**SRCA Module - Case Study 1**

**Sustainability Root cause analysis of the steam methane reforming process**

Steam methane reforming is the most widely used method of producing syngas from natural gas. The Aspen Plus process flow diagram (PFD) for the steam methane reforming process is shown below:

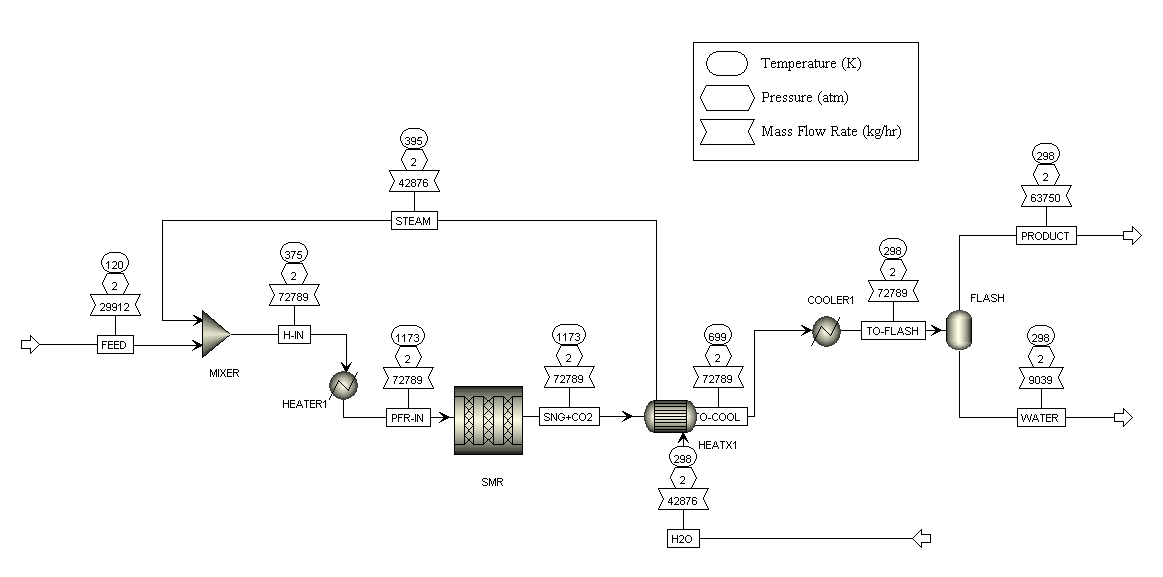


Figure 1. Process Flow Diagram of the Steam Methane Reforming Process

The mass flow rate of the major streams and corresponding component mass fractions are:

Table 1: Mass flow rates and mass fractions:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Name | FEED (Methane) | H2O (Inlet Water) | PRODUCT (Syngas) | WATER (Outlet Water) |
| Type | Inlet | Inlet | Product | Outlet waste |
| Flow rate (kg/hr) | 2.99E+04 | 4.29E+04 | 6.37E+04 | 9.04E+03 |
| X(water) | 0 | 1 | 0.0248 | 1 |
| X(carbon) | 0 | 0 | 0.2089 | 0 |
| X(methane) | 0.9813 | 0 | 0.086 | 0 |
| X(ethane) | 0 | 0 | 0 | 0 |
| X(propane) | 0 | 0 | 0 | 0 |
| X(nitrogen) | 0.0187 | 0 | 0.0088 | 0 |
| X(sulfur) | 0 | 0 | 0 | 0 |
| X(hydrogen) | 0 | 0 | 0.1507 | 0 |
| X(carbon monoxide) | 0 | 0 | 0.5209 | 0 |

(X denotes mass fraction)

**(a) Economic Evaluation**

|  |  |  |
| --- | --- | --- |
| Raw Material Costs | | |
| Raw Material | **Price** | **Quantity Needed** |
| Natural Gas | $3.5/MMBtu ($35.28/ton) | (Determine from Table 1) |
| Water | (0.46/m3)($0.46/ton) |
| Utility Costs | | |
| Utility | **Price** | **Usage** |
| Heating | $3.5/MMBtu | 169 MMBtu/h |
| Electricity | $0.067/kWh | 31518 kWh |

(Note: Here, ton denotes metric ton. Also, electricity is used in COOLER1 for refrigeration (the refrigerant could be propylene, etc.) since cooling water cannot cool the stream down to room temperature)

With the given consumption details and cost data, calculate raw material and utility costs of the plant per hour. Using a Pareto chart, determine which factor(s) contribute most significantly to the operating cost.

**(b) Safety Evaluation**

The calculated sub-indices for process inherent safety index are:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Equipment | Inventory | Process Temperature | Process Pressure | Equipment Safety |
| HEATER 1 | 3 | 4 | 0 | 1 |
| SMR | 3 | 4 | 0 | 2 |
| HEATX 1 | 3 | 4 | 0 | 1 |
| COOLER 1 | 3 | 4 | 0 | 1 |
| FLASH | 3 | 0 | 0 | 1 |

Calculate the process safety index and identify the units that have the highest impact on safety score using a Pareto chart.

**(c) Environmental Evaluation**

Using the mass flow rates and mass fractions given in Table 1 in the WAR Algorithm, evaluate the potential environmental impact of the outlet stream. Which of the eight categories have an impact score? Which are the chemicals that contribute to the PEI score? Which (if any) of these chemicals in the output (product and waste) streams can be controlled? How would you do it?

**(d) Fish-bone diagram:** Construct a fish bone diagram showing the major causes in the categories of operating cost, equipment safety and environmental impact. What process modifications would you suggest to improve the sustainability performance?

**SRCA Module - Case Study 2**

**Sustainability Root cause analysis of a polygeneration process**

**Problem Statement:** Polygeneration systems use multiple feeds (i.e., coal, biomass, natural gas, etc.) to produce a number of products like chemicals, fuels and power. In this problem, the system under consideration uses coal and natural gas to generate syngas, which is then used to produce di-methyl ether, DME (a diesel substitute) and power in gas and steam turbines. Natural gas undergoes autothermal reforming while coal is gasified to produce syngas. The syngas is then used to generate electricity in a gas turbine and steam turbines, and DME in a two-step process, with methanol as the intermediate.

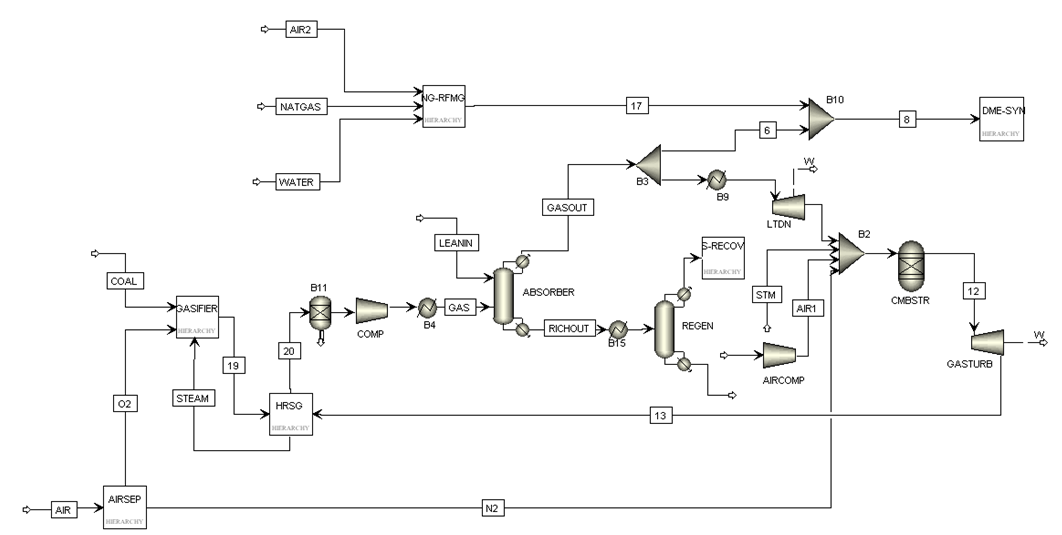


Figure 1. Process Flow Diagram of the Polygeneration Process

The breakdown of costs is:

|  |  |
| --- | --- |
| Section | Cost |
| Coal Handling | $74,657,240 |
| Water Systems | $59,069,820 |
| Gasifier Section | $172,468,680 |
| Air Separation Unit | $131,525,000 |
| Gas Cleaning | $65,350,840 |
| CO2 Compression | $4,487,070 |
| NG Reforming | $10,455,100 |
| Power Generation | $179,519,000 |
| DME Synthesis | $57,194,083 |
| Solvents and Catalysts | $96,000 |
| Plant Accessories | $114,871,550 |
| Total | **$869,695,130** |

The inherent safety score is calculated as:

|  |  |
| --- | --- |
| Chemical | Chemical Inherent Index, ICI |
| Coal | 16.14 |
| Natural Gas | 25.00 |
| Oxygen | 19.60 |
| Sulfur | 0.30 |
| Air | 0.00 |
| Water | 0.00 |
| DME | 117.85 |
| Nitrogen | 19.62 |
| Carbon dioxide | 17.94 |
| Chemical Inherent Index, ICI | **216.46** |
| Equipment | **Process Inherent Index, IPI** |
| Pump | 24 |
| Heat Exchanger | 148 |
| Reactor | 54 |
| Distillation Column | 25 |
| Separator / Extractor | 37 |
| Compressor/Turbine | 96 |
| Process Inherent Index, IPI | **384** |
| TOTAL INHERENT SAFETY INDEX, ITI | **600.5** |

The potential environmental impacts (in eight categories) of the various chemicals in the process are calculated as:

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Chemical | HTPI | HTPE | TTP | ATP | GWP | ODP | PCOP | AP |
| Carbon | 7.8236 | 0.068 | 7.8236 | 0 | 0 | 0 | 0 | 0 |
| Hydrogen Sulfide | 0 | 0.0085 | 0 | 6.9459 | 0 | 0 | 0 | 1.8603 |
| Sulfur | 2.9569 | 0 | 2.9569 | 0.0233 | 0 | 0 | 0 | 0 |
| Ammonia | 1.0729 | 0.0068 | 1.0729 | 0.0566 | 0 | 0 | 0 | 1.8603 |
| Chlorine | 0 | 0.0793 | 0 | 3.9592 | 0 | 0 | 0 | 0 |
| Hydrogen Chloride | 0.1998 | 0.034 | 0.1998 | 0.0008 | 0 | 0 | 0 | 0.8708 |
| Sulfur Dioxide | 0 | 0.0183 | 0 | 0 | 0 | 0 | 0.1441 | 0.9895 |
| Carbonyl Sulfide | 0.5707 | 0 | 0.5707 | 0 | 0 | 0 | 0 | 0 |
| Methanol | 0.0667 | 0.0009 | 0.0667 | 0 | 0 | 0 | 0.2122 | 0 |
| Dimethyl Ether | 0.0177 | 0 | 0.0177 | 0.0001 | 0.0002 | 0 | 0.2468 | 0 |
| Methyl Diethanolamine | 0.0786 | 0 | 0.0786 | 0.0001 | 0 | 0 | 0 | 0 |
| Propane | 0 | 0.0001 | 0 | 0 | 0 | 0 | 0.1476 | 0 |
| Ethane | 0 | 0.0002 | 0 | 0 | 0 | 0 | 0.0851 | 0 |
| Carbon Monoxide | 0 | 0.0043 | 0 | 0 | 0 | 0 | 0.0169 | 0 |
| Methane | 0 | 0.0004 | 0 | 0 | 0.0056 | 0 | 0.0045 | 0 |
| Carbon Dioxide | 0 | 0 | 0 | 0 | 0.0002 | 0 | 0 | 0 |
| Water | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Hydrogen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Oxygen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Nitrogen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Argon | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

The final PEI output score is the sum of the scores in each category.

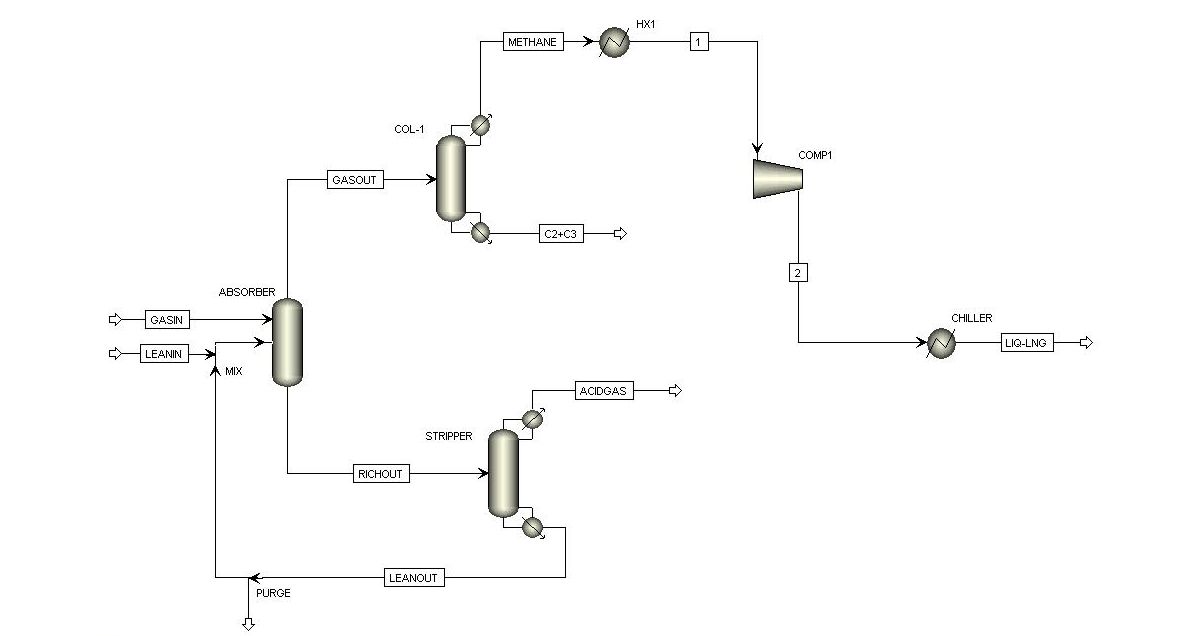
1. Construct Pareto charts for each dimension of sustainability and identify the top factors in each category (capital cost, inherent safety and environmental impact) that need attention in order to improve the sustainability performance.
2. Construct a fish bone diagram showing the major causes in these categories.
3. Examine the current prices of coal and natural gas per MMBtu. Which is cheaper? Which feedstock has a greater environmental impact? Can you conclude from the result which of the two processes (coal gasification or natural gas reforming) is cleaner?

**SRCA Module - Case Study 3**

**Sustainability Root cause analysis of a LNG Process**

**Problem Statement:** Natural gas (NG) has several advantages as a fuel since it is clean-burning and economical. In certain instances where transporting natural gas through pipelines is not feasible, the natural gas needs to be liquefied, transported by sea and further re-gasified before it can be used by the final consumer. The flow diagram and other details for NG liquefaction process are provided below. The natural gas liquefaction part involves acid gas removal using diethanolamine (DEA) solvent to remove H2S, etc., followed by compression and cooling to -123°C to convert the gas to liquid.

**Liquefaction of Natural Gas:**

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**LNG Liquefaction Process: Material Balance**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | GASIN | LEANIN | ACIDGAS | METHANE | C2+C3 | LNG |
| Total Flow (kg/hr) | 35140.12 | 42583.46 | 1563.57 | 30030.26 | 3679.75 | 30030.26 |
| Total Flow (l/min) | 10275.43 | 690.76 | 9201.90 | 6858.51 | 122.11 | 1392.51 |
| Temperature (0C) | 5.15 | 40.15 | 18.50 | -121.46 | -26.29 | -123.00 |
| Pressure (atm) | 62.00 | 62.00 | 1.67 | 62.00 | 62.00 | 70.00 |
| Vapor Frac | 1.00 | 0.00 | 1.00 | 1.00 | 0.00 | 0.00 |
| Mass Flow (kg/hr) |  |  |  |  |  |  |
| METHANE | 29518.68 | 0.00 | 18.99 | 29470.19 | 29.50 | 29470.19 |
| ETHANE | 2165.01 | 0.00 | 1.31 | 0.00 | 2163.70 | 0.00 |
| PROPANE | 1411.09 | 0.00 | 0.54 | 0.00 | 1410.55 | 0.00 |
| NITROGEN | 560.27 | 0.00 | 0.20 | 560.07 | 0.00 | 560.07 |
| CO2 | 1144.25 | 0.00 | 1191.23 | 0.00 | 1.44 | 0.00 |
| WATER | 0.00 | 30296.83 | 8.97 | 0.00 | 71.82 | 0.00 |
| DEA | 0.00 | 12000.51 | 0.00 | 0.00 | 0.00 | 0.00 |
| H2S | 340.82 | 0.00 | 342.34 | 0.00 | 2.74 | 0.00 |

Safety Scores:

Process Safety Scores

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Natural Gas | Water | DEA | Hydrogen Sulfide | Carbon dioxide |
| Flammability | 140.56 | 0 | 12 | 0 | 0 |
| Explosiveness | 35.14 | 0 | 12 | 0.68 | 0 |
| Toxic Limit | 0 | 0 | 60 | 1.37 | 1.19 |
| Corrosiveness | 70.28 | 0 | 0 | 0.68 | 0 |

Chemical Safety Scores

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Pump | Heat Exchanger | Distillation Column | Compressor/Turbine |
| Inventory | 0 | 4 | 7 | 2 |
| Process Temperature | 0 | 2 | 2 | 1 |
| Process Pressure | 0 | 6 | 9 | 3 |
| Equipment Safety | 0 | 2 | 3 | 3 |

1. Using the given data, conduct an inherent safety analysis of the processes. Which are the main factors that contribute to the safety concern in the process?

Another important factor to be considered in the design of processes is the energy efficiency. The total inlet enthalpy is calculated by adding the enthalpy of all the inlet streams and enthalpy used by all the equipments. The total outlet enthalpy is calculated by adding the enthalpy of all outlet streams. The energy efficiency is calculated by dividing the total outlet enthalpy by the sum of total inlet enthalpy and work done by the equipment. The tables below show the enthalpy details for the process.

|  |  |  |
| --- | --- | --- |
| Enthalpy of Inlet Streams | GASIN | 44761.49 kW |
| Work done by Equipments | HX1  COMP1  CHILLER | 2032.10 kW  107.63 kW  4689.92 kW |
| Enthalpy of Outlet Streams | LNG | 44315.65 kW |

(b) Calculate the energy efficiency of the processes. Is the efficiency high? How would you improve the efficiency?