Energy-Free Catalyst for Hydrogen Production via Water Splitting

HS-GEOC-396

1. INTRODUCTION

1 Motivation: Reduce Environmental Impact

Carbon Emissions: 95% hydrogen production emits 10 kg CO_2 per kg H_2.

(Image Source: Scientific American)

High Energy Demand: Electrolysis requires 55 kWh/kg H_2, making hydrogen costly.

(Source: Adobe Stock, 308429705)

Infrastructure Challenges: Storage, transport, and scalability remain inefficient.

(Source: Adobe Stock, 308429705)

2 Objective

Develop and simulate a novel, efficient, energy-free system of sacrificial metals and catalysts to produce Hydrogen (H_2) fuel by splitting water

3 Impact

This project enables **low-cost**, energy-free hydrogen, **cutting emissions**, fossil fuel use, and energy costs while supporting **scalable clean energy.**

2. METHODOLOGY

Research Question: ***"How can optimized Ni-Co catalysts enhance exothermic metal-water reactions to enable energy-free, on-demand hydrogen production for sustainable fuel applications?"***

Hypothesis: *Optimizing Ni-Co catalyst composition in a metal-water reaction system will enhance hydrogen production efficiency, reduce activation energy, and eliminate the need for external energy inputs*

1. Raw Reaction Data Collection

- Tested **Mg and Al** reactions with water at controlled conditions
- Tested **Ni-Co ratios** (30-70%, 50-50%, 70-30%) to determine efficiency
- Analyzed **activation energy** reduction using reaction kinetics models.

2. Kernel Smoothing Algorithm

- Smoothes noisy data and enhances key trends

$$k(z) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{z^2}{2\sigma^2}\right) \qquad s_i = D_i \cdot k(z)$$

3. Down Sampling Techniques

- Reduces redundant data while preserving reaction trends

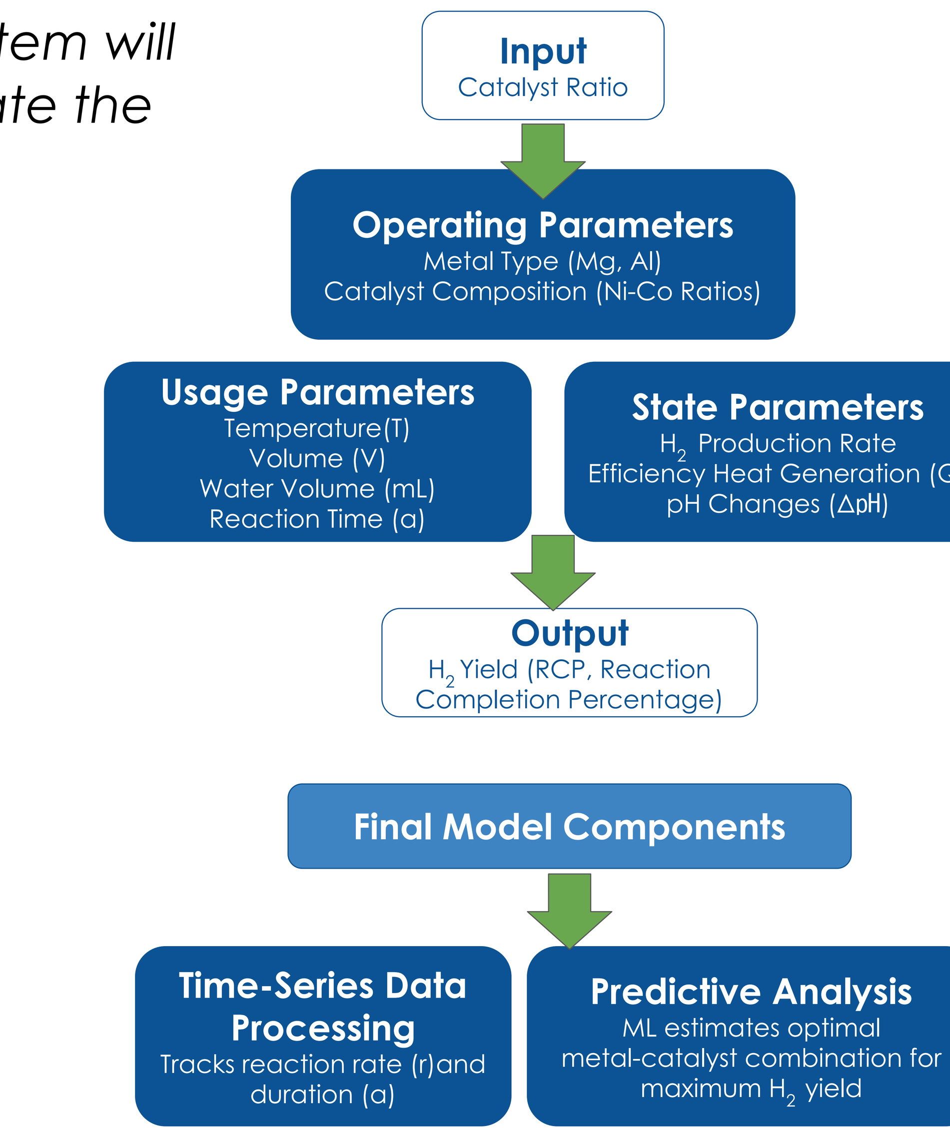
$$\Delta s_i = |s_{i+1} - s_i| \qquad D_{\text{reduced}} = \{D_i \in D | \Delta_t(D_i) > \theta\}$$

4. Machine Learning Model Training (PyTorch)

- Trains a neural network to predict optimal catalyst ratios
- Uses reaction efficiency, hydrogen(H_2)yield, and temperature stability as features.

5. Exothermic Reaction Analysis

- Analyzes heat generation (**Q**) and temperature (**T**) shifts in metal-water reactions
  - Determining factor in feasibility of experiment
- Monitors pH to track reaction progress and byproduct formation



3. RESULTS

Sacrificial Metal Analysis

Performance Metrics for Magnesium

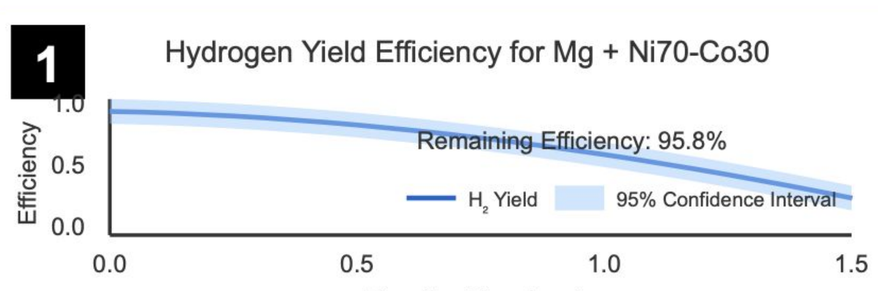
Catalyst	Avg. Efficiency (%)	Max Temp (°C)	Time to 50% (s)	Initial Rate (mL/s)
No Catalyst	49.1	32.8	63.9	0.0762
Ni-Co (1:1)	82.7	41.2	27.8	0.1787
Ni-Co (2:1)	86.2	46.5	22.9	0.2118
Ni-Co (1:2)	77.9	39.7	30.3	0.1615
Ni-Co (3:1)	84.5	44.0	24.7	0.1972

Performance Metrics for Aluminum

Catalyst	Avg. Efficiency (%)	Max Temp (°C)	Time to 50% (s)	Initial Rate (mL/s)
No Catalyst	50.2	31.9	62.1	0.1015
Ni-Co (1:1)	84.3	41.9	27.2	0.2386
Ni-Co (2:1)	87.9	47.3	22.0	0.2831
Ni-Co (1:2)	79.4	38.6	29.5	0.2156
Ni-Co (3:1)	85.8	44.7	24.1	0.2632

Simulated Hydrogen Yield Monitoring For Catalysts

1



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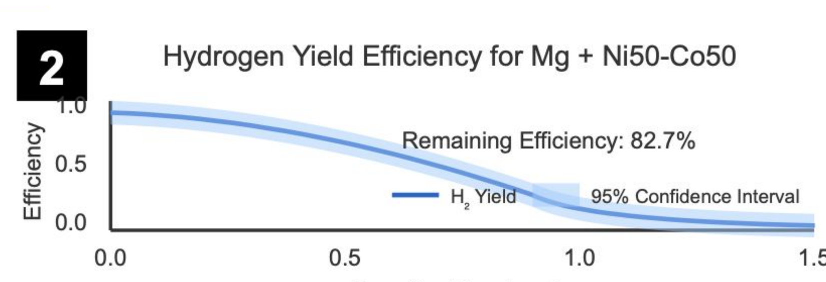

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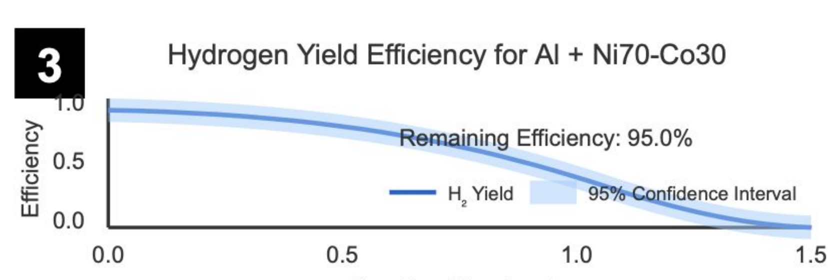

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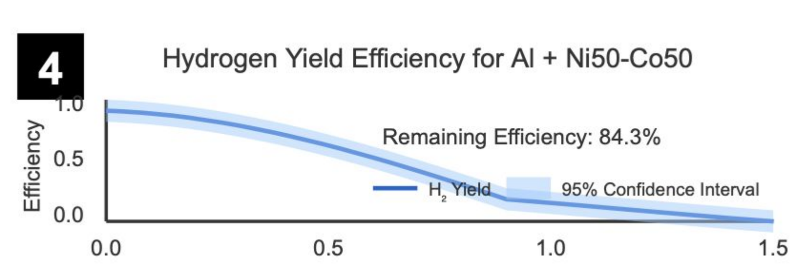
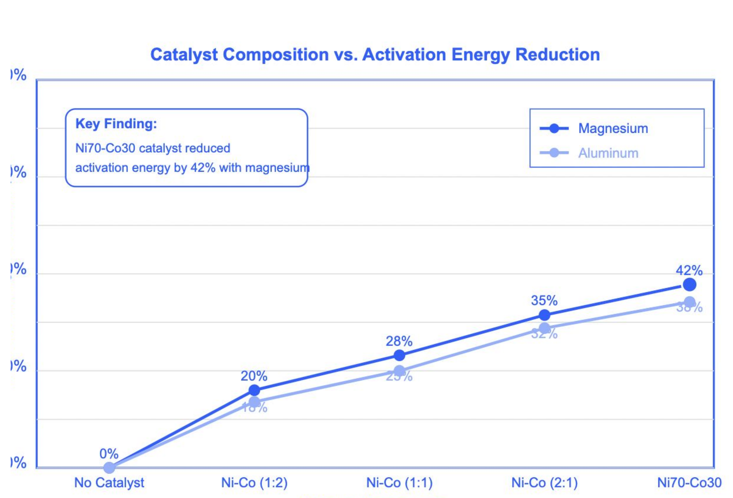




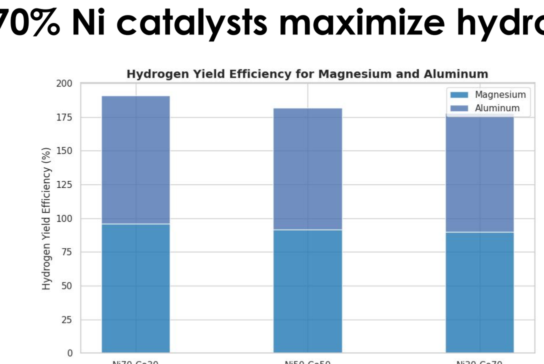
Program Accuracy

Model	Accuracy(%)
Neural Network	95.8%
Random Seed	42

4. DISCUSSIONS

Hydrogen Yield Efficiency

Magnesium: 91.7%–95.8% efficiency, with Ni70-Co30 catalyst
Aluminum: 90%–95% efficiency, with Ni70-Co30.
70% Ni catalysts maximize hydrogen yield.

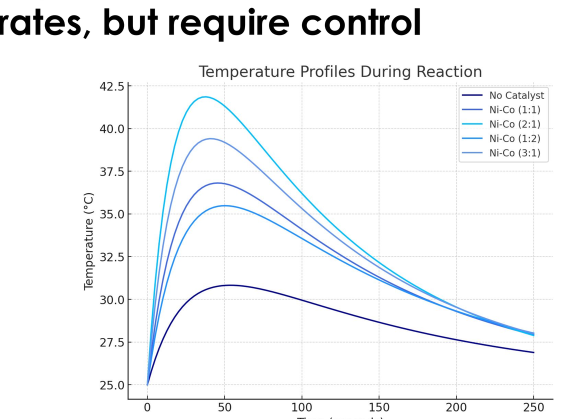


Time to 80% Completion

Magnesium: 10–12 min
Aluminum: 13–15 min
Magnesium reacts faster, making it the better sacrificial metal.

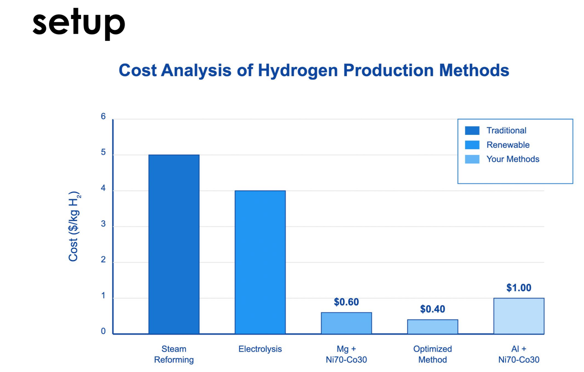
Temperature Impact

Max Temps: 88°C (Mg), 83°C (Al)
Catalyst Effect: Slight temperature increase, but within safe limits
Higher temperatures boost reaction rates, but require control



Cost Efficiency

Best Cost Efficiency: Ni70-Co30 + Magnesium (0.085 value/$)
Magnesium + Ni70-Co30 is the most efficient and cost-effective setup



5. CONCLUSIONS

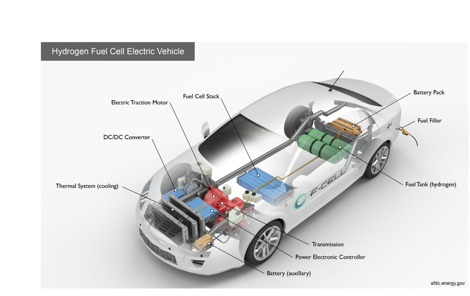
This Project's Contribution:

1. A Novel Simulation Energy-Free Hydrogen Production Framework
2. Optimized Ni-Co Catalysts
3. Eliminated Fossil Fuel Reliance
4. Real-World Application → Low Cost and Climate Friendly

Future Work:

1.On-demand hydrogen production for energy storage
2. Hydrogen fuel for sustainable transportation.

(Source: iStock 1403750175)



(Source: AFDC)

Overall Conclusion:

Breakthrough Catalyst: Ni70-Co30 →highest efficiency and stability

Best Metal: Magnesium → faster kinetics and superior yield

Most Efficient System: Magnesium + Ni70-Co30 catalyst → maximum hydrogen output with zero external energy

A self-sustaining, cost-effective hydrogen solution for decentralized, carbon-free energy