1. Catalyst Performance Analysis

A. Turnover Frequency (TOF) vs. Temperature (°C)

- Why? Higher temperatures often improve reaction rates but may also cause catalyst deactivation.

- Expected Insight: Identify the optimal temperature range for maximum TOF without compromising stability.

- Plot Type: Scatter Plot

B. Selectivity (%) vs. Adsorption Energy (eV)

- Why? Adsorption energy influences how well reactants bind to the catalyst, impacting product selectivity.

- Expected Insight: Find the optimal adsorption energy range for maximizing selectivity.

- Plot Type: Scatter Plot

C. Stability (h) vs. TOF (s⁻¹)

- Why? High TOF may lead to faster catalyst deactivation, reducing stability.

- Expected Insight: Determine which catalysts balance high TOF with long-term stability.

- Plot Type: Scatter Plot

2. Emissions Reduction & Sustainability

A. CO₂ Conversion Efficiency (%) vs. Stability (h)

- Why? A catalyst must sustain high CO₂ conversion for a long time to be effective in emissions reduction.

- Expected Insight: Identify which catalysts maintain high efficiency over extended operational hours.

- Plot Type: Scatter Plot

B. CO₂ Conversion Efficiency (%) vs. Temperature (°C)

- Why? Higher temperatures may enhance CO₂ conversion but could also increase energy consumption.

- Expected Insight: Find the temperature range that maximizes CO₂ conversion without excessive energy use.

- Plot Type: Line Plot

C. Emissions Reduction (kg CO₂-eq) vs. Catalyst Type

- Why? Different catalyst types contribute differently to emissions reduction.

- Expected Insight: Rank catalysts based on their contribution to lowering carbon emissions.

- Plot Type: Bar Chart

3. Process Efficiency & Operating Conditions

A. Activation Energy (kJ/mol) vs. TOF (s⁻¹)

- Why? Lower activation energy often leads to higher reaction rates (TOF).

- Expected Insight: Identify catalysts with the best trade-off between low activation energy and high TOF.

- Plot Type: Scatter Plot

B. Pressure (bar) vs. TOF (s⁻¹)

- Why? Some reactions require high pressure for optimal conversion, but excessive pressure increases costs.

- Expected Insight: Determine the optimal pressure range for maximizing TOF.

- Plot Type: Scatter Plot

4. Overall Correlation Analysis

A. Correlation Heatmap

- Why? A heatmap shows relationships between all variables in a single view.

-Expected Insight: Identify strong correlations between catalyst properties, performance, and emissions metrics.

- Plot Type: Heatmap

Research Development Plan: Catalytic Processes for Emissions Reduction

1. Define Research Objectives

- Main Goal: Explore innovative catalytic processes for low-carbon refining using computational and open-source tools.

- Specific Aims:

- Identify catalysts with high potential for emission reduction.

- Create a simulation model to evaluate catalytic efficiency under refinery-like conditions.

- Suggest practical implementations or improvements for scalable solutions.

2. Explore Open-Source Databases and Tools

Leverage these resources to gather data and support your research:

- Open Catalysis Project:

- Provides extensive catalytic reaction datasets and reaction network insights.

- [Website](<https://opencatalysisproject.org>)

- Material Project:

- Access properties of materials used in catalysts.

- [Website](<https://materialsproject.org>)

- Python Libraries for Modeling:

- ASE (Atomic Simulation Environment): Simulate catalytic reactions.

- RDKit: Analyze chemical reactions and molecular structures.

3. Research Methodology

- Step 1: Literature Review

- Analyze key papers on low-carbon catalytic innovations.

- Highlight gaps in current studies and practical limitations for scaling.

- Step 2: Dataset Analysis

- Use data from open-source repositories to identify promising catalysts.

- Step : Simulation Development

- Build a Python-based model using ASE or a similar tool.

- Simulate catalytic processes under variable conditions (temperature, pressure, reactant concentration).

- Step 4: Emissions Analysis

- Quantify reductions in emissions based on catalytic reaction efficiencies.

- Step 5: Comparative Study

- Evaluate the simulated results against existing lab-scale and industrial benchmarks.

4. Proposed Deliverables

- A detailed report showcasing:

- Simulation framework and methodology.

- Data visualization of catalytic performance (graphs, charts).

- Recommendations for implementation in industrial processes.

- A computational model or script that other researchers/students can replicate.