Sustainability Assessment
of Coal based Energy and Chemical Processes

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Energy usage spectrum: the world and China

World

- Coal: 35.6%
- Hydroelectric: 28.6%
- Nuclear: 23.8%
- Natural gas: 6.4%
- Oil: 5.6%

China

- Total Consumption in CPI: 70.4%
  - Coal: 47%
  - Other: 53% (coal usage in CPI includes coking and gasification)
In the next 20 years, half demand growth of China’s primary energy/resources supply will remain depending on coal.

Source: International Energy Agency (IEA, 2010)
Background

- In the last few decades, there have been many new coal processes developed and deployed in China.
- However, there has been a lack of quantitative integrated evaluation, either on their technological-economic performance, long-term influence on supply chain, or impact on society and ecological environment.
Base case: Coal syngas derived product chains

- Coal → Gasification
- Gasification → Syngas
- Syngas → Indirect → FT diesel
- Syngas → Ethylene, propylene → PE, PP
- Syngas → Formaldehyde → Paraformaldehyde, formaldehyde resin
- Syngas → Isobutyl alcohol, isobutylene
- Syngas → H2 → DME
- Syngas → Methanol → Acetic acid, Acetic oxide, Methyl formate, Formic acid, Oxalic acid
- Syngas → IGCC → Power, Heat
Sustainability concerns in the CPI

- **Technical and Economics**
  - Efficiency of resource utilization: material, energy, water.
  - Return on Investment capitals.

- **Environmental Impacts**
  - Water, Toxics waste
  - Air pollutant dispersion (especially PM$_{2.5}$)
  - GHG emission

- **Social Benefits**
  - Business: supply chain, market
  - Occupational: health and safety, social responsibility
  - Geographical: urban planning, land use, river and hydrology
Objectives

• To establish life cycle models for alternative coal processes from feedstock, to production, market, and recycling. To rationalize the decision-making on resource allocation and process design;

• To reduce investment and operating costs, raise efficiency and minimize environmental impacts. To explore integrated approaches for balance of efficiency and sustainability.
Approaches for system sustainability analysis

- **Process System Analysis**
  - Input-output analysis (yield, conversion rate)
  - Resource conversion efficiency
  - Exergy analysis

- **Sustainability**
  - Environmental impact assessment
  - Life cycle costing
  - Emergy analysis (ecological analysis)
  - Tech-economic–environ–social: multi-objective coordination
Basic PSE approaches: modeling, simulation, evaluation, and integration

Coal to Methanol

Flowsheeting

Unit modeling

Evaluation

Decision

Integration

optimization

MeOH Synthesis

Coal slurry preparation

Air separation

Cooler & Scrubber Particulate Removal

Gasification

Sulfur Removal

COS hydrolysis

CLAUS

Carbon Removal

Water Gas Shift

MeOH Syn.

De-sulfur

Gasification

optimization

Integration

Decision

Evaluation

Simulation

Flowsheeting

Unit modeling

MeOH Syn.

Coal to Methanol
coal to IGCC/methanol co-production

Gasification

Coal → gasify → Syn-gas → IGCC → Electricity → MeOH → Olefins

Combined Cycle

MeOH Synthesis

Coal slurry preparation → Air separation → Cooler & Scrubber Particulate Removal → Gasification → Sulfur Removal → COS hydrolysis → H2S

MeOH Synthesis

MeOH Synthesis

Carbon Removal

Water Gas Shift

MeOH Synthesis

Gasification

Combined Cycle

MeOH Synthesis
Process improving

- Identify bottlenecks;
- Energy integration and material flow re-distribution were conducted.
- Exergy efficiency improves 5%.
Problem of the single-feedstock gasification process

*Hydrogen to carbon ratio:*
H/C ratio of coal-based syn-gas: 0.5-1;
H/C ratio of NG-based syn-gas: 4-5;
H/C ratio to produce chemicals: 2.

*Energy loss of the key units:*
Coal gasification exothermic, high temperature syngas to be cooled.
NG steam reforming endothermic, 35% extra gas burns to heat.

*Process Innovation: Coal/Gas Co-feed, Chem/Power Co-generation*

Key structural variables:
co- feed factor $P_1$
co-generation factor: $P_2$
NG-Coal co-feed co-generation process

Coal to Syngas

NG reforming

Power

Methanol
Heat Integration

Resource Integration

Rational Reaction

Higher carbon utilization, higher exergy efficiency.

Mass/exergy flow diagram for integration & optimization
Modeling with Eco-indicator 99

1. Establish LCA model and simulation of the process;
2. Sort out environmental impact factor through inventory analysis;
3. Characterization in several major concerning catalogues.
Industrial Case: Coal to Olefins

The first commercial CTO plant in the world was built by China Shenghua Group Co. in 2011, with a capacity of 0.6 Mt/a olefins and annual return $0.16 Billion USD.
There is a big gap between olefins demand and production capacity in China. Ethylene and propylene are produced only 50% and 70% of market demand, respectively.

Coal is relatively abundance and low price in China.

Cost evaluation of CTO

- Coal feedstock cost accounts for 39% of olefins product cost, much lower than 88% of OTO. It may, however, be offset with oil/coal price fluctuation, beside of high utility/investment cost.
- CTO efficiency could be improved with better process integration, utility, operation, equipment.
- On the other hand, CTO is challenged with lower price Middle-east NGTO.
# CTO Energy efficiency, in comparison with OTO

<table>
<thead>
<tr>
<th>Item</th>
<th>OTO</th>
<th>CTO</th>
<th>LHV</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Consumption</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Naphtha (t/t olefins)</td>
<td>1.4</td>
<td>N/A</td>
<td>45000MJ/t</td>
</tr>
<tr>
<td>Coal (t/t olefins)</td>
<td>N/A</td>
<td>4.1</td>
<td>28100MJ/t</td>
</tr>
<tr>
<td>Water (t/t olefins)</td>
<td>9</td>
<td>30</td>
<td>2.6 MJ/t</td>
</tr>
<tr>
<td>Electricity (kWh/t olefins)</td>
<td>74</td>
<td>1671.0</td>
<td>3.6MJ/KWh</td>
</tr>
<tr>
<td>Steam (MJ/t olefins)</td>
<td>1140</td>
<td>8753</td>
<td></td>
</tr>
<tr>
<td>Total E input(GJ/t olefins)</td>
<td>66230</td>
<td>130057</td>
<td>—</td>
</tr>
<tr>
<td><strong>Product/output</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ethylene (t/t olefins)</td>
<td>0.56</td>
<td>0.45</td>
<td>47000MJ/t</td>
</tr>
<tr>
<td>Propylene (t/t olefins)</td>
<td>0.26</td>
<td>0.45</td>
<td>47000MJ/t</td>
</tr>
<tr>
<td>C₄ (t/t olefins)</td>
<td>0.17</td>
<td>0.10</td>
<td>47000MJ/t</td>
</tr>
<tr>
<td>CO₂ (t/t olefins)</td>
<td>1.3</td>
<td>5.8</td>
<td>—</td>
</tr>
<tr>
<td>Product energy (MJ)</td>
<td>47000</td>
<td>47000</td>
<td>—</td>
</tr>
<tr>
<td><strong>Energy efficiency (%)</strong></td>
<td>71.0</td>
<td>36.1</td>
<td>—</td>
</tr>
</tbody>
</table>

We have to explore new process to improve CTO performance.
Life cycle boundary of the CTO process

Crude coal → Coal mining → Coal gangue
          |                    |
          v                    v
Coal preparation → Bitumite

Fuel & Elec. → Coal transportation → Bitumite

ASU → CG → Ethylene
      ↓  WGS → Propylene
      ↓  AGR
      ↓  MS
      ↓  MTO

Electricity → Air → Water

CC → CO₂
CLAUS → Sulfur
LCA

Goal Definition And Scoping

Exergy inventory
  1. Life cycle exergy analysis

Environmental emission inventory
  2. Life cycle environmental analysis

Cost inventory
  3. Life cycle cost analysis

Process comparison

Improvement
Life cycle exergy flow diagram of CTO
## Life cycle exergy inventory of CTO

<table>
<thead>
<tr>
<th>Stage</th>
<th>Unit</th>
<th>Input Item</th>
<th>$E_{x_{flow}}$ (MW)</th>
<th>Output Item</th>
<th>$E_{x_{dest}}$ (MW)</th>
<th>$\eta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CP</td>
<td>CM&amp;P</td>
<td>Crude coal</td>
<td>1229.38</td>
<td>Bitumite</td>
<td>1003.76</td>
<td>54.23</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Elec. and fuel</td>
<td>54.23</td>
<td>Coal gangue</td>
<td>225.62</td>
<td></td>
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<tr>
<td>CT</td>
<td>CT</td>
<td>Bitumite</td>
<td>1003.76</td>
<td>Bitumite</td>
<td>1003.76</td>
<td>1.68</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Elec. and fuel</td>
<td>1.68</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OP</td>
<td>ASU</td>
<td>Air</td>
<td>6.79</td>
<td>$O_2$</td>
<td>13.74</td>
<td>69.50</td>
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<tr>
<td></td>
<td></td>
<td>Elec.</td>
<td>95.29</td>
<td>$N_2$</td>
<td>12.05</td>
<td></td>
</tr>
<tr>
<td>CWS</td>
<td></td>
<td>Bitumite</td>
<td>1003.76</td>
<td>Slurry</td>
<td>1003.91</td>
<td>0.46</td>
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<tr>
<td></td>
<td></td>
<td>Water</td>
<td>0.15</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Elec.</td>
<td>0.46</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CG</td>
<td></td>
<td>Slurry</td>
<td>1003.91</td>
<td>Crude syngas</td>
<td>677.33</td>
<td>241.45</td>
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<tr>
<td></td>
<td></td>
<td>$O_2$</td>
<td>13.74</td>
<td>Steam</td>
<td>112.18</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cooling water</td>
<td>18.54</td>
<td>Elec.</td>
<td>5.54</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Ammonia water</td>
<td>0.30</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WGS</td>
<td></td>
<td>Crude syngas</td>
<td>677.33</td>
<td>Shifted syngas</td>
<td>659.53</td>
<td>129.98</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Steam</td>
<td>112.18</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>AGR</td>
<td></td>
<td>Shifted syngas</td>
<td>659.53</td>
<td>Cleaned syngas</td>
<td>619.88</td>
<td>3.48</td>
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<tr>
<td></td>
<td></td>
<td>$N_2$</td>
<td>12.05</td>
<td>Rich $H_2S$</td>
<td>11.49</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Elec.</td>
<td>0.03</td>
<td>Rich $CO_2$</td>
<td>36.75</td>
<td></td>
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<tr>
<td>MSU</td>
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<td>Cleaned syngas</td>
<td>619.88</td>
<td>Methanol</td>
<td>545.24</td>
<td>77.85</td>
</tr>
</tbody>
</table>

![Exergy Inventory Diagram](image_url)
LCA

Goal Definition And Scoping

1. Exergy inventory
   - Life cycle exergy analysis

2. Environmental emission inventory
   - Life cycle environmental analysis
   - Process comparison
   - Improvement
   - Life cycle cost analysis

3. Cost inventory

- GWP: Global warming potential
- OZD: Ozone depletion
- POCP: Prot-chemical potential
- AP: Acid rain potential
- HT: Health Toxion
- NP: Nutrition potential
- ETP: Ecological Toxion potential
- RDP: Resource depletion potential

- Traditional production costs
- Waste management costs
- Ecological costs
- Social costs
### Life cycle environmental inventory of CTO

<table>
<thead>
<tr>
<th></th>
<th>kg/t olefins</th>
<th>CO₂</th>
<th>CH₄</th>
<th>NO₂</th>
<th>SO₂</th>
<th>NOX</th>
<th>CO</th>
<th>VOC</th>
<th>PM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal mining stage</td>
<td></td>
<td>42.5</td>
<td>10.94</td>
<td>.003</td>
<td>0.41</td>
<td>0.11</td>
<td>0.01</td>
<td>0.11</td>
<td>0.11</td>
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<tr>
<td>Transport stage</td>
<td></td>
<td>0.1</td>
<td>0.00</td>
<td>.001</td>
<td>0.00</td>
<td>0.00</td>
<td>.000</td>
<td>.000</td>
<td>.000</td>
</tr>
<tr>
<td>Production stage</td>
<td></td>
<td>8744.0</td>
<td>1.86</td>
<td>.044</td>
<td>5.31</td>
<td>5.72</td>
<td>9.11</td>
<td>1.60</td>
<td>1.81</td>
</tr>
<tr>
<td>Utilization stage</td>
<td></td>
<td>10.9</td>
<td>6.69</td>
<td>.001</td>
<td>0.16</td>
<td>0.39</td>
<td>4.41</td>
<td>0.74</td>
<td>5.28</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td>8797.0</td>
<td>19.50</td>
<td>.048</td>
<td>5.88</td>
<td>6.22</td>
<td>13.53</td>
<td>2.45</td>
<td>7.21</td>
</tr>
</tbody>
</table>

The chart below shows the contribution of each stage to the total emissions for each pollutant.
### Life cycle cost of CTO

<table>
<thead>
<tr>
<th>CNY/t olefins</th>
<th>CO₂</th>
<th>CH₄</th>
<th>NO₂</th>
<th>SO₂</th>
<th>NOₓ</th>
<th>CO</th>
<th>VOC</th>
<th>PM</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal mining stage</td>
<td>2.1</td>
<td>9.83</td>
<td>0.02</td>
<td>13.3</td>
<td>1.7</td>
<td>0.00</td>
<td>1.6</td>
<td>12.8</td>
<td>41</td>
</tr>
<tr>
<td>Transport stage</td>
<td>0.0</td>
<td>0.00</td>
<td>0.01</td>
<td>0.0</td>
<td>0.1</td>
<td>0.00</td>
<td>0.0</td>
<td>0.01</td>
<td>0.1</td>
</tr>
<tr>
<td>Production stage</td>
<td>424.4</td>
<td>1.67</td>
<td>0.34</td>
<td>170.5</td>
<td>90.3</td>
<td>0.66</td>
<td>22.9</td>
<td>202.4</td>
<td>913</td>
</tr>
<tr>
<td>Utilization stage</td>
<td>0.5</td>
<td>6.01</td>
<td>0.00</td>
<td>5.2</td>
<td>6.2</td>
<td>0.32</td>
<td>10.6</td>
<td>589.7</td>
<td>618</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>427.0</td>
<td>17.51</td>
<td>0.37</td>
<td>189.0</td>
<td>98.3</td>
<td>0.99</td>
<td>35.1</td>
<td>804.9</td>
<td>1573</td>
</tr>
</tbody>
</table>

The external cost constitutes 1/4 of life cycle cost, mainly in the stages of production and utilization, respectively.
Life cycle cost of CTO

In LCC of CTO, PM treatment is the largest external cost. CCS cost is the second.
How to improve the sustainability of CTO? **Process innovation.**

1. **Natural Gas and Coal to Olefin (NG-CTO)**

(1) CH$_4$ introduced to a dry reformer with recycled CO$_2$. The syngas H$_2$/CO ratio 1:1, to improve mixed syngas H/C ratio.

(2) A part of pressurized hot CO$_2$ is recycled to the gasifier, as a gasification agent, to increase syngas production.

**Diagram:**

- **DMR**
- **WGS**
- **AGR**
- **MS**
- **MTO**
- **ASU**

**Flowchart A**

- CH$_4$ → DMR → α
- Coal → Preprocessing → Gasification Unit → β → WGS → AGR → MS → MTO
- Water
- Oxygen (O$_2$) from ASU
- Unshifted gas
- Recycle Gas → CO$_2$ emission
- Purge Gas
- Ethylene Propylene
- Sulfur

**Huge CO$_2$ emission (5.8t CO$_2$/ t Olefins).**
Mass and Energy Efficiency Improvement

NG-CTO efficiency for material, energy, and CO\textsubscript{2} emission.

As CO\textsubscript{2} recycle, Carbon element and energy efficiency increase, while CO\textsubscript{2} emission is reduced.

Methane dry reforming reaction is strongly endothermic. It is important to select CO\textsubscript{2} recycle rate for a rational energy integration.
NG-CTO production cost 7020 CNY/t, slightly higher than CTO 6500 CNY/t.

High NG market prices contributes to high NG-CTO cost, due to the shortage of oil and natural gas in China.

When carbon tax is applied, NG-CTO is superior to CTO at a break even point of 14 Euro.
There are 35 billion m³/yr H₂ rich coke-oven gas burned in China.

- H₂-rich coke-oven gas fed, CH₄/CO₂ reforming raise H/C ratio to 1.
- CH₄/H₂O reforming raise H/C further to 2
As introduce of coke oven gas, C utilization efficiency rises, while CO₂ emission decreases.

H/C increases with the introduce of coke-oven gas.
## Energy efficiency and CO₂ release of GCTO

<table>
<thead>
<tr>
<th>Item</th>
<th>CTO</th>
<th>CGTO</th>
<th>LHV</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Consumption</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coal (t/t olefins)</td>
<td>4.10</td>
<td>0.97</td>
<td>28100.0 MJ/t</td>
</tr>
<tr>
<td>Coke-oven gas (m³/t olefins)</td>
<td>N/A</td>
<td>3288</td>
<td>17.4 MJ/m³</td>
</tr>
<tr>
<td>Water (t/t olefins)</td>
<td><strong>30.00</strong></td>
<td><strong>48.00</strong></td>
<td>2.6 MJ/t</td>
</tr>
<tr>
<td>Electricity (kWh/t olefins)</td>
<td>1671</td>
<td>2064</td>
<td>3.6 MJ/kWh</td>
</tr>
<tr>
<td>Steam (MJ/t olefins)</td>
<td>8753</td>
<td>12498</td>
<td>—</td>
</tr>
<tr>
<td>Total energy input (MJ)</td>
<td>130056</td>
<td>104521</td>
<td>—</td>
</tr>
<tr>
<td><strong>Products output</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ethylene (t/t olefins)</td>
<td>0.45</td>
<td>0.45</td>
<td>47000.0 MJ/t</td>
</tr>
<tr>
<td>Propylene (t/t olefins)</td>
<td>0.45</td>
<td>0.45</td>
<td>47000.0 MJ/t</td>
</tr>
<tr>
<td>C₄⁺ (t/t olefins)</td>
<td>0.10</td>
<td>0.10</td>
<td>47000.0 MJ/t</td>
</tr>
<tr>
<td>CO₂ emission (t/t olefins)</td>
<td><strong>5.80</strong></td>
<td><strong>0.30</strong></td>
<td>—</td>
</tr>
<tr>
<td>Olefins energy (MJ)</td>
<td>47000</td>
<td>47000</td>
<td>—</td>
</tr>
<tr>
<td>Energy efficiency (%)</td>
<td><strong>36.10</strong></td>
<td><strong>50.70</strong></td>
<td>—</td>
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</tbody>
</table>
Economic analysis of GCTO - Product cost

Product costs comparison

Product cost of GCTO vs CTO when carbon tax is applied

Break even point: 145 CNY, or 25 USD

* Feedstock: 620 CNY/t coal, 0.8 CNY/m³ coke-oven gas.
Concluding Remarks

1. Coal based processes will still dominate the energy/chemical industries in China for next a few decades.

2. Compared with conventional OTO, although CTO is economical feasible, it suffers lower energy efficiency, higher water usage, and severe emissions. Existing CTO could be integrated with alternative feedstock to raise H/C ratio and reduce CO$_2$ release.

3. Coal based processes with higher CO$_2$ capture rate and higher purity for commercial use could improve environmental and economic performance a lot.

4. Multi-dimensional technical-economical-environmental-social models should be built for quantitative sustainability analysis, which is essentially important for innovative development of sustainable new coal based chemical processes.
Recent Publications


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Questions and comments please.

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Outline

• Background
• Objectives and approaches of sustainability analysis
• Energy efficiency analysis and process integration
• Sustainability analysis
  – Industrial Case: coal to olefins
• Concluding remarks
Coal-based Energy and Chemical Product Chains

Coal
  ↓
Chemical
    ↓
     Coking
       ↓
       Coke
       ↓
       Coal tar
       ↓
       Gas
     ↓
Liquefaction
     ↓
     Direct
       ↓
       Diesel
       ↓
       Gasoline
       ↓
       Vehicle fuel
     ↓
     Indirect
       ↓
       FT diesel
     ↓
Syngas
     ↓
     Ethylene, propylene
     ↓
     PE, PP
     ↓
     Formaldehyde
     ↓
     Paraformaldehyde, formaldehyde resin
     ↓
     Isobutyl alcohol, isobutylene
     ↓
     H2
     ↓
     Methanol
     ↓
     DME
     ↓
     Acetic acid
     ↓
     Acetic oxide
     ↓
     Methyl formate
     ↓
     Formic acid
     ↓
     Oxalic acid
     ↓
     Power
     ↓
     Heat

Analysis, evaluation, decision-making of different product chains
Alternative Co-production processes

Methanol-Power Co-production

Coal
26377kJ/kg
Gasification
MeOH synthesis
MeOH 632kJ 24%
Combined cycle
Elec. 7111kJ 27%
Total: 51%

Hydrogen-Power Co-generation

Coal
26377kJ/kg
Gasification
CO shift
PSA
H₂ 9113kJ 34.6%
Combined cycle
Elec. 5663kJ 21.5%
Total: 56%

With CO₂ Capture

Coal
26377kJ/kg
Gasification
CO shift
CO₂ Capture
PSA
H₂ 9113kJ 34.6%
Combined cycle
Elec. 5109kJ 19.4%
Total: 54%
LCA Approach

Goal Definition And Scoping

Exergy inventory

Life cycle exergy analysis

Environmental emission inventory

Life cycle environmental analysis

Cost inventory

Life cycle cost analysis

Process comparison

Improvement
Life Cycle Boundary and Scope

Life Cycle Cost = $\text{Internal Cost} + \text{External Cost}$
Life Cycle Assessment (LCA) and Sustainability Analysis

Product Life Cycle Assessment

Technical and Economic Accounting

Sustainability: Environmental, Ecological, and Social development
Eco-LCA Framework

Multi-attribute Eco-LCA Metrics

1. Sustainable exploitation
   \[ \alpha = a^{\text{aver}} \cdot a^{\text{min}} \]

2. Economic effectiveness
   \[ \lambda = \frac{\text{Money}_{\text{Prod}}}{\text{Money}_{\text{Inv}}} \]

3. Environmental compatibility
   \[ \psi = \frac{EMR}{IVP} \]

4. Resource utilization
   \[ ECDP = \frac{Ex_{\text{Prod}}}{ECEC_{\text{Prod}}} \]


2. EMR is the overall $ECEC/\text{Money}$ Ratio, IVP is the $ECEC$ per unit of economic output. \[ \psi = \frac{EMR}{(ECEC_{\text{Prod}} / \text{Money}_{\text{Prod}})} \]
Eco-LCA of Steam Production

the functional unit produces 80 kt/yr of 3.5MPa saturated steam.

Gas boiler v.s. Solar boiler

[Diagram showing the processes and flows of steam production for both gas and solar boilers, with economic investment and environmental impacts quantified in units of 10^18 sej/yr.]
Eco-LCA of Steam Production

Resource utilization
\( ECDP \)
- (Gas) \( 3.16\times10^6 \)
- (Solar) \( 10.2\times10^6 \)

Economic effectiveness
\( \lambda \)
- (Gas) 1.82
- (Solar) 1.38

Environmental compatibility
\( \psi \)
- (Gas) 0.43
- (Solar) 1.38

Sustainable exploitation
\( \alpha \)
- (Gas) 0.04
- (Solar) 1.00
## Sustainability analysis on resource, energy, environment, and economy

<table>
<thead>
<tr>
<th>Generic</th>
<th>No.</th>
<th>Indicators</th>
<th>Metric</th>
</tr>
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<tbody>
<tr>
<td>Resource</td>
<td>1</td>
<td>Mass productivity ($MP$)</td>
<td>kg/kg</td>
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<tr>
<td></td>
<td>2</td>
<td>Renewability material index ($RI_M$)</td>
<td>kg/kg</td>
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<tr>
<td>Energy</td>
<td>3</td>
<td>Energy efficiency ($\eta$)</td>
<td>kJ/kJ</td>
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<tr>
<td></td>
<td>4</td>
<td>Exergy efficiency ($\psi$)</td>
<td>kJ/kJ</td>
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<tr>
<td>Environment</td>
<td>5</td>
<td>Global warming portential ($GWP$)</td>
<td>kg/kg</td>
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<td></td>
<td>6</td>
<td>Atmospheric acidification potential ($AP$)</td>
<td>kg/kg</td>
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<td></td>
<td>7</td>
<td>Environmental loading ratio ($ELR$)</td>
<td>kSej/kSej</td>
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<tr>
<td>Economy</td>
<td>8</td>
<td>Payback period ($PBP$)</td>
<td>yr</td>
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<tr>
<td></td>
<td>9</td>
<td>Equivalent annual cost ($c_{eq}$)</td>
<td>$</td>
</tr>
</tbody>
</table>
Case 4: Coal based process with CCS
Energy consumption, economic and environmental performance with CC rate

In considering carbon tax (at 20 Euro), CTO with 80% CCR is economically attractive than OTO, MTO, or CTO without CC.
Coal gasification with CCS or CCU?

- As shown in the chart, although GWP reduced, CO₂ capture (CC) costs (90%) for oil extraction/geo-storage are of higher cost and payback period.
- On the other side, CO₂ enriched to higher concentration (99%) for commercial usage is better for resource utilization and economic performance.
- Quantitative sustainability analysis helps rational decision making on CCUS approaches.

Carbon tax = $20 USD/t equivalent CO₂
Eco-LCA of Olefin Production

Eco-LCA models of CTO and OTO are being established and quantitatively compared, as the long term strategy assessment for the industry and decision makers.
Efficiency vs. Sustainability
Coordinate, Balance, Trade off
A platform for sustainability assessment and decision-making

**Data**
- Database: DECHEMA
- Data reconciliation: DataCon
- LCA Database: Eco-Invent

**Main models**
- Process unit models
- Process flowsheeting
- Life cycle exergy
- Life cycle costing
- Environment impacts
- multi-factor Integration
- Sustainability decision-making

**Tools**
- simulator: ASPEN Plus
- LCA software: SimPro
- Optimizer: GAMS

**Outport**
- sustainability performance
- Process Improvement and innovation
Process integration, and Innovation

Alternative energy-chemical processes

- Computer Simulation
  - Unit simulation
    - Integrated system
      - Life cycle modeling
  - Theoretical analysis
    - Elements
      - Metabolic analysis
    - LCA
      - Input-Output Analysis
        - Evaluation

- Element efficiency
  - Life cycle environmental analysis
  - Life cycle cost analysis
  - Life cycle exergy analysis

- AHP approach
  - Ecological Input-Output Analysis

Life cycle evaluation of the efficiency and sustainability
Integrated innovation of new energy/chemical processes