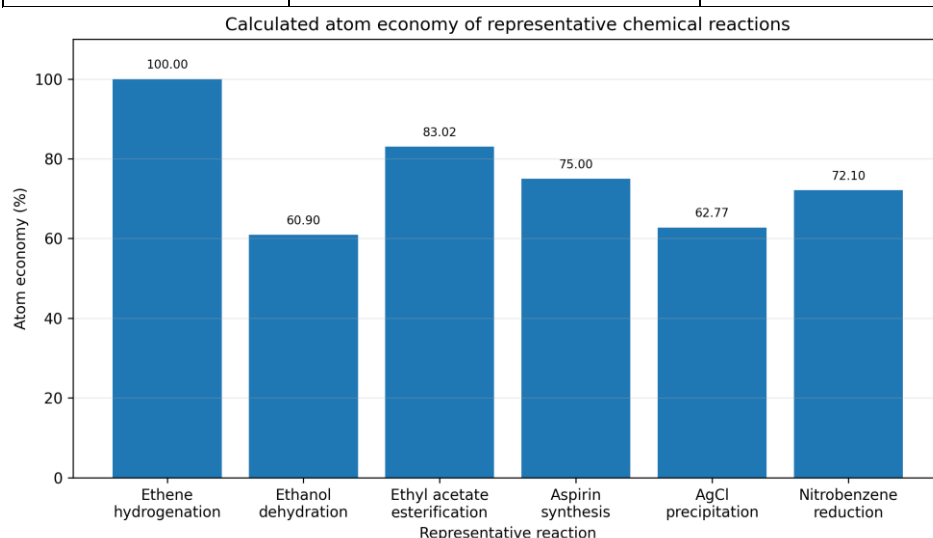


Figure 1. Calculated atom economy for the six representative reactions. Values are derived from balanced stoichiometric equations.

RESULTS

Atom Economy Comparison

The calculated atom-economy values covered a broad range. Ethene hydrogenation reached 100.00% because the atoms of both reactants are incorporated into the single desired product. Ethyl acetate esterification gave 83.02%, while aspirin synthesis gave approximately 75.00%. Nitrobenzene reduction produced 72.10% because water is formed as a stoichiometric by-product. AgCl precipitation and ethanol dehydration gave 62.77% and 60.90%, respectively. These values demonstrate that reaction class and stoichiometric structure can create substantial differences in theoretical material utilization even before yield and solvent effects are considered.

Stoichiometric Waste Potential

The SWP values provide the complementary view of the same mass balance. An SWP of 0.333 for aspirin synthesis means that, under the ideal stoichiometric equation, approximately 0.333 g of non-product stoichiometric material accompanies each gram of aspirin formed. For ethanol dehydration, the value is 0.642, reflecting the production of water as a relatively large fraction of the reactant mass. Because SWP excludes solvents, catalysts, excess reagents, work-up water, and purification losses, it should not be interpreted as a complete process E-factor.

Yield Sensitivity of Aspirin Synthesis

Aspirin synthesis was retained as the illustrative case because its theoretical atom economy is approximately 75.00%. At assumed isolated yields of 60%, 70%, 80%, 90%, 95%, and 100%, the simplified RME values are 45.00%, 52.50%, 60.00%, 67.50%, 71.25%, and 75.00%, respectively. These are calculated scenarios, not experimental measurements. To broaden the analysis, the same yield-sensitivity calculation was applied to all six reactions. The expanded results are reported in Table 4 and Figure 3, allowing the effect of yield to be compared across different stoichiometric structures.

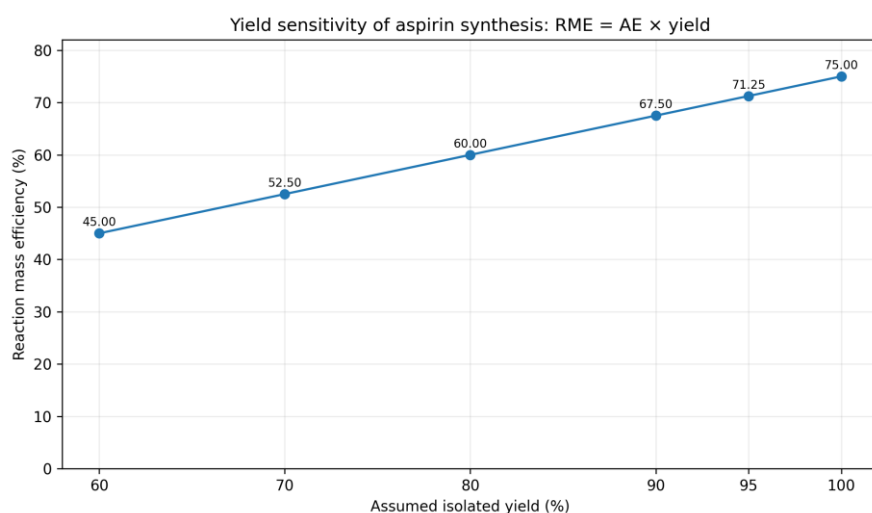


Figure 2. Calculated yield-sensitivity relationship for aspirin synthesis using the simplified $RME = AE \times \text{yield}$ expression.

Table 2. Yield-sensitivity calculation for aspirin synthesis

Assumed yield (%)	Atom economy (%)	Simplified RME (%)
60	75.00	45.00

70	75.00	52.50
80	75.00	60.00
90	75.00	67.50
95	75.00	71.25
100	75.00	75.00

Expanded Mass-Based Screening Metrics

Under the restricted stoichiometric boundary, the calculated E-factor proxy equals SWP and the PMI proxy equals $1 + \text{SWP}$. Ethene hydrogenation has an ideal stoichiometric E-factor of 0.000 and PMI of 1.000 because all stoichiometric reactant mass appears in the desired product. Ethanol dehydration has the highest stoichiometric E-factor in the selected set (0.642) and a corresponding PMI proxy of 1.642. These values should not be compared with full industrial E-factor or PMI benchmarks because process inputs such as solvents and water are excluded.

Table 4. Expanded stoichiometric mass metrics and yield-sensitivity scenarios for all six reactions.

Reaction	AE (%)	SWP / E_stoich	PMI_stoich	RME @ 60%	RME @ 80%	RME @ 100%
Ethene hydrogenation	100.00	0.000	1.000	60.00	80.00	100.00
Ethanol dehydration	60.90	0.642	1.642	36.54	48.72	60.90
Ethyl acetate esterification	83.02	0.204	1.204	49.81	66.42	83.02
Aspirin synthesis	75.00	0.333	1.333	45.00	60.00	75.00
AgCl precipitation	62.77	0.593	1.593	37.66	50.22	62.77
Nitrobenzene reduction	72.10	0.387	1.387	43.26	57.68	72.10

Broader sustainability screening requirements

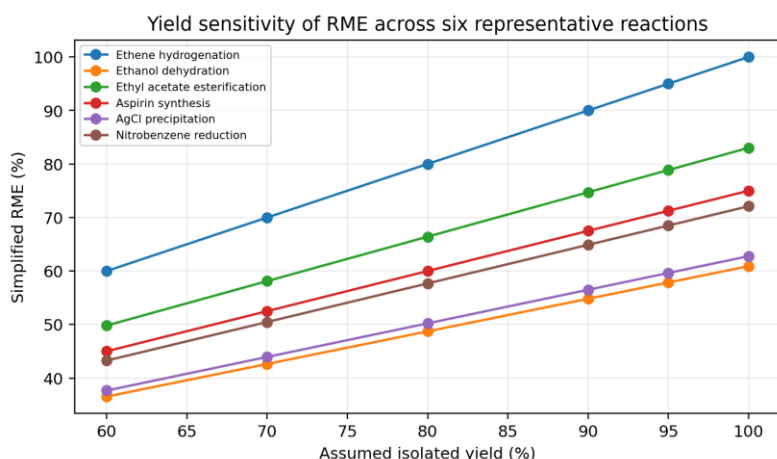
The reviewer-requested expansion beyond mass efficiency is incorporated as a defined screening framework. The present study calculates only the metrics supported by the stoichiometric dataset; the remaining metrics are specified together with their required data so that future experimental or process studies can extend the framework without mixing calculated scenarios with measured process performance.

Table 5. Data requirements for extending the stoichiometric framework to process-level sustainability assessment.

Metric dimension /	What it measures	Data required for full assessment	Status in present study
Atom economy (AE)	Theoretical incorporation of reactant mass into desired product	Balanced equation and molar masses	Calculated

RME	Mass efficiency incorporating actual yield	Reactant masses and isolated product yield	Yield scenarios calculated
E-factor	Mass of waste per mass of product	Complete material balance, including relevant waste streams	Stoichiometric proxy only
PMI	Total material input per mass of product	Reactants, solvents, water, process aids, etc.	Stoichiometric proxy only
Solvent intensity	Solvent mass per mass of product	Solvent identity and mass/volume used and recovered	Not quantified
Energy intensity	Energy consumed per mass of product	Heating, cooling, mixing, separation and other energy records	Not quantified
Hazard screening	Health, safety and environmental hazard profile	Hazard classifications, exposure information and waste characteristics	Framework identified; not scored
Life-cycle assessment	Upstream-to-downstream environmental burdens	Life-cycle inventory, system boundary and impact factors	Not performed

Figure 3. Calculated yield-sensitivity relationship for all six representative reactions using $RME = AE \times \text{yield}$. All points are mathematical scenarios, not experimental measurements.



Waste-Generation and Hazard Screening Profile

The stoichiometric equations also identify the principal reaction-level non-product streams that would require attention in a process inventory. Ethanol dehydration and nitrobenzene reduction generate water as stoichiometric by-product; ethyl acetate esterification also generates water; aspirin acylation generates acetic acid; and AgCl precipitation generates sodium nitrate. Ethene hydrogenation has no stoichiometric by-product under the selected equation. These are reaction-level waste profiles only and do not include solvent, excess-reagent, catalyst, work-up, purification, or treatment streams. Accordingly, they are not substitutes for a complete process waste inventory.

A qualitative hazard screen was added to prevent material-efficiency metrics from being interpreted as safety indicators. Publicly documented hazard information identifies hydrogen and ethene as highly flammable substances, while ethanol is classified as a highly flammable liquid. Acetic anhydride and concentrated acetic acid have important flammability and corrosivity hazards; silver nitrate is an oxidizing, corrosive substance with high aquatic toxicity; and nitrobenzene and aniline have significant acute, chronic and environmental hazard classifications. These observations are used only as qualitative flags, not as a

numerical hazard score, because hazard magnitude depends on concentration, exposure conditions, handling context, and system boundary (PubChem, 2026a–2026h).

DISCUSSION

Why Yield and Atom Economy Answer Different Questions

A high percentage yield indicates that a large fraction of a limiting reactant has been converted into the desired product under the stated experimental conditions. Atom economy asks a different question: what fraction of the stoichiometric reactant mass can, in principle, appear in the desired product? A reaction may therefore have a high yield but a modest atom economy if a substantial fraction of reactant atoms are necessarily expelled as by-products.

Conversely, a reaction with excellent atom economy can still have poor practical efficiency if conversion is incomplete or large quantities of excess reagents and solvents are required (Dicks & Hent, 2015; Sheldon, 2018).

Interpretation of the Aspirin Example

The aspirin equation provides a clear example. Salicylic acid and acetic anhydride combine to form aspirin and acetic acid. The calculated atom economy is about 75%, consistent with the commonly used stoichiometric calculation for this reaction (Dikobe et al., 2026). The remaining 25% is not evidence of laboratory failure; it is inherent to the balanced reaction because acetic acid is a stoichiometric coproduct. Improving isolation yield can increase RME, but it cannot change the atom economy unless the chemical transformation itself is redesigned.

Educational Implications

Green-metric calculations can be integrated into existing lessons on mole concept, stoichiometry, limiting reagent, percentage yield, organic reactions, and chemical equations. Students can first balance a reaction, calculate molar masses, determine theoretical yield, and then calculate atom economy. The same dataset can subsequently be expanded to discuss solvent selection, hazard, energy demand, and life-cycle thinking. This sequence turns green chemistry from a qualitative slogan into a quantitative decision framework.

Process-Level Interpretation

The present analysis deliberately stops at the reaction-equation level. A complete industrial assessment would need to include excess reagents, solvents, catalysts, extraction and purification materials, water use, energy, emissions, toxicity, recovery, recycling, and the fate of all coproducts. The literature on green metrics emphasizes that atom economy and other mass-based indicators are valuable but incomplete when used alone (Trost, 1991; Sheldon, 2018). Thus, the numerical comparisons in this study should be interpreted as an early-stage stoichiometric screen rather than a full life-cycle assessment.

Relevance to Safer Chemistry

Atom economy is also connected to the prevention principle because avoiding the formation of unwanted material can reduce the need for treatment and disposal. However, material efficiency should not be confused with chemical safety. A reaction can have excellent atom economy while using hazardous substances.

Therefore, any practical selection of a reaction should combine material metrics with hazard and exposure information, consistent with the broader twelve principles of green chemistry (Anastas & Warner, 1998).

Table 6. Interpretation of the metrics used in the present study

Metric	What it measures	Main limitation
Atom economy	Theoretical incorporation of stoichiometric reactant mass into desired product	Does not include yield, excess reagents, solvents or work-up
Stoichiometric waste potential	Non-product stoichiometric mass relative to desired product mass	Not a complete process waste measure
Simplified RME	Effect of yield on theoretical atom economy	Requires broader mass accounting for real process assessment
E-factor / PMI	Broader process material or waste intensity	System boundaries and data quality strongly affect interpretation

Extended Interpretation: Solvent, Energy, Hazard and Life-Cycle Dimensions

A recent aspirin-focused chemistry-education study demonstrates the value of combining atom economy, carbon efficiency, RME, E-factor, mass balances, energy considerations, and life-cycle thinking in a process-oriented teaching context (Dikobe et al., 2026). In a broader process-sustainability context, Lucas et al. (2024) also showed why mass- and energy-based process metrics should be interpreted alongside life-cycle impact indicators. Together, these studies support extending the present framework while maintaining a strict distinction between published process evidence and the present study's calculated stoichiometric scenarios.

The expanded framework clarifies why a reaction cannot be labelled universally “green” from atom economy or stoichiometric mass efficiency alone. Solvents and water can dominate material inputs in real processes, while energy demand can contribute substantially to environmental burden. Hazard assessment is also independent of atom economy: a reaction may use reactants or solvents with significant health or environmental hazards even when its material efficiency is high.

Accordingly, the recommended decision sequence is to use atom economy and stoichiometric mass metrics as early screens, then add actual yield, complete material inventories, solvent and energy data, hazard information, and life-cycle indicators as process data become available (Sheldon, 2018; Jiménez-González et al., 2011).

The revised approach also improves applicability beyond a single educational example. Yield sensitivity is now demonstrated across all six selected reactions, while the process-level metric table explicitly shows which additional data are required to move from theoretical screening to experimental or industrial assessment. This distinction prevents unsupported numerical claims while making the framework directly extensible to laboratory records, published process data, or future experimental studies.

Metric Divergence Analysis

The six-reaction dataset illustrates an important analytical point: green metrics can change when the assessment boundary changes. Atom economy is fixed by the balanced reaction and desired product definition, whereas yield-sensitive reaction mass efficiency changes when an assumed or measured yield changes. Stoichiometric E-factor and PMI proxies describe only the non-product mass contained in the reaction equation.

Once solvents, water, excess reagents, recovery, purification, energy, and hazards are introduced, the process picture can differ substantially from the stoichiometric picture. Therefore, an efficiency value

obtained at one assessment level should be interpreted as a partial observation rather than a complete sustainability conclusion.

Table 7. Integrated green-metrics matrix showing the assessment boundary and evidence status.

Assessment layer	Metric information /	Primary question	Present study
Reaction	Atom economy	How much stoichiometric reactant mass can enter the desired product?	Calculated
Reaction	SWP / stoichiometric E-factor	How much non-product stoichiometric mass accompanies product formation?	Calculated
Reaction yield +	Simplified RME	How does assumed yield alter material efficiency?	Calculated for all six reactions
Process	Full E-factor / PMI	What is the material burden when process inputs and waste streams are included?	Proxy only; full inventory required
Process	Solvent / energy intensity	What mass and utility burdens arise from processing?	Data requirements identified
Safety / life cycle	Hazard + LCA	What health, environmental and upstream/downstream burdens remain?	Framework identified; not quantified

Worked Example: Aspirin as A Stoichiometric-To-Process Bridge

For the aspirin reaction, the balanced stoichiometric equation gives an atom economy of 75.00%. At an assumed 80% isolated yield, the restricted RME expression gives 60.00%. The difference between these values is not a second kind of waste measurement; it represents the effect of yield within the deliberately simplified model.

A complete process assessment would then add the actual quantities of solvents, water, excess reagents, catalysts, purification aids, energy, and waste streams. This worked example shows how one reaction can move from a theoretical calculation to a process-data checklist without presenting unsupported process measurements.

Literature-Based Process Case Study Benchmark

To demonstrate how the proposed framework can connect with published process-oriented evidence, a literature benchmark was added separately from the six-reaction dataset. Dikobe et al. (2026) reported a chemistry-education case study comparing routes for salicylic-acid preparation within an aspirin-manufacture system.

Their published comparison included atom economy, reaction mass efficiency, isolated yield, and E-factor under the study's stated system boundary. The values below are reproduced only as a literature benchmark; they are not experimental measurements generated by the present study.

Table 8. Literature-based benchmark from Dikobe et al. (2026). Values are reported under that study's stated system boundary and are not part of the present six-reaction calculations.

Published route	Atom economy (%)	RME (%)	Yield (%)	E-factor
Route 1 (phenol-based)	65.22	41.42	84.44	1306.51
Route 3 (methyl-salicylate-based)	54.88	27.86	87.96	3471.50

The literature case also demonstrates why yield and atom economy should not be interpreted in isolation. In the cited study, the route data were embedded in a broader systems-thinking and life-cycle framework. This provides an external example of the transition from reaction metrics to process and life-cycle assessment without treating the present stoichiometric calculations as a substitute for a complete process inventory.

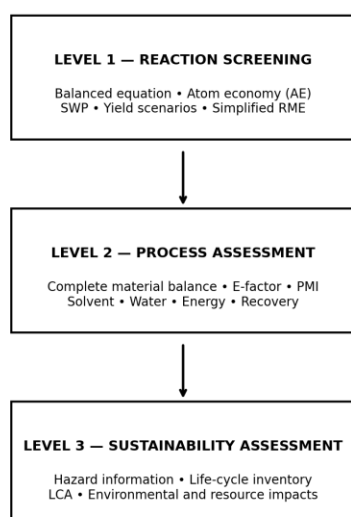
Industrial Context and Data Scaling

Industrial use of green metrics requires a wider system boundary than the balanced-equation calculations used here. Published green-chemistry literature has long shown that waste intensity varies substantially across sectors, and recent process-oriented reviews continue to emphasize the importance of combining mass-based indicators with energy and life-cycle information. Accordingly, the six reactions in the present paper should be viewed as reaction-level teaching and screening examples, while industrial assessment requires plant-specific material balances, solvent and water inventories, utility data, recovery rates, waste treatment, and defined life-cycle boundaries.

Proposed Stoichiometric-to-Process Green Assessment Pathway

The framework proposed in this study is intentionally staged. Level 1 can be completed directly from a balanced equation and molar masses, preserving the reproducibility of the present calculations. Level 2 requires complete material and utility records, while Level 3 requires hazard information and life-cycle inventory data. This structure allows future experimental or literature-based datasets to be added without replacing or retrospectively altering the stoichiometric results.

PROPOSED STOICHIOMETRIC-TO-PROCESS GREEN ASSESSMENT PATHWAY



Present study: Level 1 fully calculated + selected Level 2 proxies + Level 3 data requirements identified

Figure 4. Proposed Stoichiometric-to-Process Green Assessment Pathway. Each level adds information; higher-level assessment does not replace the transparent reaction-level calculations.

LIMITATIONS

The study remains a stoichiometric secondary analysis and therefore does not provide new experimental measurements. The selected reactions are representative educational examples rather than a statistically representative sample of industrial chemistry. Atom economy and the stoichiometric E-factor/PMI proxies depend on the chosen reaction equation, desired product definition, and system boundary. The extended yield-sensitivity analysis uses assumed yields solely as mathematical scenarios and should not be interpreted as literature or laboratory yield data. Full process E-factor, PMI, solvent intensity, energy intensity, hazard assessment, and life-cycle indicators require complete process inventories that were not available for all six reactions. Future work should therefore incorporate experimentally measured or carefully documented literature process data and apply the expanded framework at laboratory and industrial scales.

CONCLUSION

This study demonstrates that balanced chemical equations can be transformed into reproducible green-chemistry metrics and that different metrics reveal different dimensions of reaction efficiency. Across six representative reactions, calculated atom economy ranged from 60.90% to 100.00%. The expanded yield-sensitivity analysis shows how assumed yield changes simplified RME across the complete reaction set while leaving atom economy unchanged. Stoichiometric E-factor and PMI proxies further expose differences in non-product material generation under a clearly defined boundary. The results reinforce that reaction yield, atom economy, E-factor, PMI, solvent use, energy demand, hazard, and life-cycle information are complementary rather than interchangeable measures.

The revised framework is transparent, reproducible, and suitable for chemistry education and preliminary process screening. Its principal value is not to declare a single reaction universally greener, but to demonstrate how reaction structure and yield influence measurable efficiency indicators and to make the missing process information explicit. Future studies can integrate actual experimental or literature-based mass balances, solvent and water consumption, energy use, hazard scores, carbon efficiency, complete E-factor and PMI calculations, and life-cycle indicators. Such integration would move the assessment from stoichiometric screening toward a comprehensive sustainability evaluation while preserving the reproducibility of the present calculations.

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Declarations

Ethical approval

Not applicable. The study used published chemical information and stoichiometric calculations and did not involve human participants, animals, or identifiable personal data.

Conflict of interest

The author declares that there is no known financial or personal conflict of interest that could have influenced the work reported in this paper.

Data availability

All numerical results reported in the manuscript are reproducible from the balanced equations, molar masses, formulas, and metric definitions. The core reaction dataset is provided in Table 1; the aspirin yield-

sensitivity dataset is in Table 2; and the expanded six-reaction yield-sensitivity and stoichiometric mass-metric dataset is provided in Table 4. No experimental process inventory, solvent log, energy record, or hazard score is represented as measured data.

Author contribution

The author conceived the study, performed the stoichiometric calculations, interpreted the results, and prepared the manuscript.

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