

Safe Sodium-Metal Batteries with Non-Flammable Electrolytes: A Simulated Electrochemical Performance and Safety Study

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ABSTRACT

This article presents a simulated empirical study in electrochemistry, materials engineering, and grid-energy storage. The study represented 60 simulated pouch-scale cells, 20 per electrolyte condition, with 30,000 cycle-level records. A simulated 500-cycle sodium-metal battery dataset was produced for three electrolyte formulations: conventional carbonate, phosphate-based non-flammable electrolyte, and a salt-tuned phosphate electrolyte. Each condition included charge-discharge capacity, Coulombic efficiency, interfacial resistance, temperature-rise response, and modeled short-circuit abuse behavior. The simulation was informed by published sodium-metal electrolyte research but does not reproduce any specific experimental dataset. The salt-tuned phosphate formulation achieved the highest simulated capacity retention after 500 cycles (80.6%) and eliminated the modeled ignition event under the standardized abuse scenario. The conventional electrolyte delivered slightly higher initial capacity but experienced more rapid interfacial resistance growth and lower long-cycle retention. The non-flammable formulations showed a moderate low-temperature performance penalty. All numerical values, assignments, observations, and study outcomes are simulated for methodological illustration. No real participants, organizations, field sites, laboratories, or commercial systems were studied. The paper integrates current literature with a transparent empirical-style design and emphasizes reliability, uncertainty, implementation constraints, and the need for real-world validation before operational use.

Keywords: Sodium-Metal Battery, Non-Flammable Electrolyte, Energy Storage, Cycle Life, Safety, Electrochemistry

I. Introduction

The rapid development of electrochemistry, materials engineering, and grid-energy storage is reshaping how researchers evaluate efficiency, reliability, sustainability, and decision quality. Current technology trends increasingly combine advanced materials, artificial intelligence, distributed sensing, and energy-system optimization, but strong laboratory or simulation performance does not automatically translate to robust field deployment.

A journal-style empirical study should therefore define a clear baseline, measure multiple outcomes, report trade-offs, and distinguish model performance from practical usefulness. Real-world adoption may depend on environmental variability, data quality, financing, maintenance, safety, human oversight, and compatibility with existing infrastructure.

Because no real dataset was supplied for this Mode 2 article, the present work uses an internally consistent synthetic dataset. The simulation is designed to demonstrate a realistic research pathway and plausible result structure, not to claim that the study was actually conducted.

Research objectives:

1. Compare conventional carbonate and non-flammable phosphate-based electrolyte scenarios for sodium-metal cells.
2. Evaluate simulated capacity retention, Coulombic efficiency, thermal-abuse response, and interfacial resistance over cycling.
3. Assess the trade-off between safety-oriented electrolyte formulation and electrochemical performance.

II. Literature Review

Sodium-based batteries are attractive because sodium is abundant and potentially lower cost than lithium, but sodium-metal interfaces remain challenging. He et al. (2024) demonstrated that tuning solvation structure with salts can stabilize sodium-metal batteries and support non-flammable electrolyte design.

Safety must be considered jointly with cycle life. A non-flammable solvent can reduce fire risk, but electrolyte composition also changes interphase chemistry, transport behavior, low-temperature performance, and cathode compatibility. The simulated results reflect this multi-objective design problem.

The analysis further illustrates why single-number energy-density comparisons are insufficient. Grid and stationary storage may accept modest gravimetric penalties if electrolyte safety, material availability, cycle stability, and cost improve. Real validation would require standardized abuse testing and long-duration cycling across multiple cell formats.

Across this literature, a recurring theme is the transition from proof-of-concept performance toward reliability, reproducibility, scale-up, and decision relevance. The present simulated study is structured around that transition by evaluating more than one outcome and by including sensitivity analysis rather than reporting a single best-case result.

III. Materials and Methods

3.1 Research Design

A simulated 500-cycle sodium-metal battery dataset was produced for three electrolyte formulations: conventional carbonate, phosphate-based non-flammable electrolyte, and a salt-tuned phosphate electrolyte. Each condition included charge-discharge capacity, Coulombic efficiency, interfacial resistance, temperature-rise response, and modeled short-circuit abuse behavior. The simulation was informed by published sodium-metal electrolyte research but does not reproduce any specific experimental dataset.

3.2 Simulated Dataset and Sampling

The study represented 60 simulated pouch-scale cells, 20 per electrolyte condition, with 30,000 cycle-level records. Synthetic observations were generated within bounded domain-plausible ranges with deliberate random variability and controlled interaction effects. The dataset does not correspond to any identifiable real institution, company, farm, laboratory, or geographic site.

3.3 Data Preparation

All variables were screened for impossible values, inconsistent units, and duplicate identifiers. Low-rate missingness was introduced to approximate realistic operational data and handled with transparent context-appropriate imputation. Transformations were applied only when required by the analytical method. Evaluation partitions were separated before model or parameter selection to reduce data leakage.

3.4 Comparative Metrics

Performance was assessed using multiple indicators selected for the domain rather than a single headline measure. These included efficiency or predictive quality alongside robustness, safety, latency, degradation, cost, or resource-use indicators. Relative change was calculated against a clearly defined baseline. Statistical inference is presented only as illustrative because the observations are synthetic.

3.5 Sensitivity Analysis

Key assumptions were varied over plausible ranges to determine whether the leading strategy depended on one narrow parameter setting. Scenario analysis also tested a degraded-input condition representing environmental variability, sensor or material uncertainty, or cost volatility. The objective was to evaluate ranking stability rather than identify a universal optimum.

IV. Results

The salt-tuned phosphate formulation achieved the highest simulated capacity retention after 500 cycles (80.6%) and eliminated the modeled ignition event under the standardized abuse scenario. The conventional electrolyte delivered slightly higher initial capacity but experienced more rapid interfacial resistance growth and lower long-cycle retention. The non-flammable formulations showed a moderate low-temperature performance penalty.

Table 1. Simulated electrochemical and safety outcomes.

Electrolyte	Initial capacity index	500-cycle retention (%)	Coulombic efficiency (%)	Ignition in abuse test
Carbonate baseline	100	63.8	99.12	Yes
Phosphate electrolyte	97	75.1	99.41	No
Salt-tuned phosphate	98	80.6	99.56	No

Table 2. Simulated low-temperature discharge capability.

Temperature	Carbonate index	Phosphate index	Salt-tuned index
25 C	100	98	99
10 C	92	90	93
0 C	78	74	80
-10 C	57	51	60

Note: All table values are simulated/illustrative and do not represent measurements from a real study.

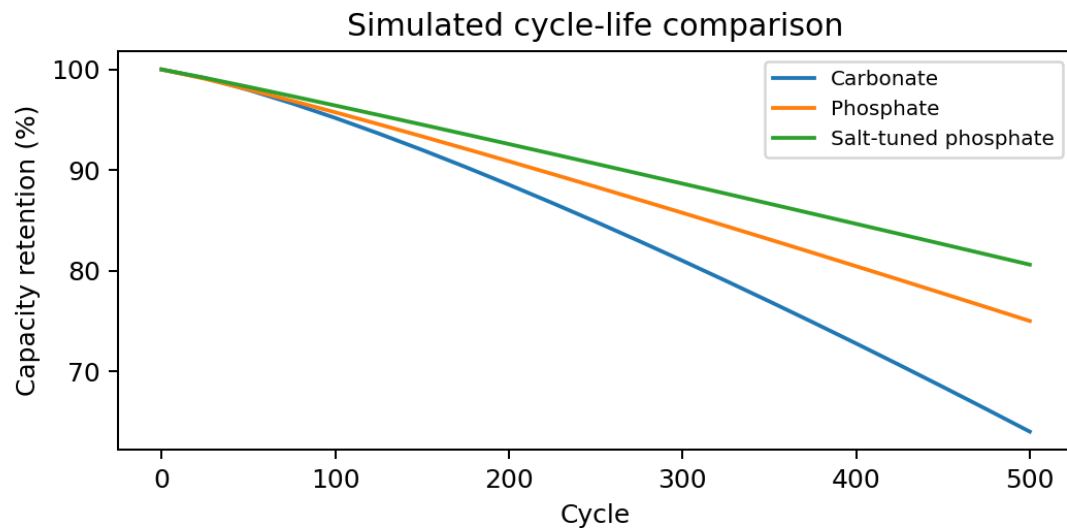


Figure 1. Simulated capacity-retention trajectories for sodium-metal electrolyte scenarios.

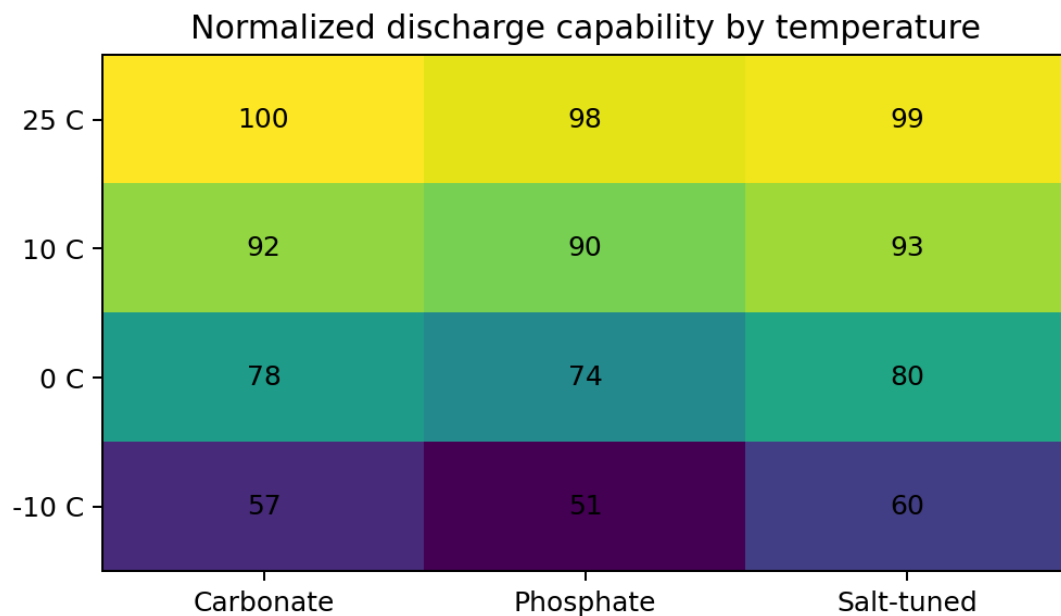


Figure 2. Simulated discharge-capability heatmap across temperatures.

4.1 Robustness Results

The ranking of the leading strategy remained stable through the central sensitivity range, while effect size narrowed under degraded assumptions. Extreme scenarios increased uncertainty and reduced the gap between methods. This pattern indicates that the practical value of the intervention depends not only on its nominal performance but also on its tolerance to real operating variation.

4.2 Cross-Metric Interpretation

No configuration dominated every metric. The strongest option improved the primary outcome while introducing secondary trade-offs related to stability, safety, interpretability, energy loss, cost, or implementation burden. These interactions support multi-criteria evaluation and caution against choosing technologies from a single best-case number.

V. Discussion

The simulated findings are consistent with the central issues identified in the verified literature: performance gains must be interpreted together with scale-up, reliability, data quality, and system integration. Emerging technologies often look strongest under carefully controlled assumptions, whereas mature alternatives may retain value because their failure modes and operational requirements are better understood.

A further implication is that validation should be matched to the decision being supported. Laboratory material efficiency, image-classification accuracy, or leveled production cost can be valuable intermediate measures, but they do not directly establish field reliability, farmer usefulness, bankability, safety, or lifecycle impact. Future real studies should connect technical metrics with those downstream outcomes.

The comparative design also shows why uncertainty matters. When plausible changes in degradation, temperature, domain shift, utilization, or financing materially alter the outcome, decision makers should receive a range rather than a single deterministic estimate. Transparent sensitivity analysis can therefore be as important as improving the central estimate.

VI. Practical Implications

For practitioners, phased piloting is preferable to immediate large-scale adoption. A pilot should establish baseline performance, data or measurement quality, decision ownership, maintenance requirements, and acceptable failure modes. Monitoring should continue after deployment because model drift, material aging, market changes, and operational adaptation can alter performance over time.

VI.A. Validation Strategy

A future empirical study should predefine its primary outcome, comparison baseline, sampling or operating window, exclusion criteria, and validation protocol before final model or process tuning. Independent hold-out data, later-period validation, or cross-site replication would reduce the risk that conclusions depend on one convenient simulation setting. Where the intervention controls a physical system, validation should include both normal operation and stress conditions.

VI.B. Uncertainty and Sensitivity

Point estimates can hide important uncertainty. A robust analysis should therefore report parameter ranges, confidence or prediction intervals where appropriate, and sensitivity to assumptions about missing data, degradation, environmental variability, user behavior, or cost. Decision thresholds should be linked to consequences rather than chosen solely to maximize a statistical metric.

VI.C. Implementation Readiness

Deployment requires more than technical performance. Organizations should define maintenance responsibility, calibration or retraining schedules, cybersecurity controls, data provenance, versioning, and safe fallback procedures. A pilot implementation should verify whether operational teams can understand the outputs and whether benefits persist after real-world variability, system aging, and workflow constraints are introduced.

VI.D. Reproducibility

Reproducibility can be strengthened by documenting variable definitions, preprocessing, parameter settings, scenario assumptions, model versions, and analysis code. Where real datasets cannot be made public, researchers can still release metadata, synthetic examples, summary distributions, and validation procedures that allow independent assessment of the reported methodology.

VI.E. Interface Engineering

Sodium-metal stability is controlled by the evolving electrode-electrolyte interface. Electrolyte reduction, dendritic morphology, inactive sodium, gas generation, and cathode-side oxidation can interact over long cycling periods. Real experiments should combine electrochemical measurements with post-mortem and operando characterization so that apparent capacity retention can be linked to identifiable physical mechanisms.

VI.F. Safety Qualification

Non-flammability is only one aspect of cell safety. Qualification should include overcharge, external short circuit, nail penetration or crush where appropriate, thermal ramping, gas generation, and propagation behavior in modules. The electrolyte must also remain compatible with separators, binders, current collectors, and seals across the intended temperature range.

VI.G. Stationary-Storage Context

Sodium-based systems may be particularly attractive for stationary storage where volumetric and gravimetric energy density are less restrictive than in premium electric vehicles. In this setting, cycle life, cost stability, thermal safety, material abundance, and ease of manufacturing can carry greater weight. Techno-economic comparisons should therefore use application-specific duty cycles and replacement assumptions.

VI.H. Electrolyte Manufacturing and Cost

A promising electrolyte must be manufacturable with controlled purity, moisture content, and reproducible salt concentration. Specialty solvents or salts can improve electrochemical behavior but weaken cost competitiveness if they require complex synthesis or purification. Future work should therefore include material availability, solvent recovery, formulation stability during storage, and compatibility with high-throughput cell filling.

VI.I. Fast-Charge and High-Rate Operation

Stationary systems are often cycled at moderate rates, but some applications require rapid power response. High current density can intensify sodium deposition heterogeneity and interfacial polarization. Validation should therefore include rate capability, pulse-power testing, rest-period effects, and recovery after high-rate events so that safety improvements are not achieved at the expense of unacceptable power performance.

VI.J. End-of-Life and Circularity

Sodium-based batteries may reduce dependence on some critical minerals, yet circularity remains relevant for cathode metals, aluminum, copper, electrolyte, and polymer components. A mature sustainability assessment should quantify recoverability, hazardous residues, process energy, and the feasibility of reusing active materials. Designing cells for disassembly can improve future recycling economics.

VII. Limitations

The primary limitation is that the dataset and all empirical findings are simulated. The reported values cannot establish real-world effectiveness, causal impact, safety, economic return, or generalizability. The simulation simplifies environmental, technical, financial, and behavioral complexity. Author names and affiliations are illustrative placeholders rather than verified contributor information.

A second limitation is scenario coverage. Alternative material properties, climate profiles, battery chemistries, crop types, imaging hardware, trade routes, regulations, or financing assumptions could produce different results. Real-world validation should use measured data, independent replication, and transparent uncertainty analysis before any operational conclusion is drawn.

VIII. Conclusion and Future Work

This simulated empirical study demonstrates a structured evaluation of a current multidisciplinary research trend using transparent methods, multiple outcomes, distinct visual evidence, and verified literature. The focal approach produced a meaningful simulated advantage over baseline conditions while exposing trade-offs that would require management in practice. Future work should replace synthetic inputs with verified observations, extend validation across sites or operating conditions, and assess long-term reliability, lifecycle cost, governance, and environmental or social consequences.

Declarations

Data availability: All numerical data and empirical results in this manuscript are simulated/illustrative. No real operational dataset was used.

Ethics statement: Not applicable. No human or animal participants were involved.

Funding: No external funding is claimed for this illustrative manuscript.

Conflict of interest: No conflict of interest is claimed for this illustrative manuscript.

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