

Goals & Motivation

- P&G has a net zero greenhouse gas (GHG) emissions target to reach by 2040.
 - Relevance: Primary consumer of propylene-derivatives (high GHG emissions) to package their products.
- Project Goal: To assess production emissions and costs from bio-sourced propylene instead of petroleum-sourced.
- Examples of products that P&G develop:



Scope

1. Quantify the GHG emissions of propylene produced from ethanol.
2. Quantify the total production cost (TPC) of propylene produced from ethanol.
3. Compare the GHG emissions and TPC of bio-sourced and petroleum-sourced propylene.

Mass and Energy Balances

Mass Balances:

- In = Out
- Reaction conversions from industry sources
- Basis of 1,000 tons of propylene produced per day (~10.5 kg/s)
- Assumed perfect separations

Energy Balances:

- Reactor and separator conditions from industry sources
- Reactors
 $\Delta H_{rxn} = \sum(m\Delta H_f)_{out} - \sum(m\Delta H_f)_{in}$
- Separators
 $\Delta S_{mix} = -nR\sum y_i \ln y_i$
 $\Delta G = T\Delta S_{mix}$

Baseline Ethanol Feed Requirement	17.6 kg/s	Model Ethanol Feed Requirement	27.8 kg/s
Baseline Energy Requirement	632 kJ/kg C3	Model Energy Requirement	18,238 kJ/kg C3

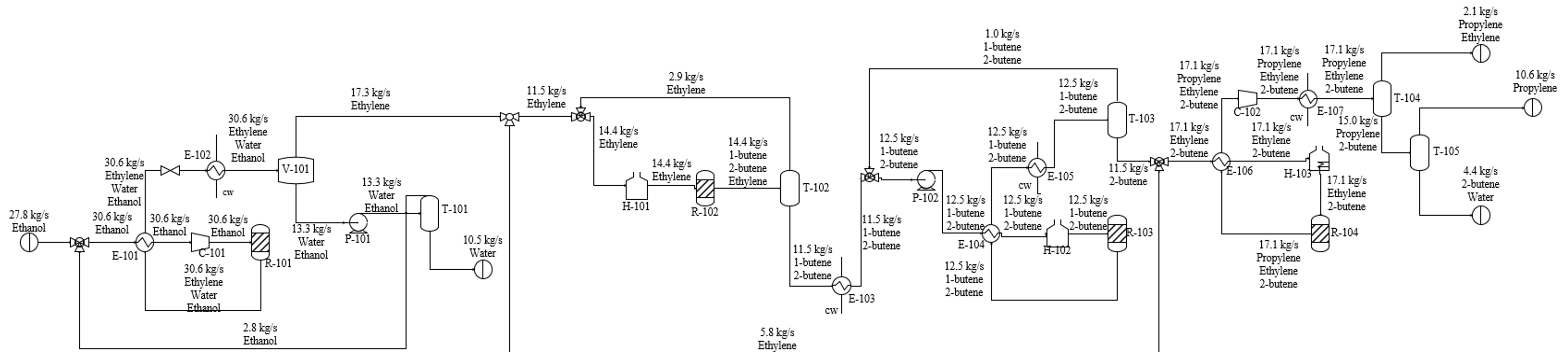
Process Reactions

Order	Chemical Formula	Description
1	$C_2H_5OH \rightarrow C_2H_4 + H_2O$	Dehydration of ethanol to ethylene and water.
2	$2C_2H_4 \rightarrow C_4H_8$	Dimerization of ethylene to 1-butene.
3	$C_4H_8 \rightarrow C_4H_8$	Isomerization of 1-butene to 2-butene.
4	$C_4H_8 + C_2H_4 \rightarrow 2C_3H_6$	Metathesis of 2-butene and ethylene to propylene.

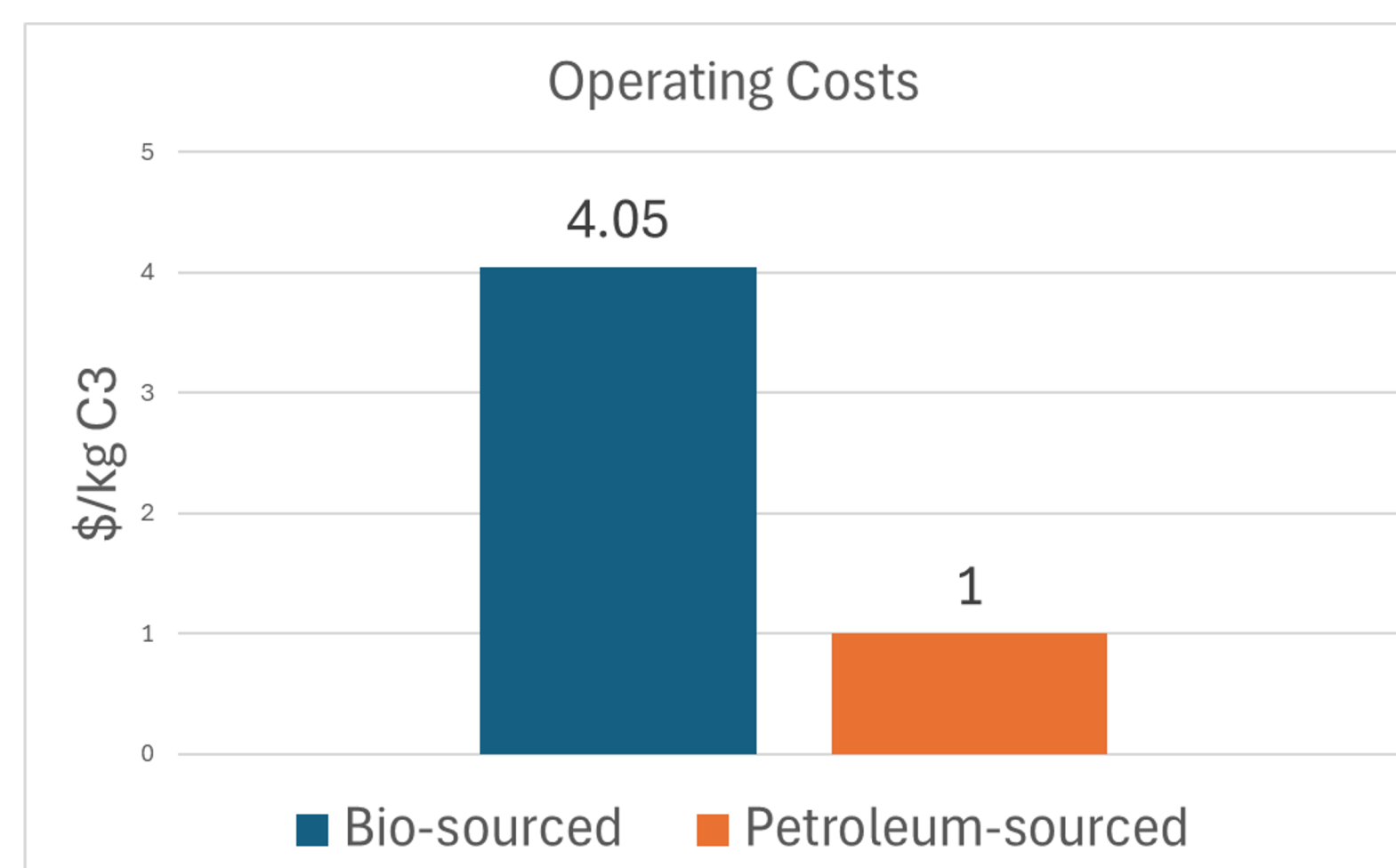
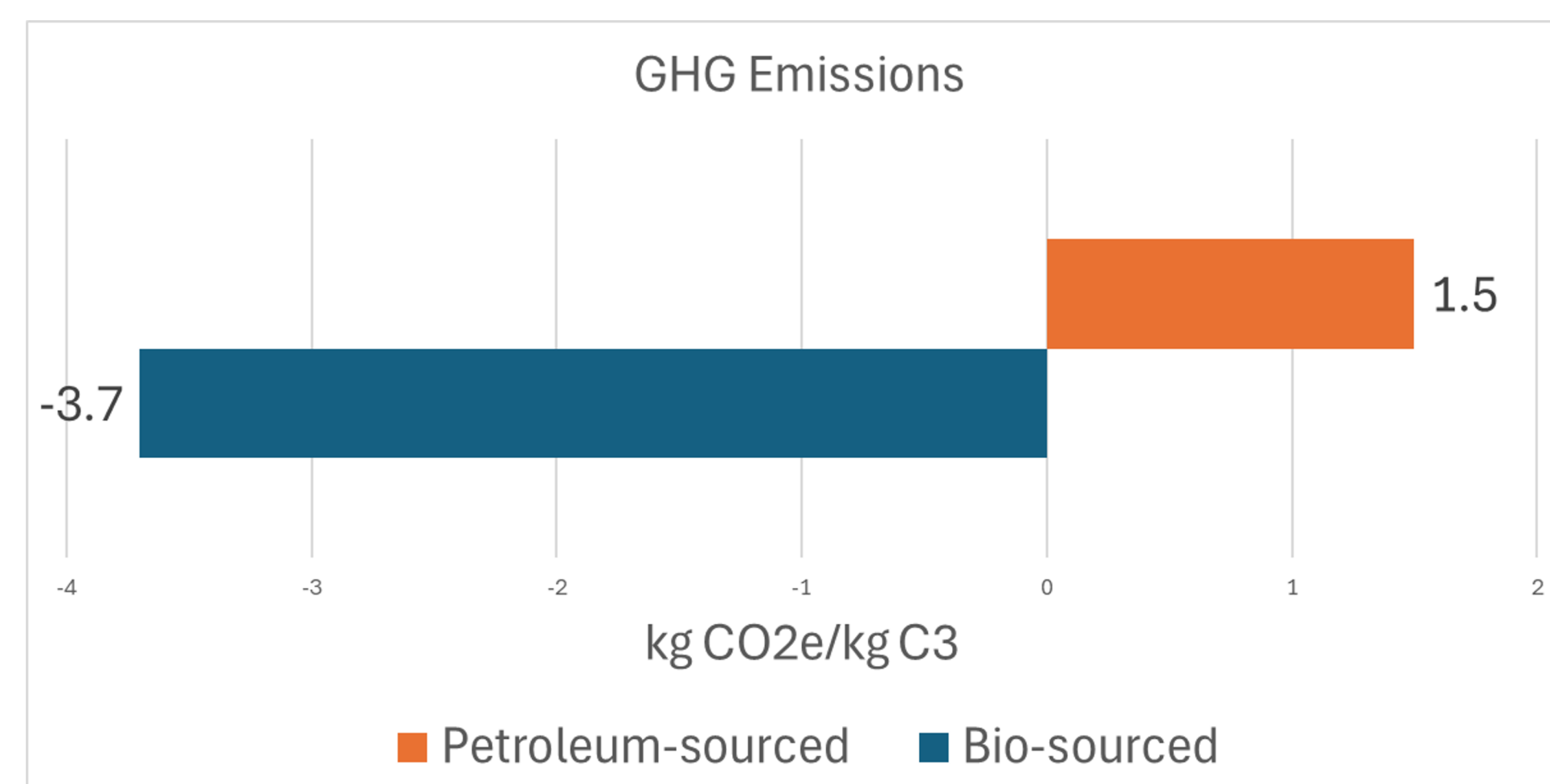
Process Model

- Modeled in Aspen Plus software
 - Used heaters, heat exchangers, and compressors to achieve ideal conditions
 - Used reactors to achieve new chemical species
 - Used distillation columns and flash tanks to achieve separations
- Model provided mass flows and heat and electricity requirements

Process Flow Diagram



Results



- **Total Module Cost:** \$20.9 million
- **Equipment Purchase Cost:** \$7 million

Conclusion

- Make the transition from petroleum to bio-sourced propylene
- Higher cost is necessary to meet net zero GHG emissions target
- Opportunity to lower total module cost through process optimization in the future

Citations

Scan QR code for a complete list of references.

