Sustainable Process Development and Evaluation

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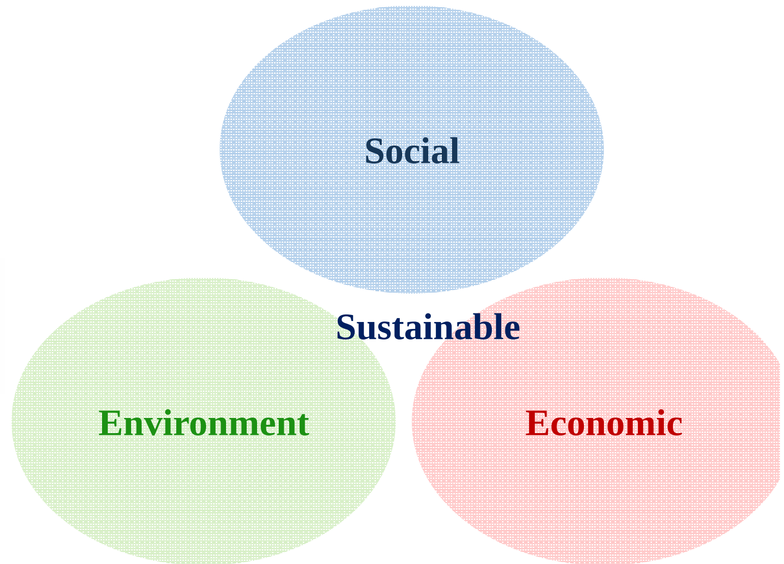
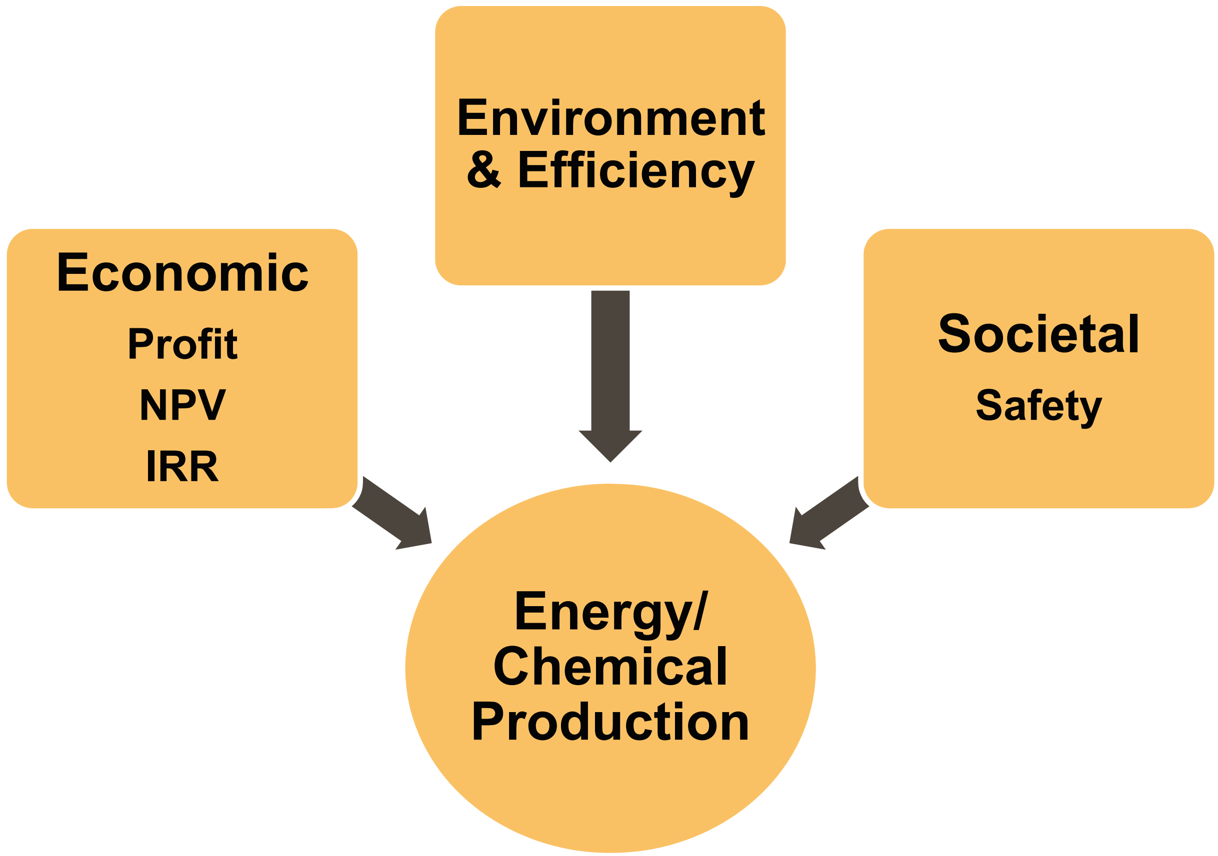
Design for Sustainability



A Systematic, Life-Cycle Based Approach

Criteria for Sustainability Assessment



Economic Evaluation

- **Profit**
- **NPV (Net Present Value)**

NPV = $-C_{TCI} + \sum C_{A,m} / (1+r)^m$

C_{TCI} : Total capital investment before base year composed of total fixed capital cost, working capital cost

C_A : Total annual income cash flow after base year m

r : The interest rate

m: The project life after base year

- **IRR/DPV (Internal Rate of Return/Discounted cash flow rate of return)**

IRR = $FV / (1+i)^n = FV (1-d)$

FV : The nominal value of a cash flow amount in a future period

i : The interest rate **d : The discount rate**

n : The time in years before the future cash flow occurs

NPV and IRR take into account the economic life cycle including initial investment, annual profit, annual depreciation, salvage value and interest on investment

Environmental & Safety Analysis

- Potential Environmental Impact (PEI) from EPA WAR Algorithm is used for environmental analysis

- Enhanced Inherent Safety Index
  - Chemical Inherent Safety Index
  - Process Inherent Safety Index
    - Considers safety score and quantity of process equipment

Exergy Analysis

- The First Law of Thermodynamics
  - The basis of energy analysis. It states that energy can neither be created nor destroyed and it just changes forms
  - However, it does not provide enough information regarding the potential work that a form of energy can produce or the potential work lost in energy transformation processes
- Different types of energy display different qualities
  - For example, high temperature steam can produce more potential work than low temperature steam
- How to compare the efficiency of different feedstock to the same product, or the same feedstock to different products?

Exergy Analysis (cont'd)

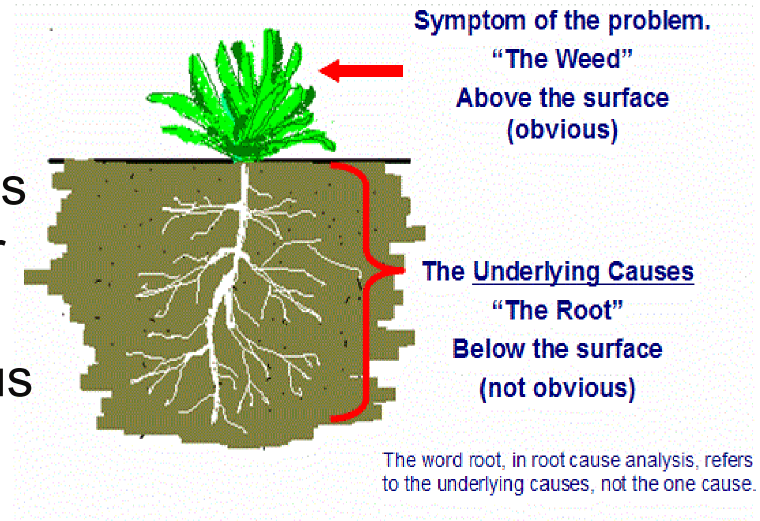
- Based on the First and Second Laws of Thermodynamics, exergy analysis allows accounting for irreversibilities in the process, providing a more detailed tracking mechanism for energy and chemical generation and consumption

- The exergy of a system is the maximum available work that can be extracted from that system until it reaches equilibrium with its environment

- Exergy analysis differentiates the "quality" of energies and chemicals

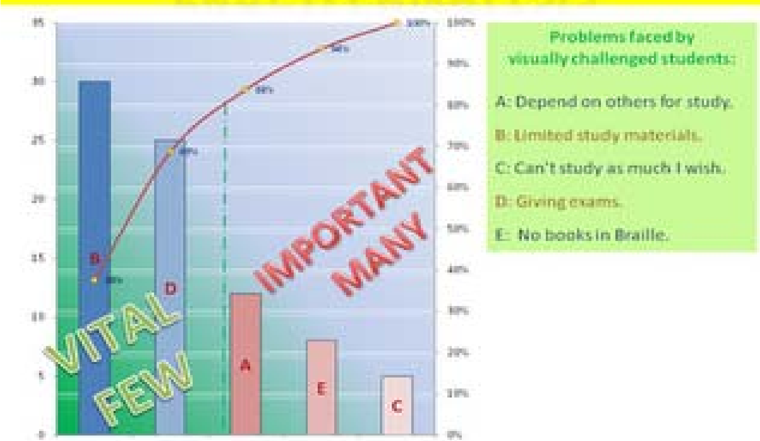
Root Cause Analysis (RCA)

- Root cause analysis (RCA) aims at identifying the root causes of problems
- The RCA works on the belief that problems are best solved by attempting to correct or eliminate root causes, as opposed to merely addressing the immediately obvious symptoms

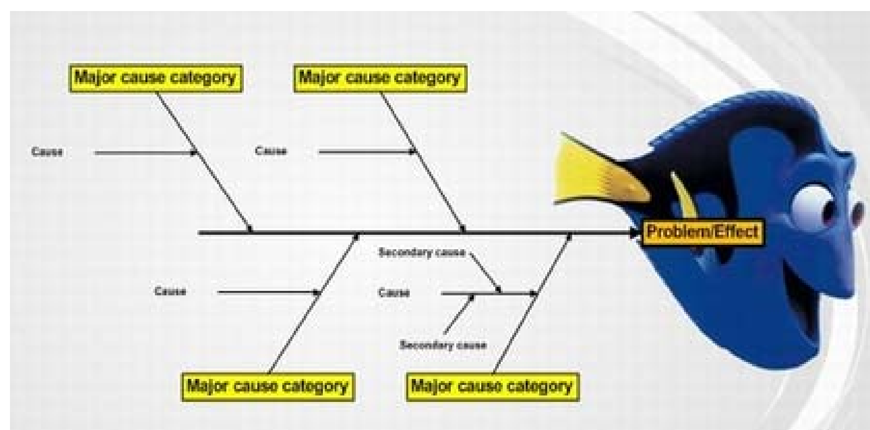


RCA includes

PARETO ANALYSIS



FISH BONE DIAGRAM

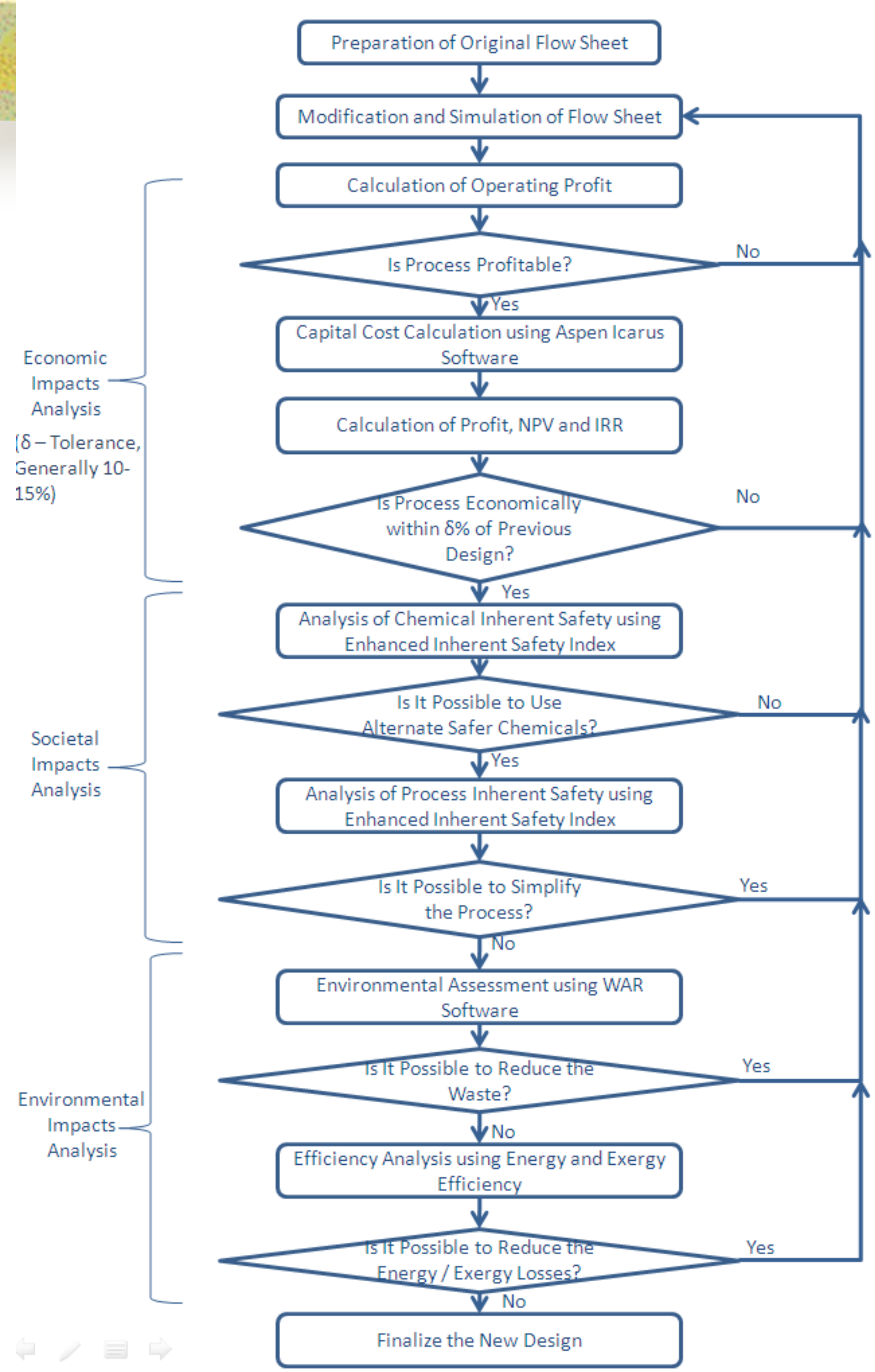


The F-28 Methodology for Sustainability RCA

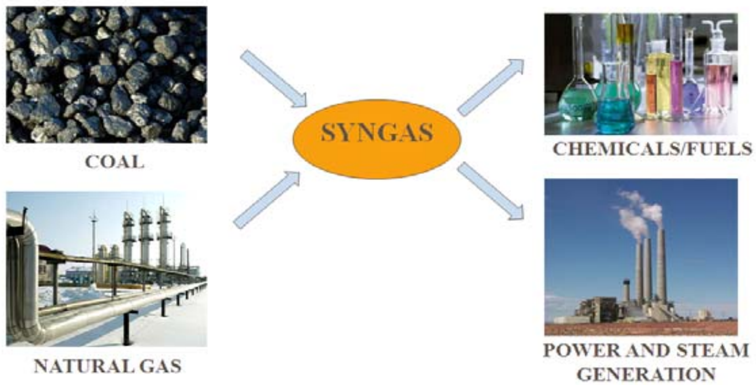
Perform sustainability root cause analysis in two steps:

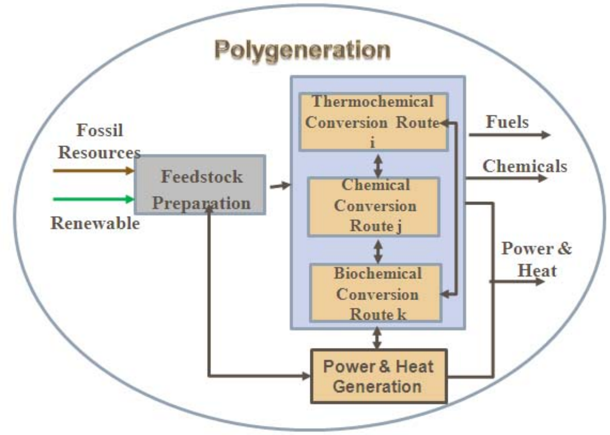
- **The Pareto analysis**
  - **To screen out significant factors and correlations for sustainability improvement**
- **The Fishbone diagram**
  - **To visualize various relationships, and convey the important relationships between seeming disconnected elements**

Decision Making in Design for Sustainability

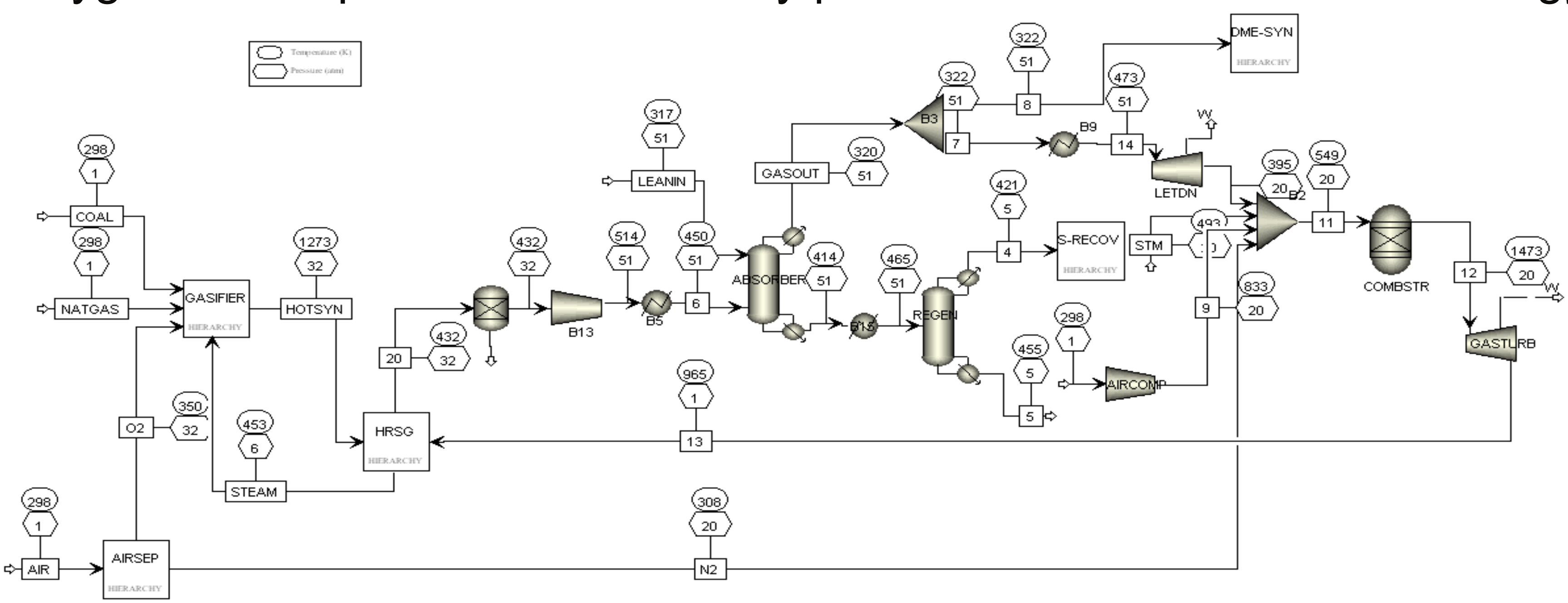


Case Study 1: Polygeneration





Polygeneration plants simultaneously produce chemicals/fuels and energy



Syngas to DME and Power

- DME (dimethyl ether) produced by a 2-stage process

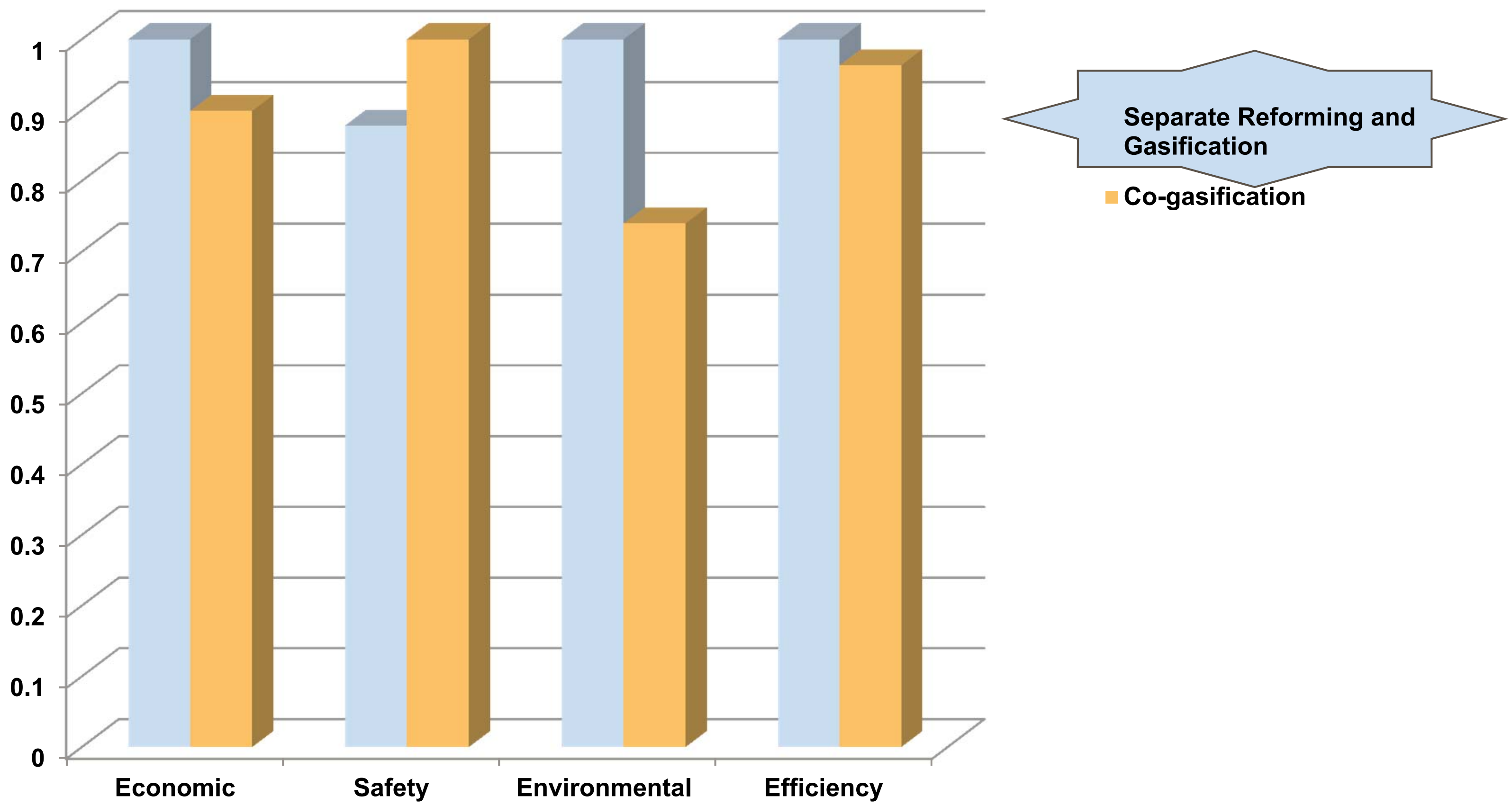
- H_2:CO ratio in syngas:
  - Natural gas reforming ~ 3:1
  - Coal gasification ~ 0.7:1
  - DME synthesis requirement: 2:1

- Two proposed schemes:
  - Separated Natural Gas Reforming and Coal Gasification
  - Co-gasification of Natural Gas and Coal

Input & Output

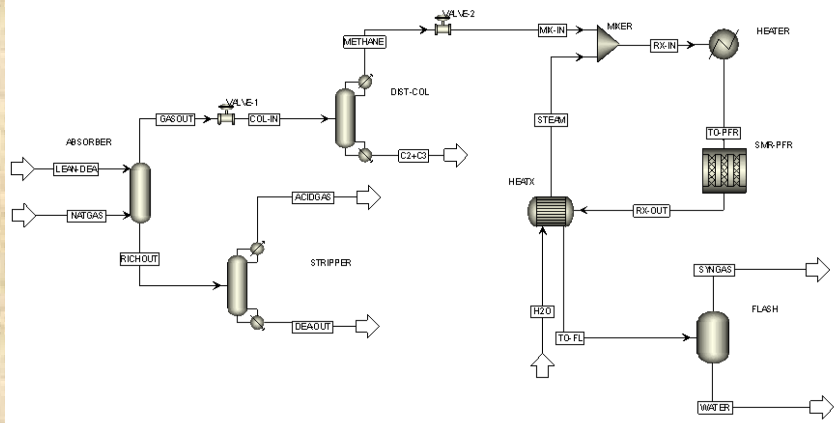
	Coal and Natural Gas Gasification	Cogasification of Coal and Natural Gas
Coal Input (t/h)	80.70	100.00
Natural Gas Input (t/h)	50.00	40.00
Total Thermal Input (MMbtu)	4550.00	4550.00
DME Production (ton/h)	117.8	112.3
Electricity Production (kW/h)	136831.78	157871.70

Overall Sustainability Assessment Results



Case Study 2: Syngas Technologies

Steam Reforming of Methane

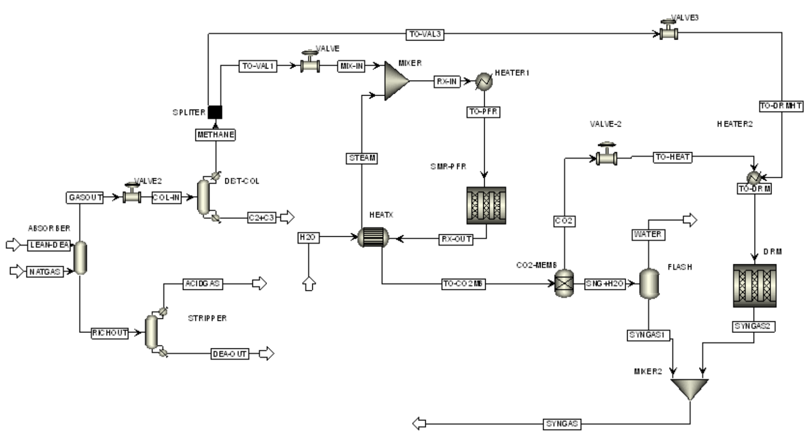


Steam reforming: Exothermic, H_2:CO = 3:1 (molar ratio)

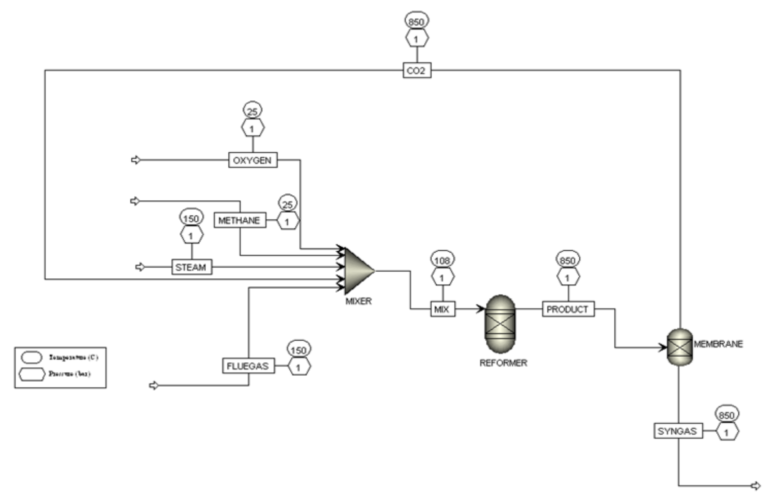
Dry reforming and tri-reforming:

- Endothermic
- produces syngas with a H_2:CO molar ratio suitable for F–T fuels and DME
- consumes greenhouse gases: CO_2, CH_4

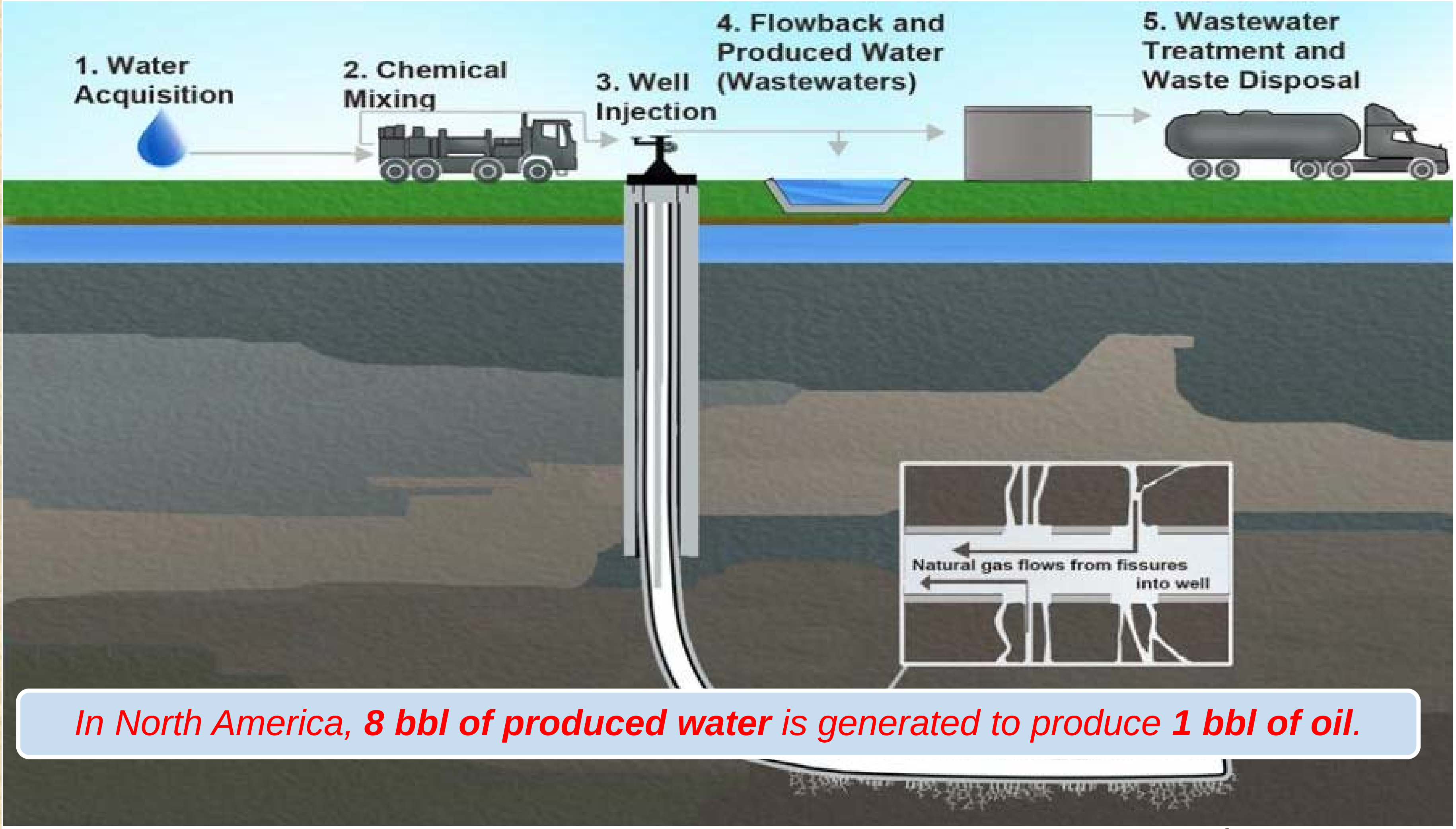
Combined Steam Reforming and Dry Reforming



Tri-reforming of Methane



Case Study 3: Produced Water Treatment Technologies



*In North America, **8 bbl of produced water** is generated to produce **1 bbl of oil**.*

source: environmental protection agency

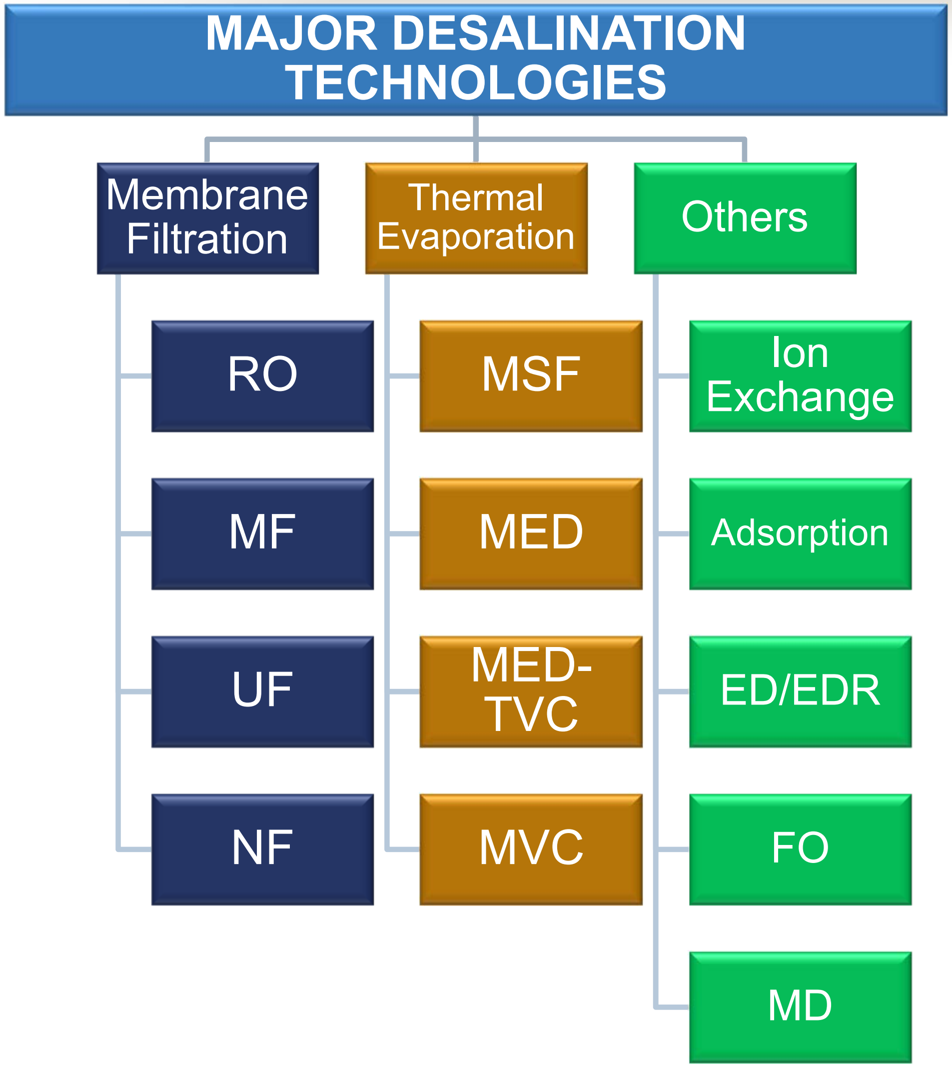
Composition

TDS: 8000 - 360,000 ppm, oil and grease, varies inorganic and organic chemicals, NORM (naturally-occuring radioactive material), etc.

Parameter	Minimum value	Maximum value	Heavy metal	Minimum value (mg/l)	Maximum value (mg/l)
Density (kg/m^3)	1014	1140	Calcium	13	25 800
Conductivity (µS/cm)	4200	58 600	Sodium	132	97 000
Surface tension (dyn/cm)	43	78	Potassium	24	4300
pH	4.3	10	Magnesium	8	6000
TOC (mg/l)	0	1500	Iron	<0.1	100
TSS (mg/l)	1.2	1000	Aluminium	310	410
Total oil (IR; mg/l)	2	565	Boron	5	95
Volatile (BTX; mg/l)	0.39	35	Barium	1.3	650
Base/neutrals (mg/l)	—	<140	Cadmium	<0.005	0.2
Chloride (mg/l)	80	200 000	Copper	<0.02	1.5
Bicarbonate (mg/l)	77	3990	Chromium	0.02	1.1
Sulphate (mg/l)	<2	1650	Lithium	3	50
Ammoniacal nitrogen (mg/l)	10	300	Manganese	<0.004	175
Sulphite (mg/l)	—	10	Lead	0.002	8.8
Total polar (mg/L)	9.7	600	Strontium	0.02	1000
Higher acids (mg/l)	<1	63	Titanium	<0.01	0.7
Phenol (mg/l)	0.009	23	Zinc	0.01	35
Volatile fatty acids (mg/l)	2	4900	Arsenic	<0.005	0.3
			Mercury	<0.005	0.3
			Silver	<0.001	0.15
			Beryllium	<0.001	0.004

1% = 10,000 ppm (mg/L)

Source: Igunnu et al. 2012 Produced water treatment technologies



Salinity ranges from 1,000 ppm to 300,000 ppm (typically 60,000 ppm)

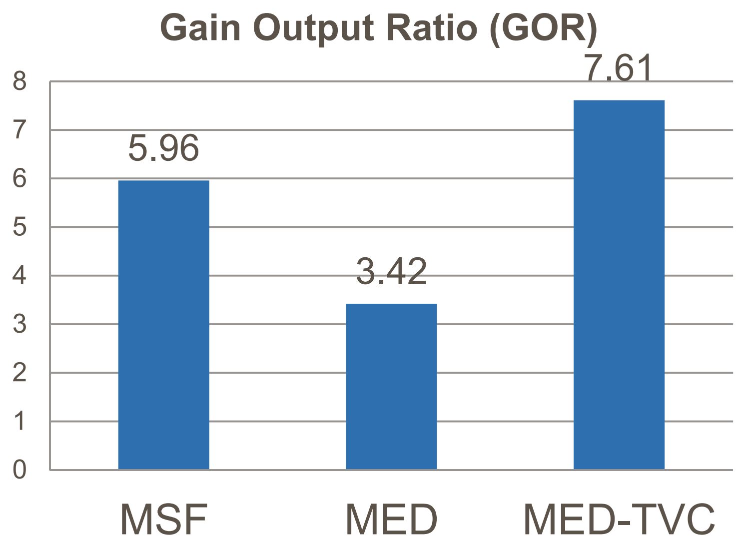
Sustainability Analysis

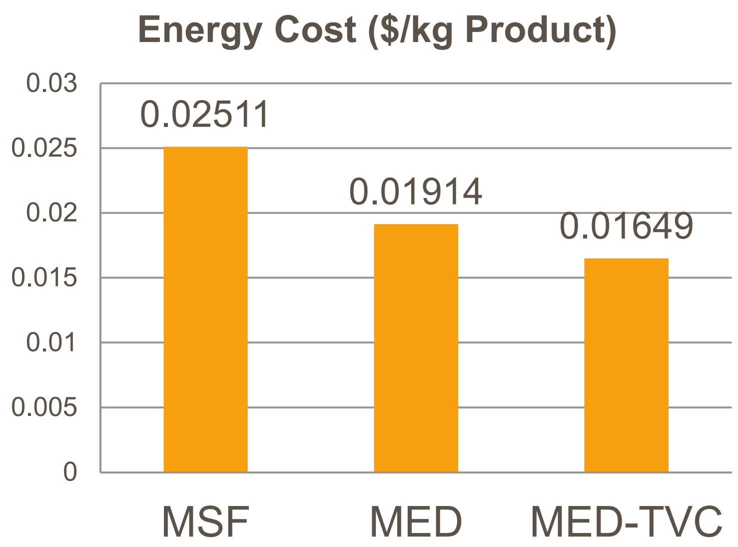
Technological — Gain Output Ratio (GOR), Water Recovery

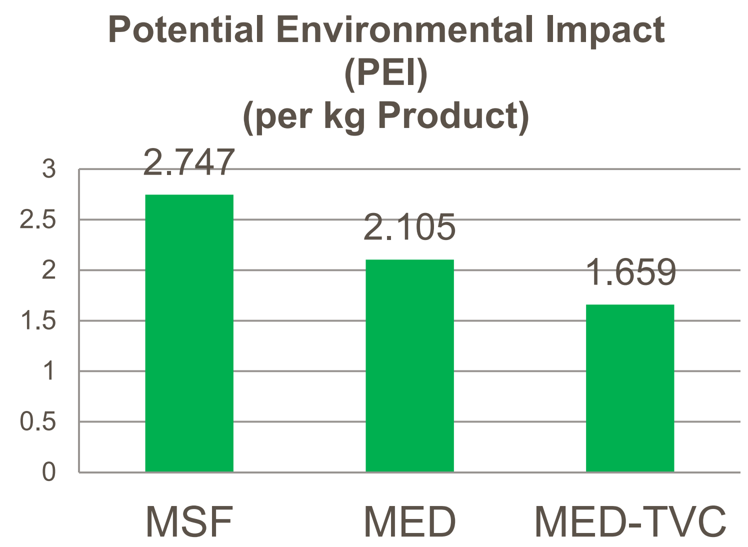
Economic — Capital Cost, Operation Cost

Environmental — Potential Environmental Impacts (PEI)

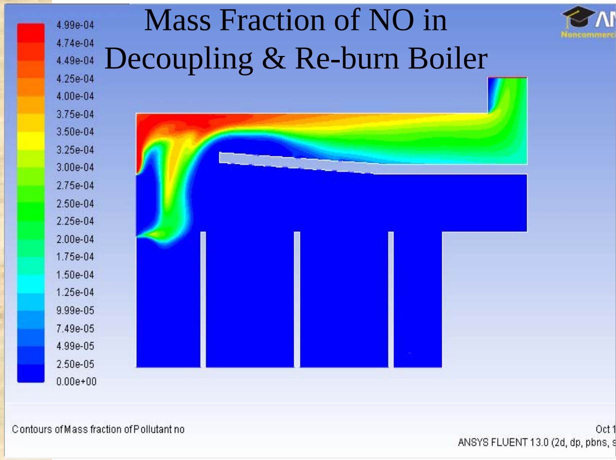
Results Summary

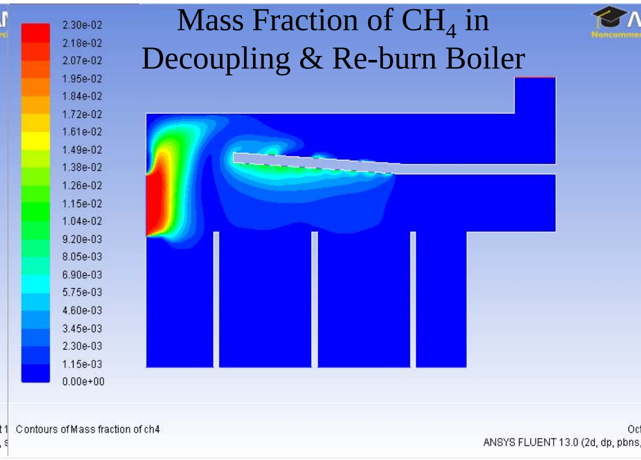


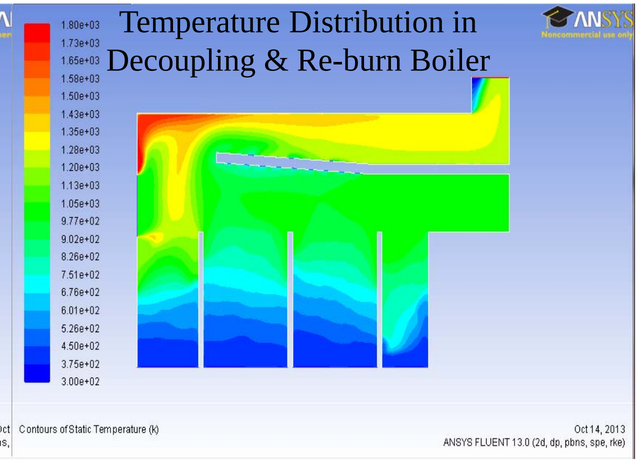


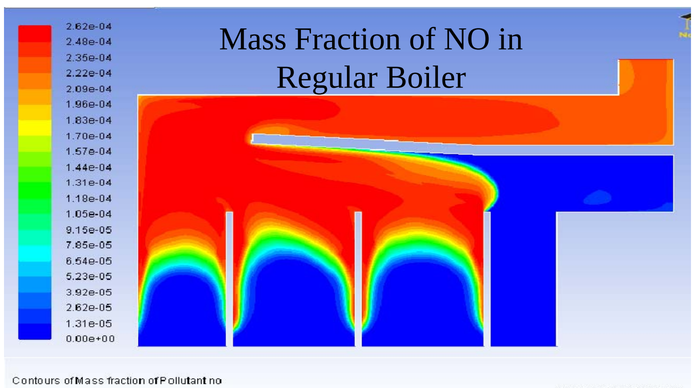


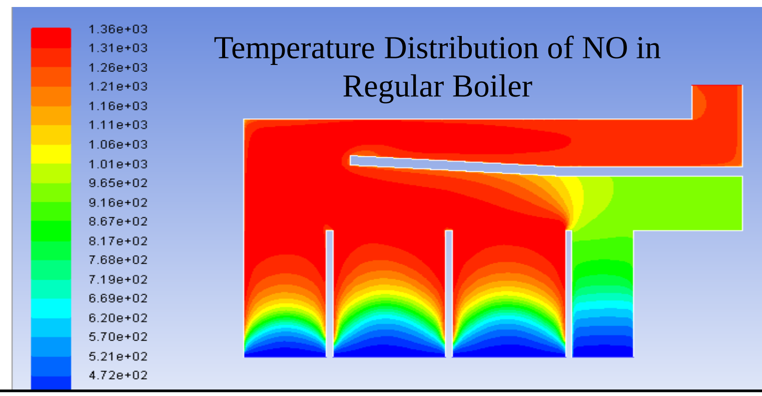
Case Study 4: Low Nox Boiler Development











Comparison of Boilers			
	Regular	New Design	Nox Reduction (%)
Average Mass Fraction of NOx	186.9 ppm	141.1 ppm	24.47%

Conclusions and Discussions

- **Sustainability Assessment**
  - A sequential decision-making procedure for conceptual designs
- **The F-28 Root Cause Analysis methodology**
  - Combines Pareto analysis and the Fishbone diagram
  - Identify the key areas for further improvement
  - A effective tool for process design, analysis and improvement

Acknowledgement

- NSF
- Texas Hazardous Waste Research Center
- Entergy

THANK YOU