# **Tyche Example for Simple Electrolysis**

# Set up.

One only needs to execute the following line once, in order to make sure recent enough packages are installed.

```
In [ ]: #!pip install 'numpy>=1.17.2' 'pandas>=0.25.1'
```

## Import packages.

```
In [1]:
        import os
        import sys
        sys.path.insert(0, os.path.abspath("../src"))
        import numpy
In [2]:
                                  as np
        import matplotlib.pyplot as pl
        import pandas
                                  as pd
        import re
                                  as re
        import scipy.stats
                                  as st
        import seaborn
                                  as sb
        # The `tyche` package is located at <https://github.com/NREL/portfoli
        o/tree/master/production-function/framework/src/tyche/>.
        import tyche
                                  as ty
        from copy import deepcopy
```

# Load data.

The data are stored in a set of tab-separated value files in a folder.

```
In [3]: designs = ty.Designs("../data/simple_electrolysis")
In [4]: investments = ty.Investments("../data/simple_electrolysis")
```

## Compile the production and metric functions for each technology in the dataset.

```
In [5]: | designs.compile()
```

## Examine the data.

## The functions table specifies where the Python code for each technology resides.

In [6]:	designs.functions									
Out[6]:		Style	Module	Capital	Fixed	Production	Metrics	Notes		
	Technology	Otyle	Module	Capitai	Tixeu	Troduction	Metrics	Holes		
	Simple electrolysis	numpy	simple_electrolysis	capital_cost	fixed_cost	production	metrics			

Right now, only the style numpy is supported.

# The indices table defines the subscripts for variables.

In [7]: designs.indices Out[7]:

		Offset		Description	Notes
Technology	Type	Index			
	Capital	Catalyst	0	Catalyst	
	Fixed	Rent	0	Rent	
	Input Metric	Electricity	1	Electricity	
		Water	0	Water	
Simple electrolysis		Cost	0	Cost	
		GHG	2	Greenhouse gas emissions	
		Jobs	1	Jobs	
	0.4	Hydrogen	1	Hydrogen	
	Output	Oxygen	0	Oxygen	

The designs scenario.	table contains the cost, input, efficiency, and price data for a

In [8]: designs.designs

				value	Units	Notes
Technology	Scenario	Variable	Index			
Simple		lanut	Electricity	279	kJ/mole	
electrolysis		Input	Water	19.04	g/mole	
		Input	Electricity	0.85	1	
		efficiency	Water	0.95	1	
		Input	Electricity	3.33e-5	USD/kJ	
		price	Water	4.8e-3	USD/mole	
	Base Electrolysis	Lifetime	Catalyst	3	yr	Effective lifetime of Al-Ni catalyst.
		Output	Hydrogen	0.90	1	
		efficiency	Oxygen	0.90	1	
		Output	Hydrogen	1.0e-2	USD/g	
		price	Oxygen	3.0e-3	USD/g	
		Scale	NaN	6650	mole/yr	Rough estimate for a 50W setup.
		la a d	Electricity	279	kJ/mole	
		Input	Water	19.04	g/mole	
		Input	Electricity	st.truncnorm(-3, 0.75, loc=0.97, scale=0.04)	1	
		efficiency	Water	st.truncnorm(-3, 2, loc=0.97, scale=0.01)	1	
		Input	Electricity	3.33e-5	USD/kJ	
		price	Water	4.8e-3	USD/mole	
	Fast Progress on Electrolysis	Lifetime	Catalyst	3	yr	Effective lifetime of Al-Ni catalyst.
		Output	Hydrogen	st.beta(3, 2, loc=0.90, scale=0.03)	1	
		efficiency	Oxygen	st.beta(3, 2, loc=0.90, scale=0.06)	1	
		Output	Hydrogen	1.0e-2	USD/g	
		price	Oxygen	3.0e-3	USD/g	
		Scale	NaN	6650	mole/yr	Rough estimate for a 50W setup.
	Moderate	Innut	Electricity	279	kJ/mole	
	Progress on Electrolysis	Input	Water	19.04	g/mole	

Value

Units

Notes

Not	Units	Value				
			Index	Variable	Scenario	Technology
	1	st.truncnorm(-2, 1.75, loc=0.93, scale=0.04)	Electricity	Input		
	1	st.truncnorm(-2, 3, loc=0.97, scale=0.01)	Water	efficiency		
	USD/kJ	3.33e-5	Electricity	Input		
	USD/mole	4.8e-3	Water	price		
Effect lifetime Al cataly	yr	3	Catalyst	Lifetime		
	1	st.beta(2, 2, loc=0.90, scale=0.03)	Hydrogen	Output		
	1	st.beta(2, 2, loc=0.90, scale=0.06)	Oxygen	efficiency		
	USD/g	1.0e-2	Hydrogen	Output		
	USD/g	3.0e-3	Oxygen	price		
Rou estimation for a 50 set	mole/yr	6650	NaN	Scale		
	kJ/mole	279	Electricity			
	g/mole	19.04	Water	Input		
	1	st.truncnorm(-1, 2.75, loc=0.89, scale=0.04)	Electricity	Input		
	1	st.truncnorm(-1, 4, loc=0.96, scale=0.01)	Water	efficiency		
	USD/kJ	3.33e-5	Electricity	Input		
	USD/mole	4.8e-3	Water	price		
Effect lifetime Al cataly	yr	3	Catalyst	Lifetime	Slow Progress on Electrolysis	
	1	st.beta(1, 2, loc=0.90, scale=0.03)	Hydrogen	Output		
	1	st.beta(1, 2, loc=0.90, scale=0.06)	Oxygen	efficiency		
	USD/g	1.0e-2	Hydrogen	Output		
	USD/g	3.0e-3	Oxygen	price		
Rou estima for a 50 set	mole/yr	6650	NaN	Scale		

The parameters each technology.	table contains additional techno-economic parameters for

In [9]: designs.parameters

			Offset	Value	Units	Notes
Technology	Scenario	Parameter				
Simple electrolysis		Electricity consumption	3	237	kJ	
		GHG factor for electricity	9	0.138	gCO2e/kJ	based on 1 kWh = 0.5 kg CO2e
		GHG factor for water	8	0.00108	gCO2e/g	based on 244,956 gallons = 1 Mg CO2e
	Base Electrolysis	Hydrogen production	1	2.00	g	
	Edde Electrolycle	Jobs	4	1.5e-4	job/mole	
		Oxygen production	0	16.00	g	
		Reference capital cost for catalyst	6	0.63	USD	
		Reference fixed cost for rent	7	1000	USD/yr	
		Reference scale	5	6650	mole/yr	
		Water consumption	2	18.08	g	
		Electricity consumption	3	237	kJ	
		GHG factor for electricity	9	0.138	gCO2e/kJ	based on 1 kWh = 0.5 kg CO2e
		GHG factor for water	8	0.00108	gCO2e/g	based on 244,956 gallons = 1 Mg CO2e
	Fast Progress on	Hydrogen production	1	2.00	g	
	Electrolysis	Jobs	4	1.5e-4	job/mole	
		Oxygen production	0	16.00	g	
		Reference capital cost for catalyst	6	0.63	USD	
		Reference fixed cost for rent	7	1000	USD/yr	
		Reference scale	5	6650	mole/yr	
		Water consumption	2	18.08	g	
	Moderate Progress on Electrolysis	Electricity consumption	3	237	kJ	
		GHG factor for electricity	9	0.138	gCO2e/kJ	based on 1 kWh = 0.5 kg CO2e
		GHG factor for water	8	0.00108	gCO2e/g	based on 244,956 gallons = 1 Mg CO2e

			Offset	Value	Units	Notes
Technology	Scenario	Parameter				
		Hydrogen production	1	2.00	g	
		Jobs	4	1.5e-4	job/mole	
		Oxygen production	0	16.00	g	
		Reference capital cost for catalyst	6	0.63	USD	
		Reference fixed cost for rent	7	1000	USD/yr	
		Reference scale	5	6650	mole/yr	
		Water consumption	2	18.08	g	
		Electricity consumption	3	237	kJ	
		GHG factor for electricity	9	0.138	gCO2e/kJ	based on 1 kWh = 0.5 kg CO2e
		GHG factor for water	8	0.00108	gCO2e/g	based on 244,956 gallons = 1 Mg CO2e
	Slow Progress on	Hydrogen production	1	2.00	g	
	Electrolysis	Jobs	4	1.5e-4	job/mole	
		Oxygen production	0	16.00	g	
		Reference capital cost for catalyst	6	0.63	USD	
		Reference fixed cost for rent	7	1000	USD/yr	
		Reference scale	5	6650	mole/yr	
		Water consumption	2	18.08	g	

The results table specifies the units of measure for results of computations.

```
In [10]:
            designs results
Out[10]:
                                                       Units Notes
                  Technology Variable
                                           Index
                                  Cost
                                            Cost
                                                   USD/mole
                                            Cost
                                                    USD/gH2
                                 Metric
                                           GHG
                                                 gCO2e/gH2
             Simple electrolysis
                                            Jobs
                                                     job/gH2
                                        Hydrogen
                                                      g/mole
                                Output
                                         Oxygen
                                                      g/mole
```

The tranches table specifies multually exclusive possibilities for investments: only one Tranch may be selected for each Cateogry.

In [11]:	investments.	tranches		
Out[11]:				Notes
	Category	Tranche	Scenario	
		High Electrolysis R&D	Fast Progress on Electrolysis	
	Electrolysis R&D	Low Electrolysis R&D	Slow Progress on Electrolysis	
	Election 1818 Kad	Medium Electrolysis R&D	Moderate Progress on Electrolysis	
		No Electrolysis R&D	Base Electrolysis	

The investments table bundles a consistent set of tranches (one per category) into an overall investment.

```
In [12]:
            investments.investments
Out[12]:
                                                                             Amount Notes
                       Investment
                                         Category
                                                                  Tranche
                High R&D Spending
                                   Electrolysis R&D
                                                       High Electrolysis R&D
                                                                           5000000.0
                 Low R&D Spending
                                   Electrolysis R&D
                                                       Low Electrolysis R&D
                                                                           1000000.0
             Medium R&D Spending
                                   Electrolysis R&D Medium Electrolysis R&D
                                                                           2500000.0
                  No R&D Spending
                                   Electrolysis R&D
                                                        No Electrolysis R&D
                                                                                  0.0
```

Evaluate the scenarios in the dataset.

```
In [13]: scenario_results = designs.evaluate_scenarios(sample_count=50)
```

In [14]: scenario\_results.xs(1, level="Sample", drop\_level=False)

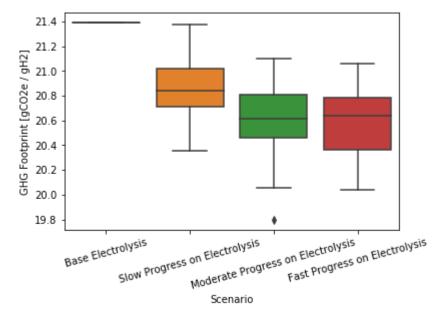
Out[14]:

					Value	Units
Technology	Scenario	Sample	Variable	Index		
			Cost	Cost	0.183900	USD/mole
				Cost	0.102121	USD/gH2
	Dago Flootrolygia	1	Metric	GHG	21.391959	gCO2e/gH2
	Base Electrolysis	ļ		Jobs	0.000083	job/gH2
			Output	Hydrogen	1.800796	g/mole
			Output	Oxygen	14.406372	g/mole
			Cost	Cost	0.183904	USD/mole
				Cost	0.100198	USD/gH2
	Fast Progress on	1	Metric	GHG	20.988579	gCO2e/gH2
	Electrolysis	'		Jobs	0.000082	job/gH2
			Output	Hydrogen	1.835406	g/mole
Simple			Output	Oxygen	14.955168	g/mole
electrolysis			Cost	Cost	0.183409	USD/mole
				Cost	0.099262	USD/gH2
	Moderate Progress on	1	Metric	GHG	20.848608	gCO2e/gH2
	Electrolysis	ı		Jobs	0.000081	job/gH2
			Output	Hydrogen	1.847728	g/mole
			Output	Oxygen	15.159795	g/mole
			Cost	Cost	0.181918	USD/mole
				Cost	0.098976	USD/gH2
	Slow Progress on	1	Metric	GHG	20.958893	gCO2e/gH2
	Electrolysis	ı		Jobs	0.000082	job/gH2
			Output	Hydrogen	1.838006	g/mole
			Output	Oxygen	15.489779	g/mole

# Save results.

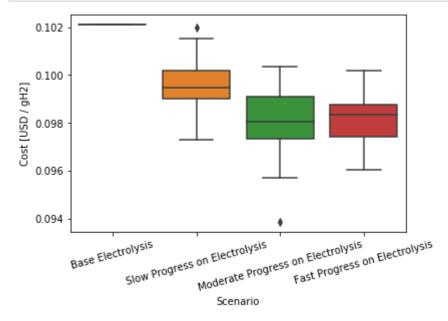
#### Plot GHG metric.

```
In [16]: g = sb.boxplot(
    x="Scenario",
    y="Value",
    data=scenario_results.xs(
        ["Metric", "GHG"],
        level=["Variable", "Index"]
    ).reset_index()[["Scenario", "Value"]],
    order=["Base Electrolysis", "Slow Progress on Electrolysis", "Moderate Progress on Electrolysis", "Fast Progress on Electrolysis"])
    g.set(ylabel="GHG Footprint [gCO2e / gH2]")
    g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



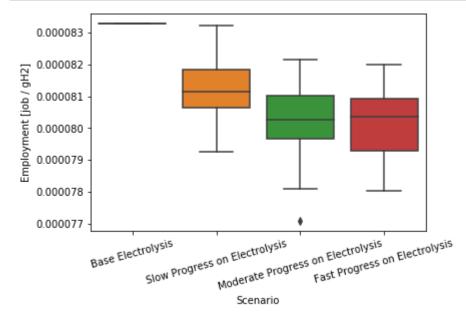
Plot cost metric.

```
In [17]: g = sb.boxplot(
    x="Scenario",
    y="Value",
    data=scenario_results.xs(
        ["Metric", "Cost"],
        level=["Variable", "Index"]
    ).reset_index()[["Scenario", "Value"]],
    order=["Base Electrolysis", "Slow Progress on Electrolysis", "Moderate Progress on Electrolysis", "Fast Progress on Electrolysis"])
    g.set(ylabel="Cost [USD / gH2]")
    g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



Plot employment metric.

```
In [18]: g = sb.boxplot(
    x="Scenario",
    y="Value",
    data=scenario_results.xs(
        ["Metric", "Jobs"],
        level=["Variable", "Index"]
    ).reset_index()[["Scenario", "Value"]],
    order=["Base Electrolysis", "Slow Progress on Electrolysis", "Moderate Progress on Electrolysis", "Fast Progress on Electrolysis"])
    g.set(ylabel="Employment [job / gH2]")
    g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



# **Evaluate the investments in the dataset.**

```
In [19]: investment_results = investments.evaluate_investments(designs, sample
    _count=50)
```

#### Costs of investments.

```
In [20]: investment_results.amounts
Out[20]:
```

**Amount** 

# Investment High R&D Spending 5000000.0 Low R&D Spending 1000000.0 Medium R&D Spending 2500000.0 No R&D Spending 0.0

# Benefits of investments.

In [21]: investment\_results.metrics.xs(1, level="Sample", drop\_level=False)

Out[21]:

							Value	Ur
Investment	Category	Tranche	Scenario	Sample	Technology	Index		
		No				Cost	0.102121	USD/g
No R&D Spending	Electrolysis R&D	No Electrolysis R&D	Base Electrolysis	1	Simple electrolysis	GHG	21.391959	gCO2e/g
		Nab				Jobs	0.000083	job/g
		∐iah	Fast			Cost	0.098317	USD/g
High R&D Spending	Electrolysis R&D	High Electrolysis	Progress on	· 1	Simple electrolysis	GHG	20.721331	gCO2e/g
- p		R&D	Electrolysis			Jobs	0.000081	job/g
Medium		Medium	Moderate			Cost	0.098472	USD/g
R&D	Electrolysis R&D	Electrolysis	Progress on	1	Simple electrolysis	GHG	20.751749	gCO2e/g
Spending		R&D	Electrolysis		, , , , , ,	Jobs	0.000081	job/g
		Law	Slow			Cost	0.099348	USD/g
Low R&D Spending	Electrolysis R&D	Low Electrolysis R&D	Progress on	1	Simple electrolysis	GHG	20.909038	gCO2e/g
		NOD	Electrolysis		Sieda diyeld		0.000081	job/g
4								

In [22]: investment\_results.summary.xs(1, level="Sample", drop\_level=False)

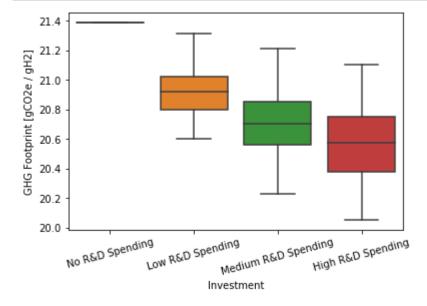
Out[22]:

			Value	Units
Investment	Sample	Index		
		Cost	0.102121	USD/gH2
No R&D Spending	1	GHG	21.391959	gCO2e/gH2
		Jobs	0.000083	job/gH2
		Cost	0.098317	USD/gH2
High R&D Spending	1	GHG	20.721331	gCO2e/gH2
		Jobs	0.000081	job/gH2
		Cost	0.098472	USD/gH2
Medium R&D Spending	1	GHG	20.751749	gCO2e/gH2
		Jobs	0.000081	job/gH2
		Cost	0.099348	USD/gH2
Low R&D Spending	1	GHG	20.909038	gCO2e/gH2
		Jobs	0.000081	job/gH2

#### Save results.

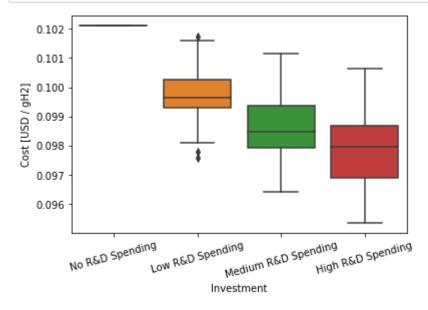
#### Plot GHG metric.

```
In [25]: g = sb.boxplot(
    x="Investment",
    y="Value",
    data=investment_results.metrics.xs(
        "GHG",
        level="Index"
    ).reset_index()[["Investment", "Value"]],
    order=["No R&D Spending", "Low R&D Spending", "Medium R&D Spending",
    "High R&D Spending"]
)
    g.set(ylabel="GHG Footprint [gCO2e / gH2]")
    g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



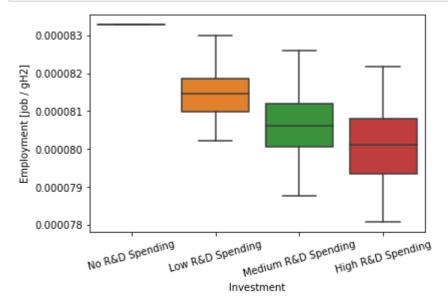
#### Plot cost metric.

```
In [26]: g = sb.boxplot(
    x="Investment",
    y="Value",
    data=investment_results.metrics.xs(
        "Cost",
        level="Index"
    ).reset_index()[["Investment", "Value"]],
    order=["No R&D Spending", "Low R&D Spending", "Medium R&D Spending", "High R&D Spending"]
)
    g.set(ylabel="Cost [USD / gH2]")
    g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



Plot employment metric.

```
In [27]: g = sb.boxplot(
    x="Investment",
    y="Value",
    data=investment_results.metrics.xs(
        "Jobs",
        level="Index"
    ).reset_index()[["Investment", "Value"]],
    order=["No R&D Spending", "Low R&D Spending", "Medium R&D Spending",
    "High R&D Spending"]
)
    g.set(ylabel="Employment [job / gH2]")
    g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



# Sensitity analysis.

## Vary the four efficiencies in the design.

# Start from the base case.

Out[30]:

				Value	Units	Notes
Technology	Scenario	Variable	Index			
		l	Electricity	279	kJ/mole	
		Input	Water	19.04	g/mole	
		Input efficiency	Electricity	0.85	1	
	Simple Base trolysis Electrolysis		Water	0.95	1	
		Input price	Electricity	3.33e- 5	USD/kJ	
Cimple			Water	4.8e-3	USD/mole	
electrolysis		Lifetime	Catalyst	3	yr	Effective lifetime of Al- Ni catalyst.
		Output efficiency	Hydrogen	0.90	1	
			Oxygen	0.90	1	
		0 1 1 1 1 1 1	Hydrogen	1.0e-2	USD/g	
		Output price	Oxygen	3.0e-3	USD/g	
		Scale	NaN	6650	mole/yr	Rough estimate for a 50W setup.

#### Out[31]:

			Offset	Value	Units	Notes
Technology	Scenario	Parameter				
		Electricity consumption	3	237	kJ	
		GHG factor for electricity	9	0.138	gCO2e/kJ	based on 1 kWh = 0.5 kg CO2e
		GHG factor for water	8	0.00108	gCO2e/g	based on 244,956 gallons = 1 Mg CO2e
		Hydrogen production	1	2.00	g	
Simple	Base	Jobs	4	1.5e-4	job/mole	
electrolysis	Electrolysis	Oxygen production	0	16.00	g	
		Reference capital cost for catalyst	6	0.63	USD	
		Reference fixed cost for rent	7	1000	USD/yr	
		Reference scale	5	6650	mole/yr	
		Water consumption	2	18.08	g	

# Generate the new scenarios and append them to the previous ones.

```
In [32]: sensitivities = deepcopy(designs)
sensitivities.designs = sensitivities.designs[0:0]
sensitivities.parameters = sensitivities.parameters[0:0]
```

```
In [33]:
         # Iterate over variables and efficiencies.
         for variable, index in variables:
             for efficiency in efficiencies:
                 # Name the scenario.
                 scenario = "Let " + variable + " @ " + index + " = " + str(ro
         und(efficiency, 3))
                 # Alter the base case.
                 vary_design = base_design.rename(index={"Base Electrolysis" :
         scenario}, level=1)
                 vary_design.loc[("Simple electrolysis", scenario, variable, i
         ndex), "Value"] = efficiency
                 # Keep the parameters the same.
                 vary_parameters = base_parameters.rename(index={"Base Electro"})
         lysis" : scenario}, level=1)
                 # Append the results to the existing table of scenarios.
                 sensitivities.designs = sensitivities.designs.append(vary des
         ign)
                 sensitivities.parameters = sensitivities.parameters.append(va
         ry parameters)
```

#### Remember to compile the design, since we've added scenarios.

```
In [34]: sensitivities.compile()
```

#### See how many rows there are in the tables now.

```
In [35]: sensitivities.designs.shape
Out[35]: (480, 3)
In [36]: sensitivities.parameters.shape
Out[36]: (400, 4)
```

In [37]: | sensitivities.designs

Out[37]:

				Value	Units	Notes
Technology	Scenario	Variable	Index			
	Let Input efficiency @ Water = 0.75	Input	Electricity	279	kJ/mole	
			Water	19.04	g/mole	
		Input efficiency	Electricity	0.85	1	
			Water	0.75	1	
		Input price	Electricity	3.33e- 5	USD/kJ	
Simple						
electrolysis	Let Output efficiency @ Hydrogen = 0.975	Output efficiency	Hydrogen	0.975	1	
			Oxygen	0.90	1	
		Output price	Hydrogen	1.0e-2	USD/g	
			Oxygen	3.0e-3	USD/g	
		Scale	NaN	6650	mole/yr	Rough estimate for a 50W setup.

480 rows × 3 columns

# Compute the results.

```
In [38]: results = sensitivities.evaluate_scenarios(1)
    results
```

## Out[38]:

					Value	Units
Technology	Scenario	Sample	Variable	Index		
		1	Cost	Cost	0.190164	USD/mole
			Metric	Cost	0.119657	USD/gH2
	Let Input efficiency @ Electricity = 0.75			GHG	24.239606	gCO2e/gH2
	•			Jobs	0.000094	job/gH2
			Output	Hydrogen	1.589241	g/mole
Simple electrolysis						
	Let Output efficiency @ Oxygen = 0.975	1	Metric	Cost	0.100121	USD/gH2
				GHG	21.391959	gCO2e/gH2
				Jobs	0.000083	job/gH2
			Output	Hydrogen	1.800796	g/mole
				Oxygen	15.606903	g/mole

240 rows × 2 columns

## Plot the cost results.

### Out[40]:

	Scenario	Value
0	Let Input efficiency @ Electricity = 0.75	0.190164
1	Let Input efficiency @ Electricity = 0.775	0.188595
2	Let Input efficiency @ Electricity = 0.8	0.187026
3	Let Input efficiency @ Electricity = 0.825	0.185457
4	Let Input efficiency @ Electricity = 0.85	0.183900
5	Let Input efficiency @ Electricity = 0.875	0.184132
6	Let Input efficiency @ Electricity = 0.9	0.184364
7	Let Input efficiency @ Electricity = 0.925	0.184597
8	Let Input efficiency @ Electricity = 0.95	0.184829
9	Let Input efficiency @ Electricity = 0.975	0.185061

```
In [41]: cost_results["Variable" ] = cost_results["Scenario"].apply(lambda x:
    re.sub(r'^Let (.*) @ (.*) =.*$', '\\1[\\2]', x))
    cost_results["Efficiency"] = cost_results["Scenario"].apply(lambda x:
    float(re.sub(r'^.*= (.*)$', '\\1', x)))
    cost_results["Cost [USD/mole]"] = cost_results["Value"]
```

In [42]: cost\_results = cost\_results[["Variable", "Efficiency", "Cost [USD/mol
e]"]]
cost\_results[0:10]

#### Out[42]:

	Variable	Efficiency	Cost [USD/mole]
0	Input efficiency[Electricity]	0.750	0.190164
1	Input efficiency[Electricity]	0.775	0.188595
2	Input efficiency[Electricity]	0.800	0.187026
3	Input efficiency[Electricity]	0.825	0.185457
4	Input efficiency[Electricity]	0.850	0.183900
5	Input efficiency[Electricity]	0.875	0.184132
6	Input efficiency[Electricity]	0.900	0.184364
7	Input efficiency[Electricity]	0.925	0.184597
8	Input efficiency[Electricity]	0.950	0.184829
9	Input efficiency[Electricity]	0.975	0.185061

Out[43]: <matplotlib.axes.\_subplots.AxesSubplot at 0x7f386f638898>

