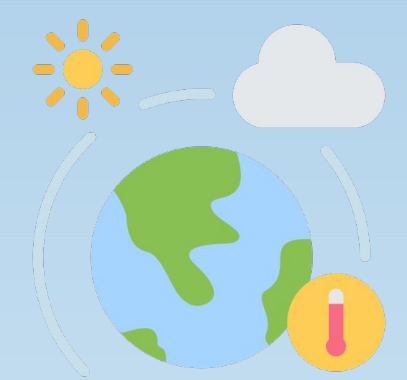


Research Motivation



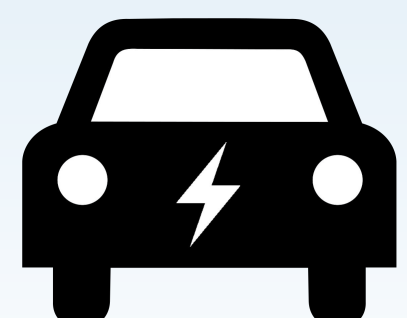
Climate change: Driven by increasing carbon dioxide emissions.



Transportation: Cars and vans accounted for 48% of transportation-related CO₂ emissions.



Natural Disasters: Rising temperatures and sea levels



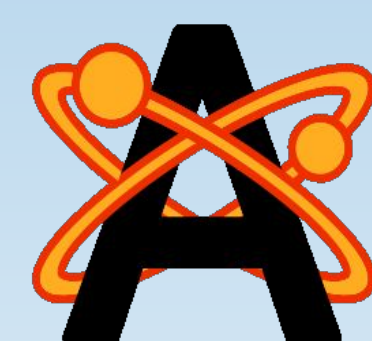
Underprivileged communities: Affected due to limited disaster relief and healthcare access.

Current solutions: EV and bio-based fuels face sustainability challenges

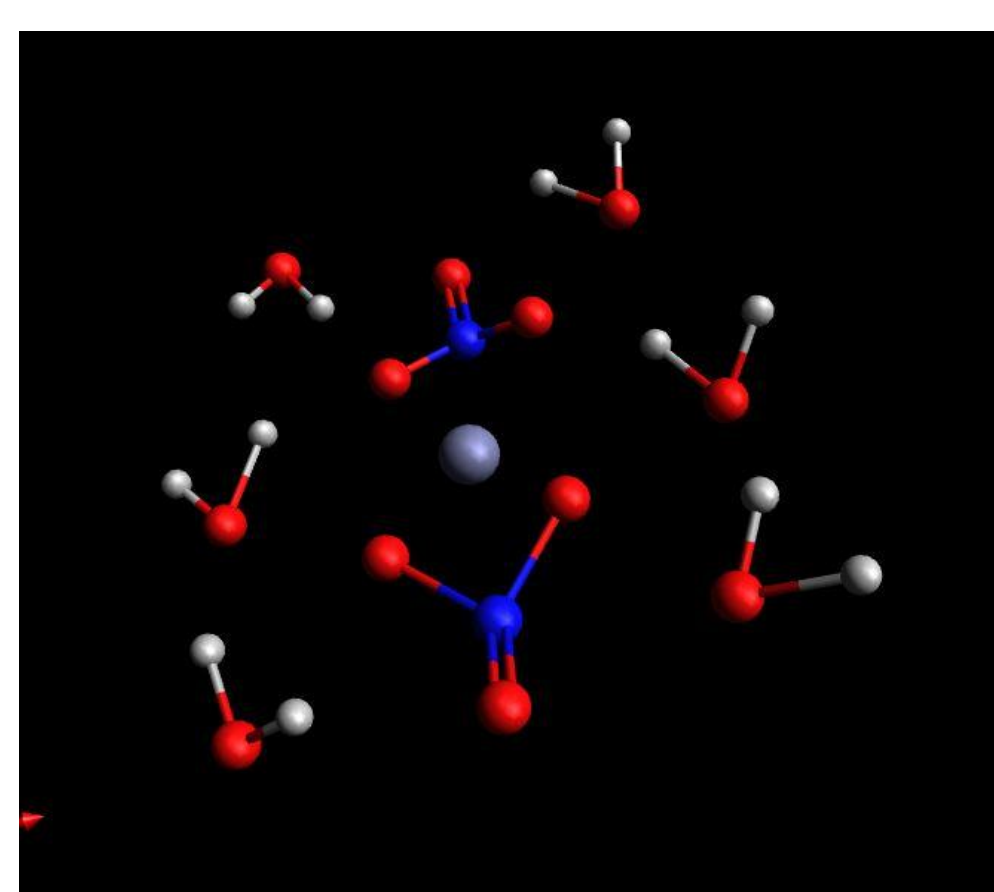
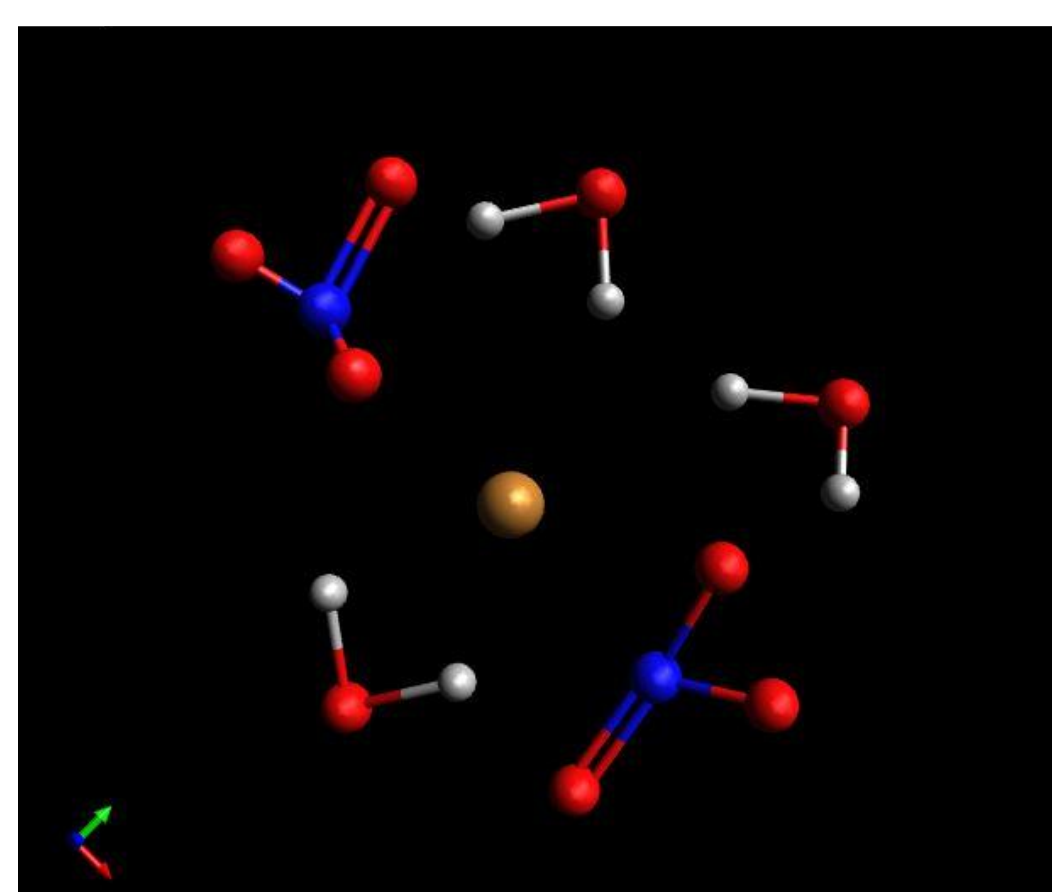
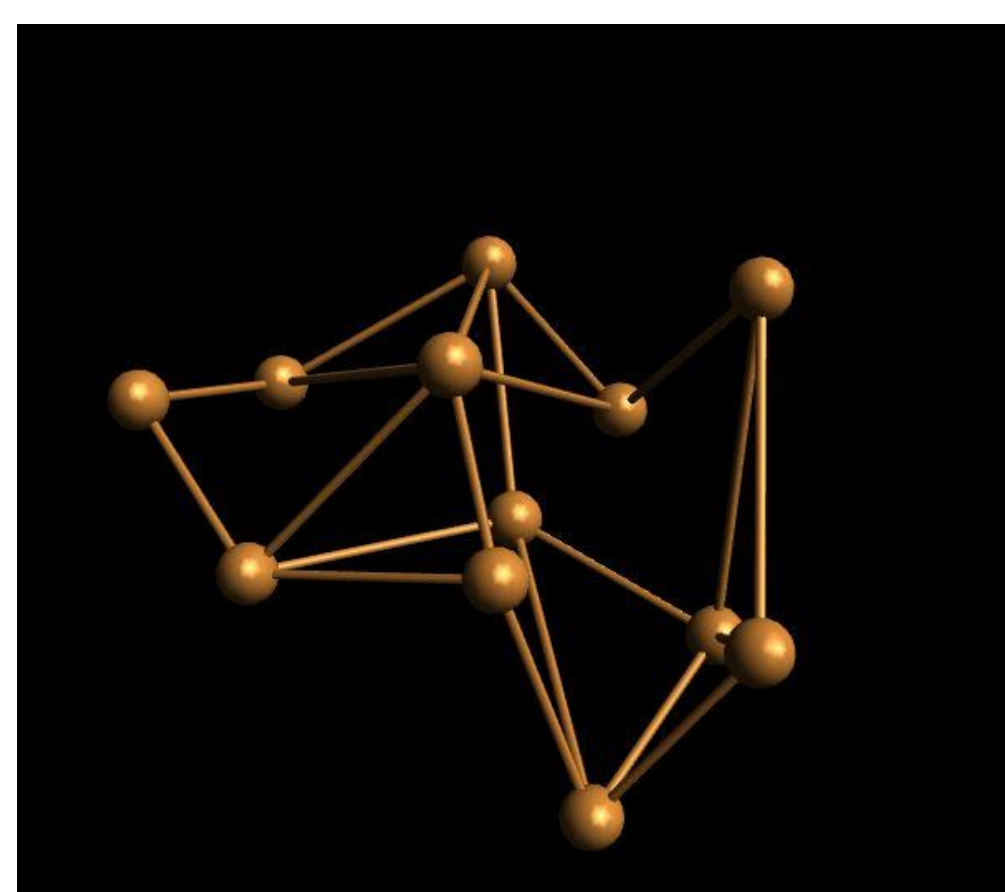
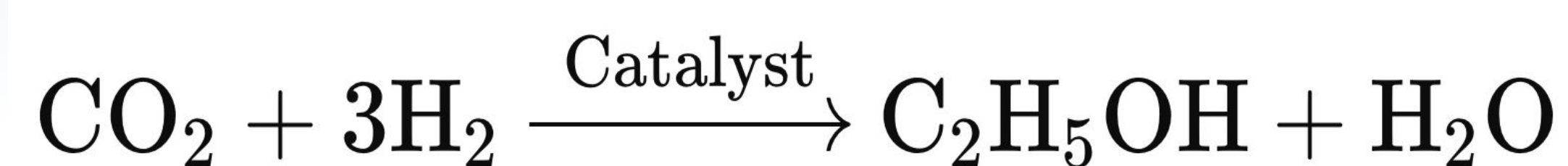
Methods & Materials

Software Used:

- Avogadro molecular modeling software
- ChemreaX modeling software
- MITSimply simulation software Catalyst



- Reaction: Conditions simulated at ambient pressure with varying temperatures (100°F - 600°F).

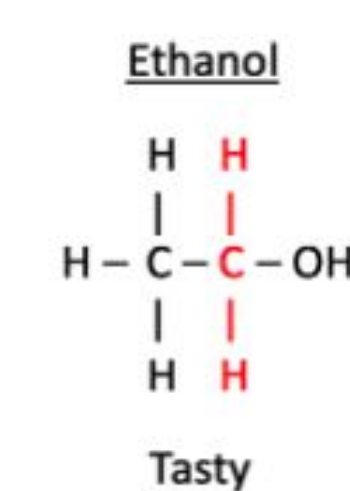
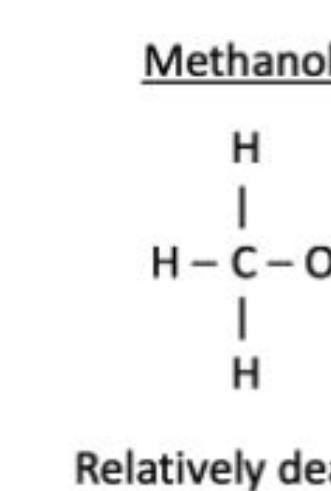
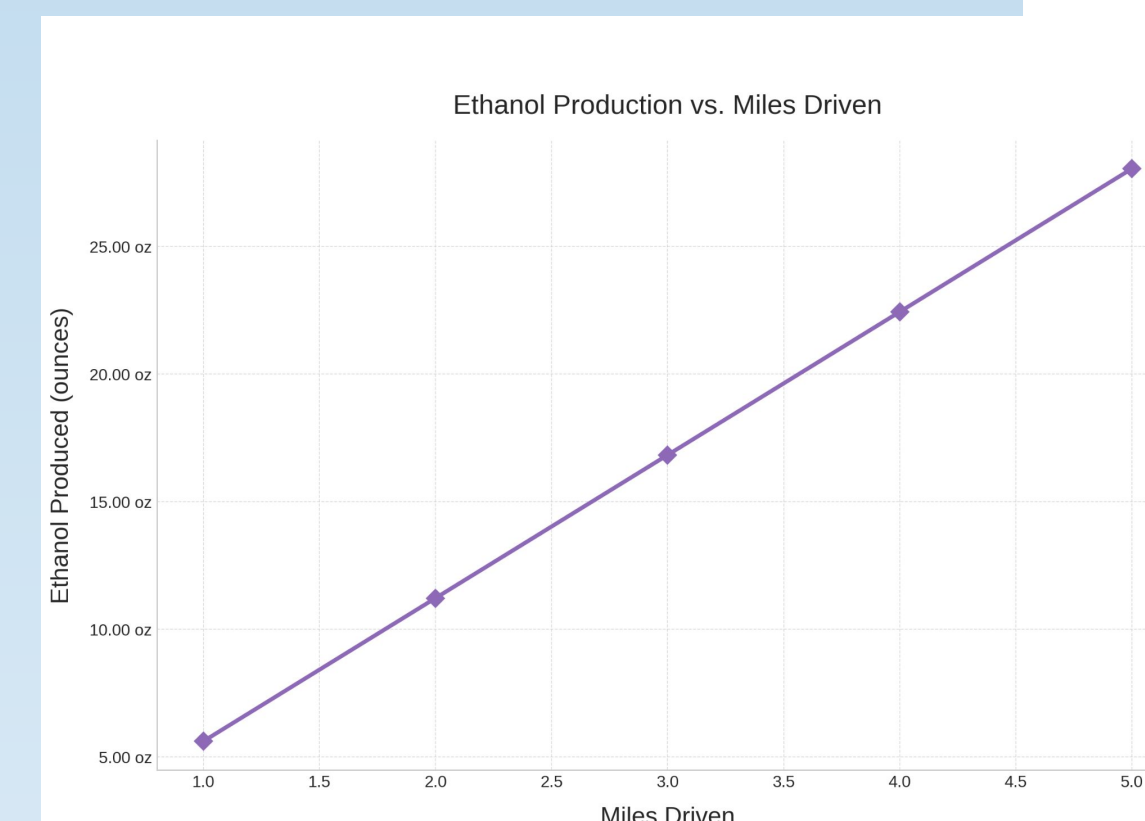
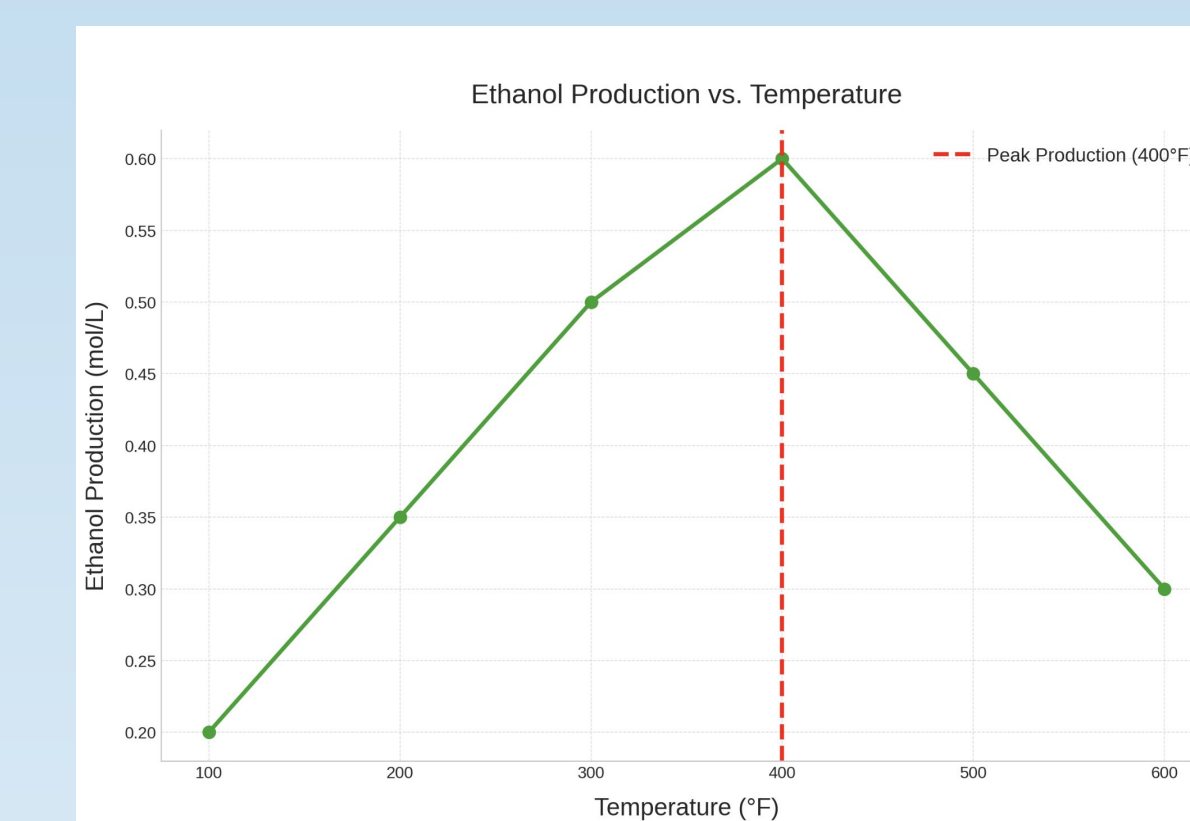
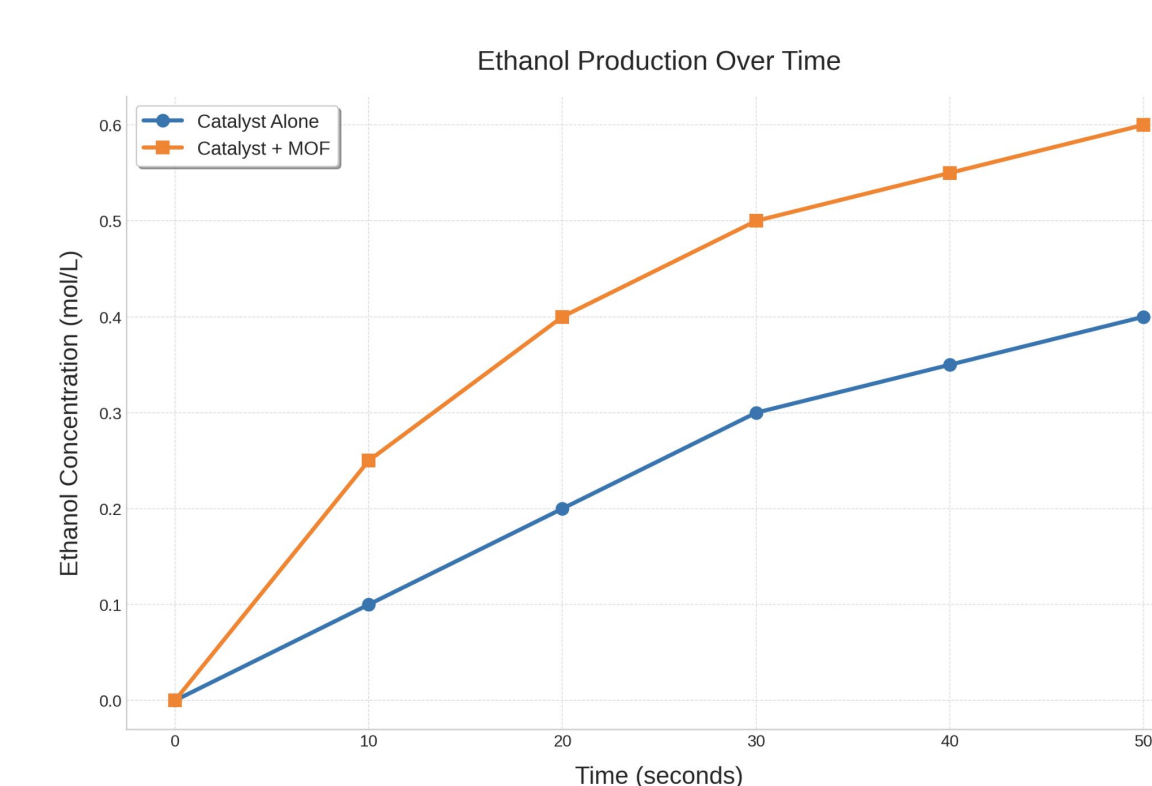
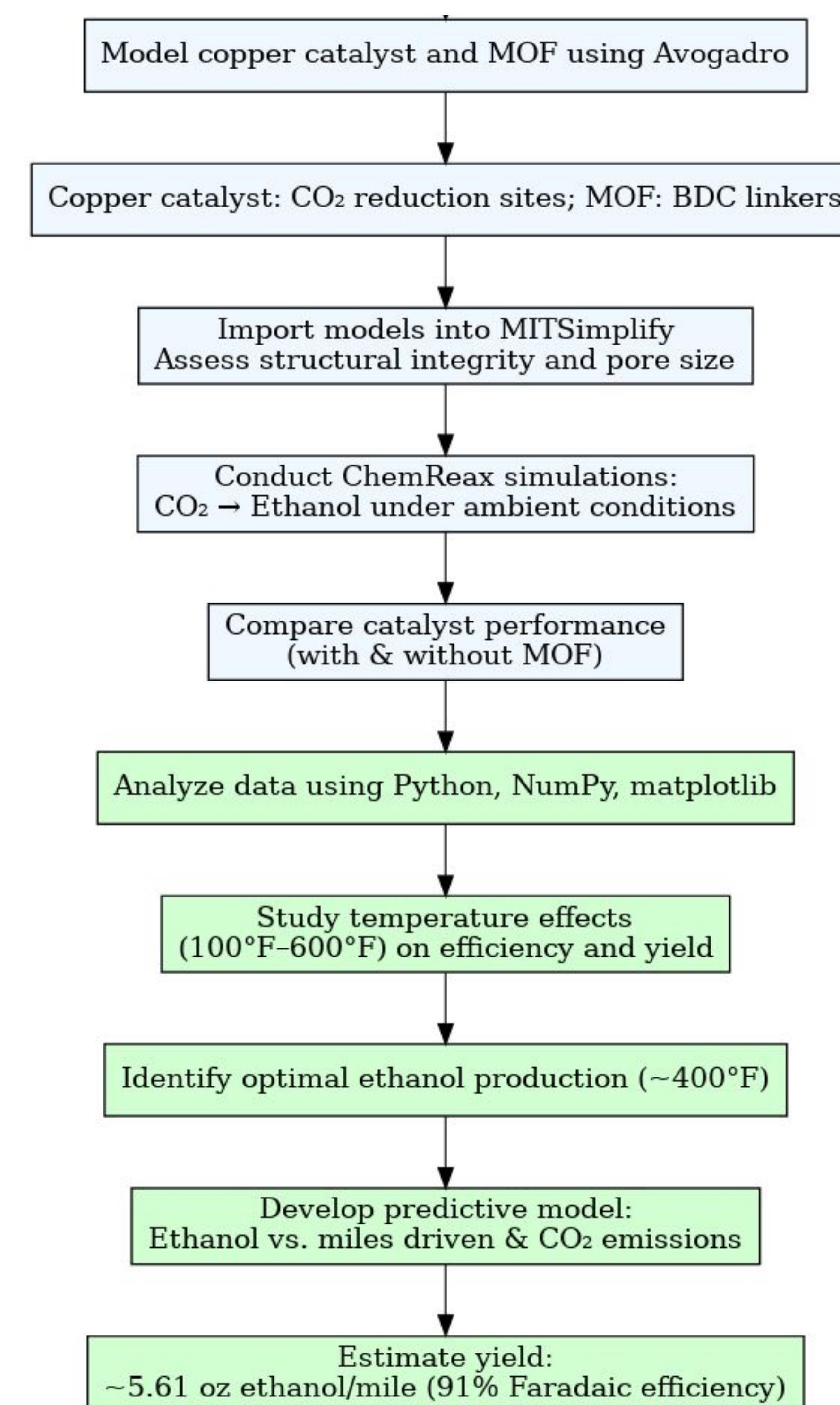


Organic compounds used in simulation

Procedure

This project captures vehicle CO₂ emissions and converts them into ethanol using MOFs and a copper catalyst, providing a sustainable way to reduce emissions and produce renewable fuel.

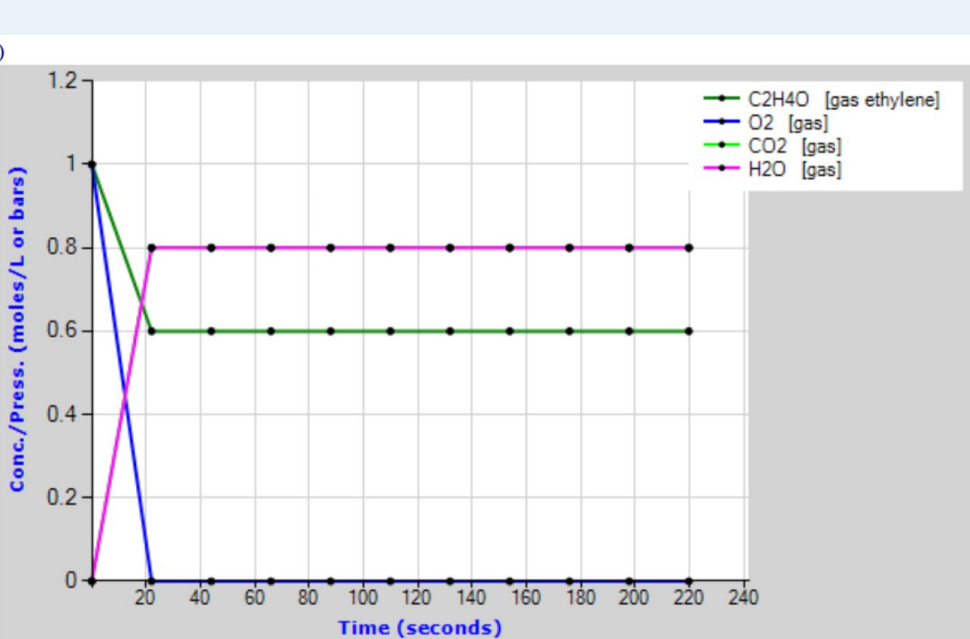
Hypothesis: MOFs and a copper catalyst are expected to efficiently capture vehicle emissions and convert them into ethanol, boosting carbon capture and sustainable fuel production.



Source: (Ethanol and Methanol for UPSC/PCS, n.d.)

Simulated Final State: (at T = 298.15 K, P = 1.00 X)

Reactants	Final Concentration	Adjusted Concentration	Excess
CO ₂ (mol)	6.000e-001	6.000e-001	0.000e+000
H ₂ (mol)	1.800e-001	1.800e-001	0.000e+000
CO ₂ (mol)	6.000e-001	6.000e-001	0.000e+000
H ₂ (mol)	1.800e-001	1.800e-001	0.000e+000



Thermodynamic Data (at T = 298.15 K)

Standard Enthalpy of Formation (kJ/mol)	Standard Entropy (J/mol·K)	Standard Gibbs Free Energy (kJ/mol)	Standard Heat Capacity (J/mol·K)	Standard Heat Capacity (J/mol·K)	Standard Heat Capacity (J/mol·K)
CO ₂ (gas)	-393.51	213.74	-393.51	213.74	213.74
H ₂ (gas)	0.00	130.68	0.00	130.68	130.68
C ₂ H ₅ OH (liquid)	-277.69	160.70	-277.69	160.70	160.70
H ₂ O (liquid)	-285.83	69.91	-285.83	69.91	69.91

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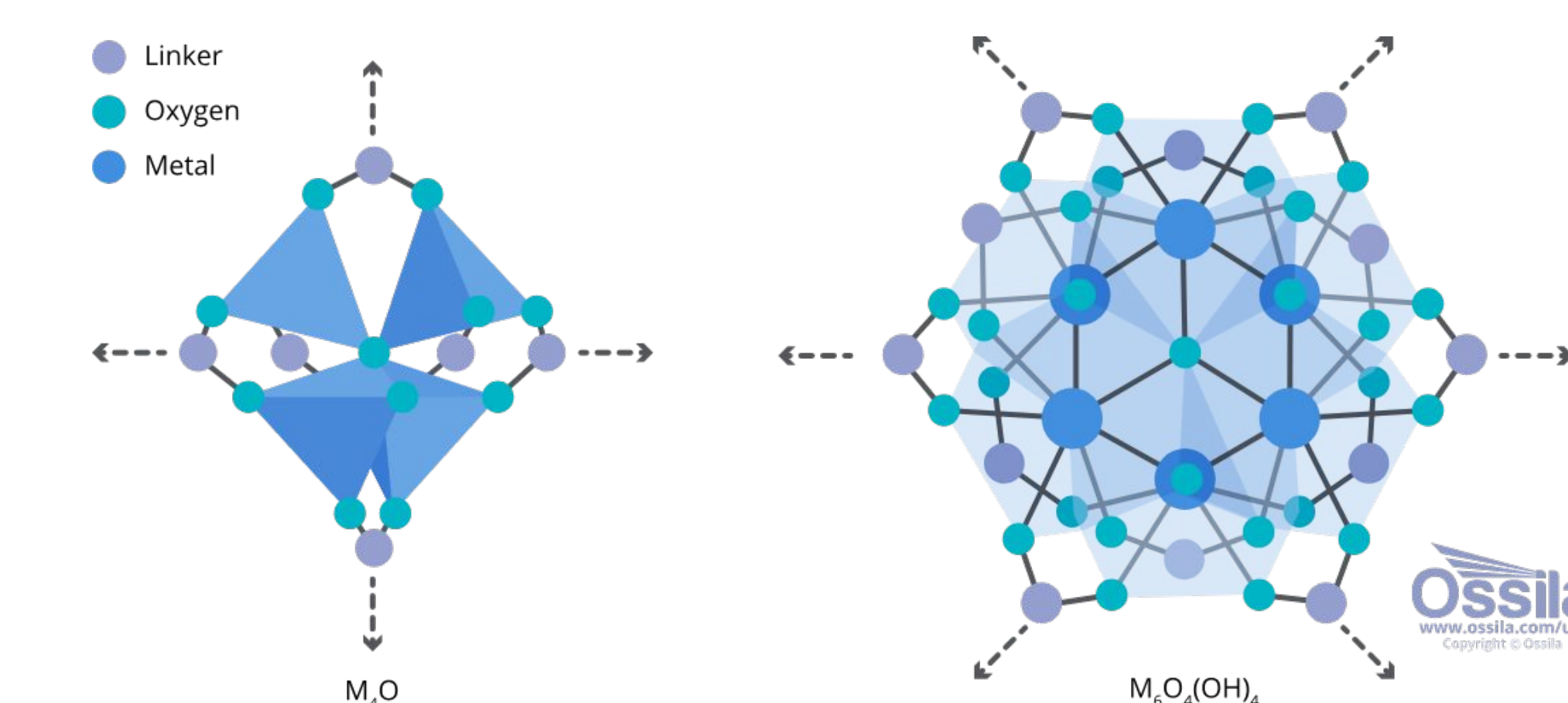


Diagram of a Metal Organic Framework(MOF)