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)
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** → Syngas → Indirect → FT diesel

- Ethylene, propylene → PE, PP
- Formaldehyde → Paraformaldehyde, formaldehyde resin
- Isobutyl alcohol, isobutylene

- H2
- Methanol → DME, Acetic acid, Acetic oxide, Methyl formate, Formic acid, Oxalic acid

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

optimization  Integration

Decision

Evaluation

Simulation

Flowsheeting

Unit modeling

MeOH Synthesis

Coal slurry preparation

Air separation

Cooler & Scrubber

Particulate Removal

Gasification

Sulfur Removal

COS hydrolysis

CLAUS

Carbon Removal

Water Gas Shift

De-sulfur

MeOH Syn.
coal to IGCC/methanol co-production
Exergy efficiency analysis

Coal 100%

ASU

Energy Flow 1.02%

Oxygen 0.79%

Nitrogen 1.23%

Exergy loss 3.53%

SPG

Syngas 78.11%

WGS

Syngas 76.34%

Exergy loss 1.40%

Energy Flow 0.37%

Exergy loss 2.52%

Energy Flow 8.12%

AGR

Nitrogen 0.59%

Hydrogen sulfide 0.44%

Exergy loss 0.37%

CLAUS

Sulfur 0.07%

Exergy loss 1.47%

Syngas 34.94%

Methanol Synthesis

Energy Flow 4.41%

Energy Flow 3.18%

Syngas 29.06%

Methanol Separate

Exergy loss 3.76%

Methanol 28.48%

HRSG-CC

Electricity 18.31%

Energy Flow 7.16%

Exergy loss 25.53%

Exergy loss 14.56%

Exergy loss 1.40%
- 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 \( P_2 \)
Multi-feed Co-production System

- Coal/Coke
- Coke Oven Gas
- Cracking
- Coal bed gas
- Natural gas
- Biomass
- Gasification
- Catforming
- Steam Reforming
- Refining
- Power Generation
- Combined Cycle
- Unreacted Gas
- Steam
- Electricity
- Chemicals Synthesis
- MeOH, F-T Fuel DME, Hydrogen

Syngas:
- H2/CO: 0.5
- H2/CO: 5
- H2/CO: 3
- H2/CO: 3
- H2/CO: 2
NG-Coal co-feed co-generation process

Coal to Syngas

NG reforming

Power

Methanol
Less exergy loss

Higher carbon utilization, higher exergy efficiency.
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.
LCA

Goal Definition And Scoping

1. Exergy inventory
   - Life cycle exergy analysis

2. Environmental emission inventory
   - Life cycle environmental analysis

3. Cost inventory
   - 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>Ex_{flow} (MW)</th>
<th>Output Item</th>
<th>Ex_{dest} (MW)</th>
<th>η</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>O₂</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>N₂</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>
</tr>
<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></td>
</tr>
<tr>
<td></td>
<td></td>
<td>O₂</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>
</tr>
<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>N₂</td>
<td>12.05</td>
<td>Rich H₂S</td>
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<td></td>
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<tr>
<td></td>
<td></td>
<td>Elec.</td>
<td>0.03</td>
<td>Rich CO₂</td>
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<tr>
<td>MSU</td>
<td></td>
<td>Cleaned syngas</td>
<td>619.88</td>
<td>Methanol</td>
<td>545.24</td>
<td>77.85</td>
</tr>
</tbody>
</table>

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**chart:**

- **Exergy input:**
  - **CP:** 1283.61 MW
  - **CT:** 1005.44 MW
  - **OP:** 1127.73 MW

- **Exergy output:**
  - **CP:** 677.33 MW
  - **CT:** 659.53 MW
  - **OP:** 619.88 MW

- **Exergy destruction:**
  - **CP:** 54.23 MW
  - **CT:** 1.68 MW
  - **OP:** 723.12 MW
## Life cycle environmental inventory of CTO

<table>
<thead>
<tr>
<th>Stage</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>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>
</tr>
<tr>
<td>Transport stage</td>
<td>0.1</td>
<td>0.00</td>
<td>.001</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Production stage</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>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>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>

![Graph showing percentage contributions of different pollutants across stages](27)
## 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>0.0</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>Total</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

<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>
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<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>
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<td>0.34</td>
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<td>90.3</td>
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<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>
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<td>618</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>427.0</strong></td>
<td><strong>17.51</strong></td>
<td><strong>0.37</strong></td>
<td><strong>189.0</strong></td>
<td><strong>98.3</strong></td>
<td><strong>0.99</strong></td>
<td><strong>35.1</strong></td>
<td><strong>804.9</strong></td>
<td><strong>1573</strong></td>
</tr>
</tbody>
</table>

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) CH₄ introduced to a dry reformer with recycled CO₂. The syngas H₂/CO ratio 1:1, to improve mixed syngas H/C ratio.

(2) A part of pressurized hot CO₂ is recycled to the gasifier, as a gasification agent, to increase syngas production.
Mass and Energy Efficiency Improvement

NG-CTO efficiency for material, energy, and CO₂ emission.

As CO₂ recycle, Carbon element and energy efficiency increase, while CO₂ emission is reduced.

Methane dry reforming reaction is strongly endothermic. It is important to select CO₂ 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.
Coke-oven Gas aided Coal to Olefins (GCTO)

- H₂-rich coke-oven gas fed, CH₄/CO₂ reforming raise H/C ratio to 1. CH₄/H₂O reforming raise H/C further to 2.

There are 35 billion m³/yr H₂ rich coke-oven gas burned in China.
Material and Environmental performance of GCTO

H/C increases with the introduce of coke-oven gas

As introduce of coke oven gas, C utilization efficiency rises, while CO₂ emission decreases.
## 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><strong>130056</strong></td>
<td><strong>104521</strong></td>
<td>—</td>
</tr>
<tr>
<td><strong>Products output</strong></td>
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<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>
</tr>
</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 145CNY, 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 CO₂ release.

3. Coal based processes with higher CO₂ 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


2011: Dynamic flexibility analysis of chemical reaction systems with time-delay reactions.
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• National Science Foundation of China (21136003);
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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

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

Methanol-Power Co-production

Coal \(\rightarrow\) Gasification \(\rightarrow\) MeOH synthesis \(\rightarrow\) Combined cycle

Gasification \(\rightarrow\) MeOH \(\rightarrow\) Combined cycle

MeOH \(\rightarrow\) 24%  
Elec. \(\rightarrow\) 27%

Total: 51%

Hydrogen-Power Co-generation

Coal \(\rightarrow\) Gasification \(\rightarrow\) CO shift \(\rightarrow\) PSA \(\rightarrow\) Combined cycle

Gasification \(\rightarrow\) CO shift \(\rightarrow\) PSA

H₂ \(\rightarrow\) 34.6%  
Elec. \(\rightarrow\) 21.5%

Total: 56%

With CO₂ Capture

Coal \(\rightarrow\) Gasification \(\rightarrow\) CO shift \(\rightarrow\) CO2 Capture \(\rightarrow\) Combined cycle

Gasification \(\rightarrow\) CO shift \(\rightarrow\) CO2 Capture

H₂ \(\rightarrow\) 34.6%  
Elec. \(\rightarrow\) 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 = Internal Cost + External Cost
Life Cycle Assessment (LCA) and Sustainability Analysis

Product Life Cycle Assessment

Technical and Economic Accounting

Sustainability: Environmental, Ecological, and Social development
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
   \[ \psi = \frac{\text{EMR}}{\text{IVP}} \]

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


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

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

Gas boiler v.s. Solar boiler

Unit: 10^18 sej/yr
Eco-LCA of Steam Production

Resource utilization ($ECDP$)
- (Gas) $3.16 \times 10^6$
- (Solar) $10.2 \times 10^6$

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>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Renewability material index ((RI_M))</td>
<td>kg/kg</td>
</tr>
<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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<tr>
<td></td>
<td>6</td>
<td>Atmospheric acidification potential ((AP))</td>
<td>kg/kg</td>
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<tr>
<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
In considering carbon tax (at 20Euro), 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 (90%) for oil extraction/geo-storage are of higher cost and PayBackPeriod.
- 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 equivalentCO₂
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: DECHHEMA
- 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

**Output**
- sustainability performance
- Process Improvement and innovation

**Tools**
- simulator: ASPEN Plus
- LCA software: SimPro
- Optimizer: GAMS
Process integration, and Innovation

Alternative energy-chemical processes

Computer Simulation → Unit simulation → Integrated system

Theoretical analysis → Elements Metabolic analysis → LCA → Input-Output Analysis → Evaluation

Aspen Plus

SimaPro

Element efficiency

Life cycle environmental analysis
Life cycle cost analysis
Life cycle exergy analysis

Ecological Input-Output Analysis

AHP approach

Life cycle evaluation of the efficiency and sustainability

Integrated innovation of new energy/chemical processes