Sustainability Assessment of Coal based Energy and Chemical Processes

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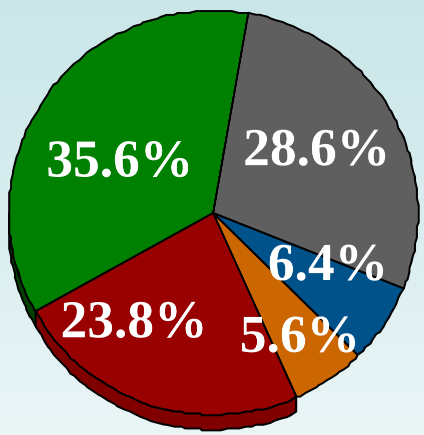
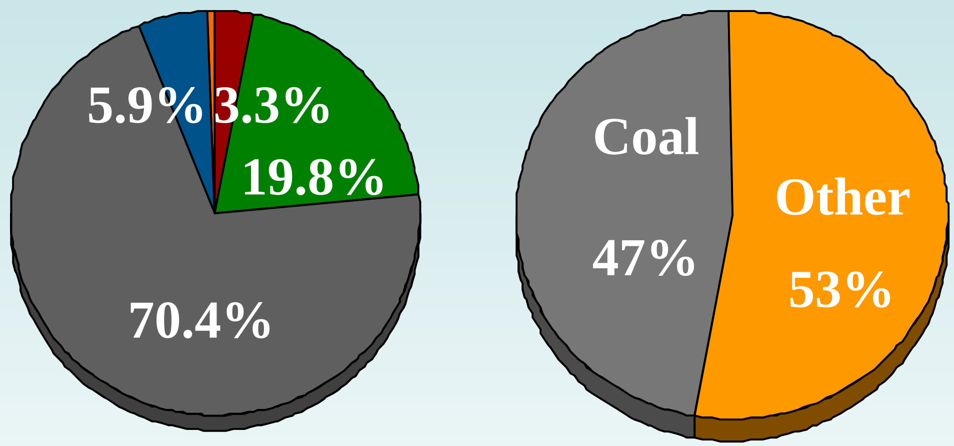
Energy usage spectrum: the world and China



World

- Coal
- Hydroelectric
- Nuclear
- Natural gas
- Oil

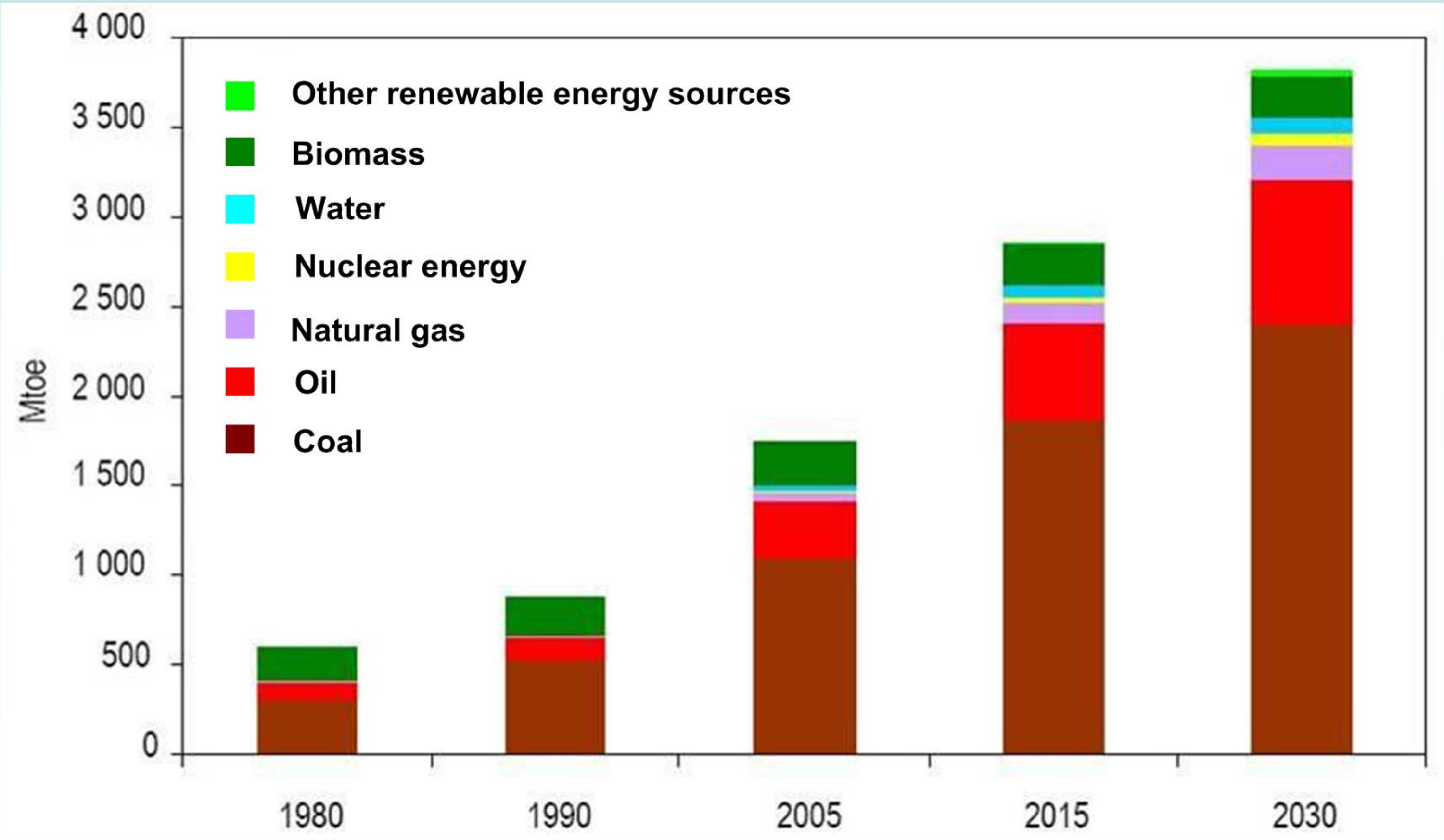


Total Consumption **in CPI**

China

coal usage in CPI includes coking and gasification

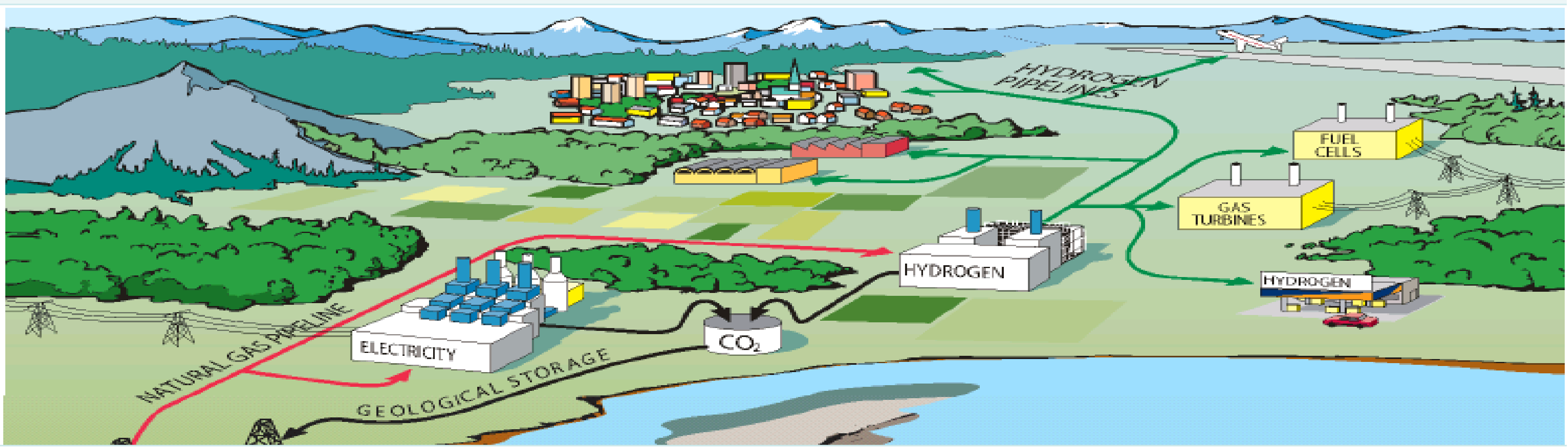
In the next 20 years, half demand growth of China's primary energy/resources supply will remain depending on coal.



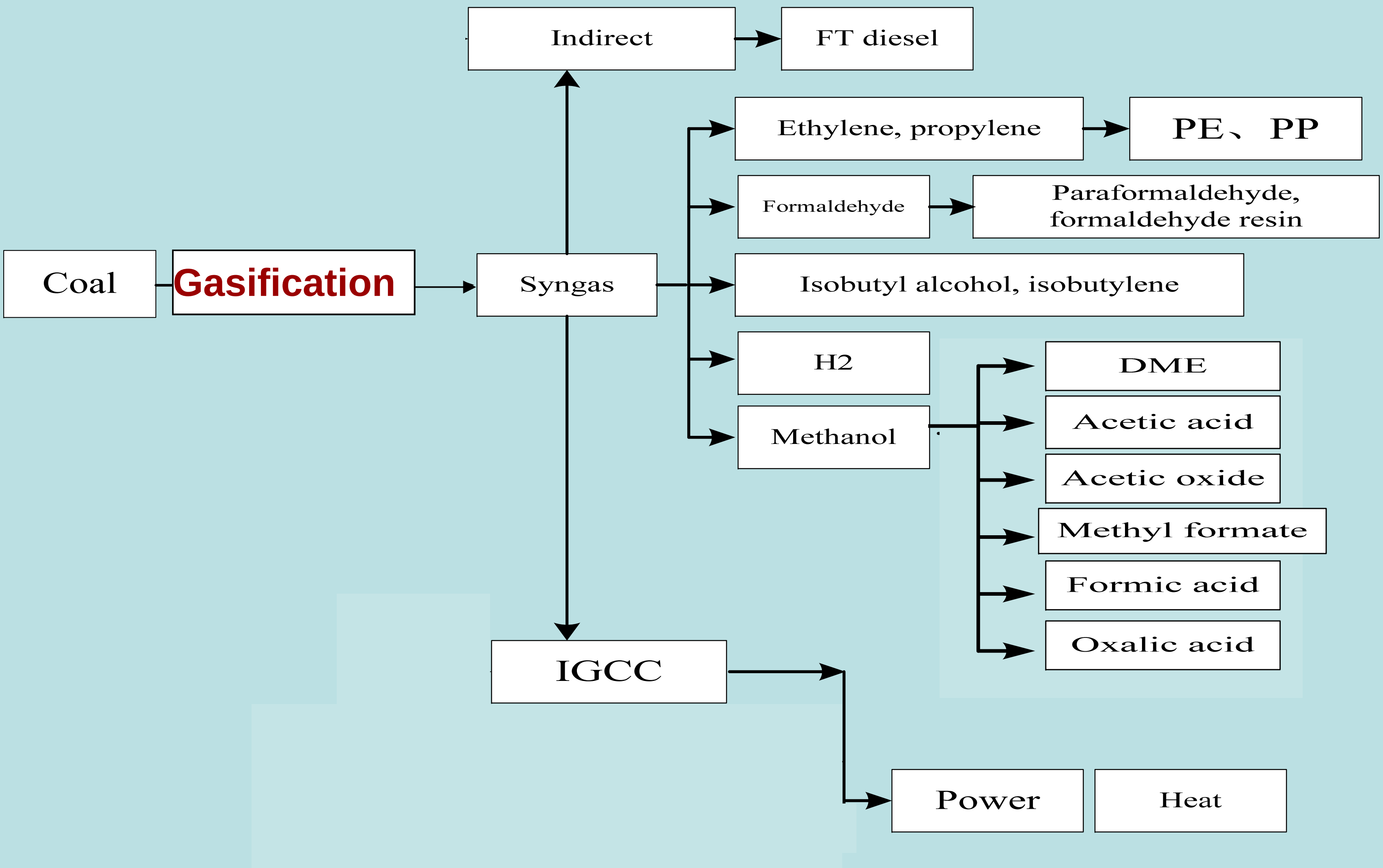
Source: International Energy Agency (IEA, 2010)

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



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

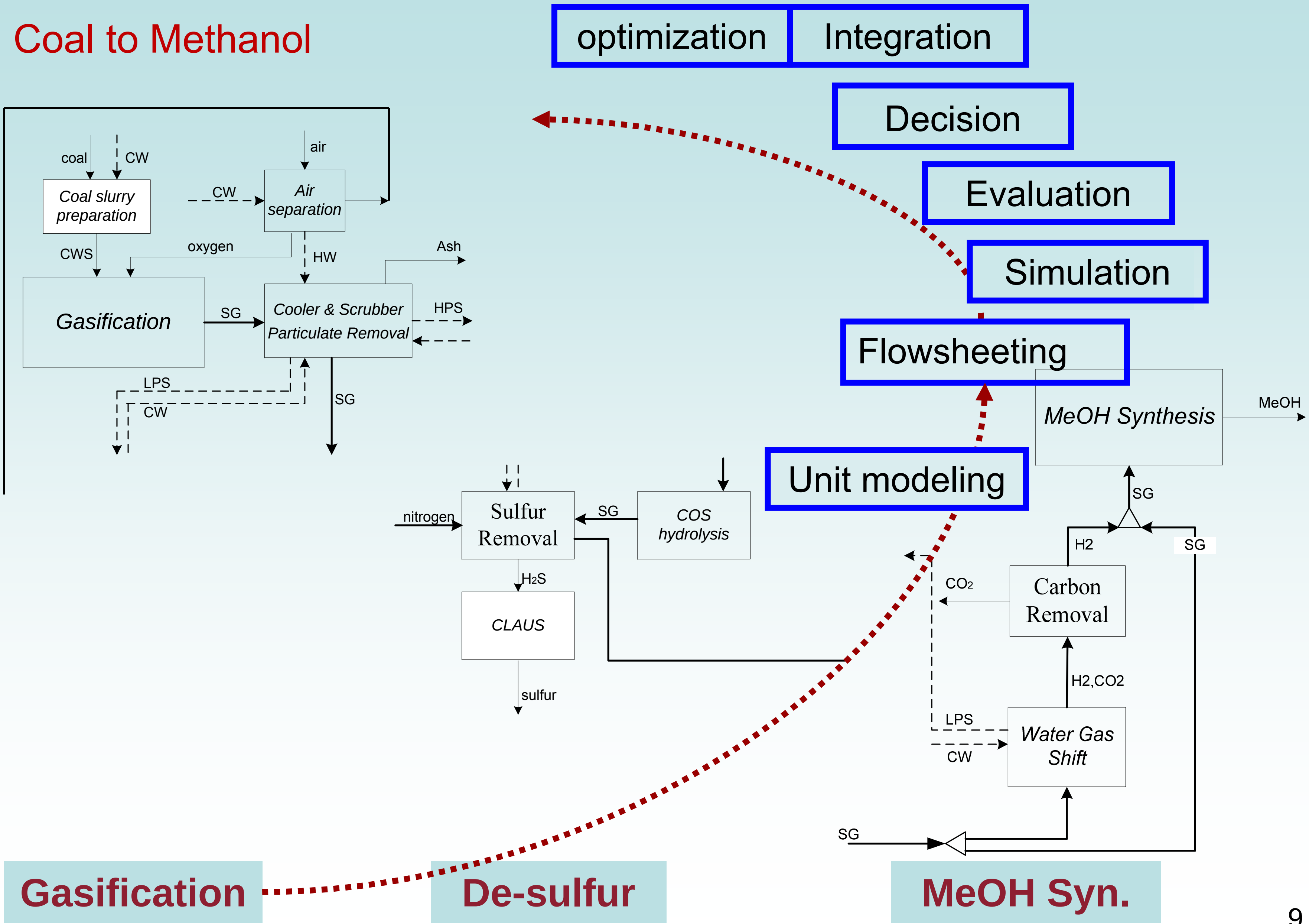
  Life cycle costing

  Emergy analysis (ecological analysis)

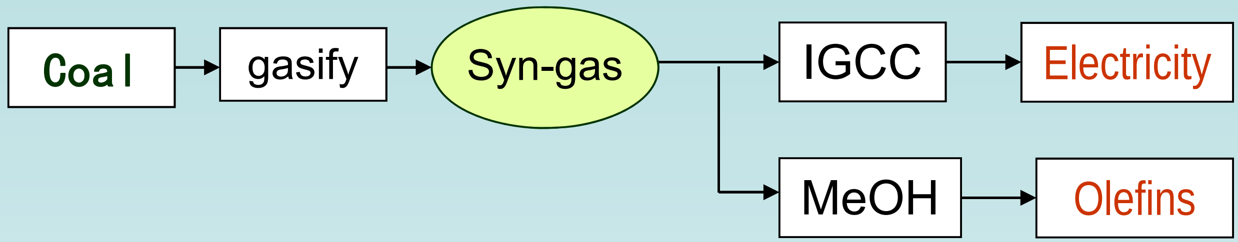
  Tech-economic–environ–social: multi-objective coordination

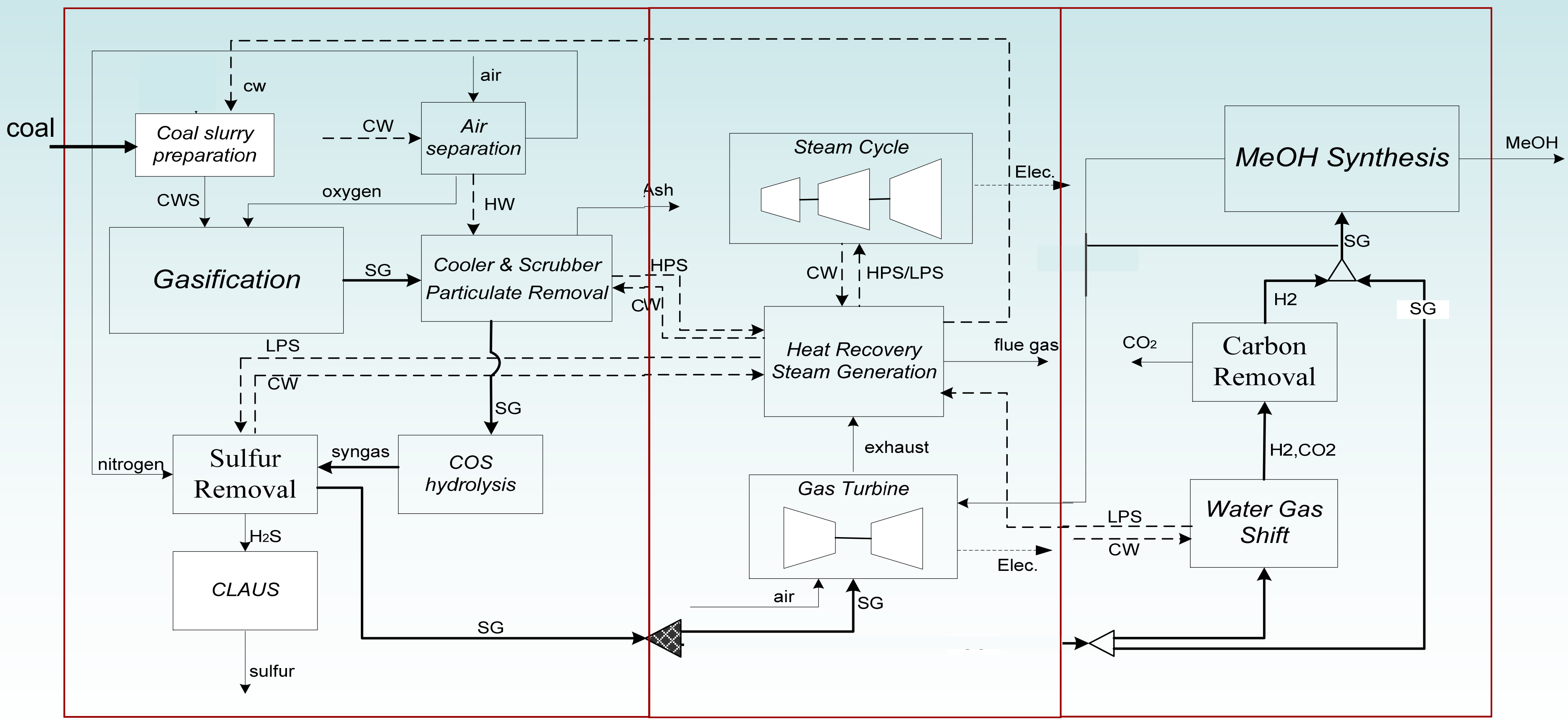
Basic PSE approaches: modeling, simulation, evaluation, and integration

Coal to Methanol



coal to IGCC/methanol co-production



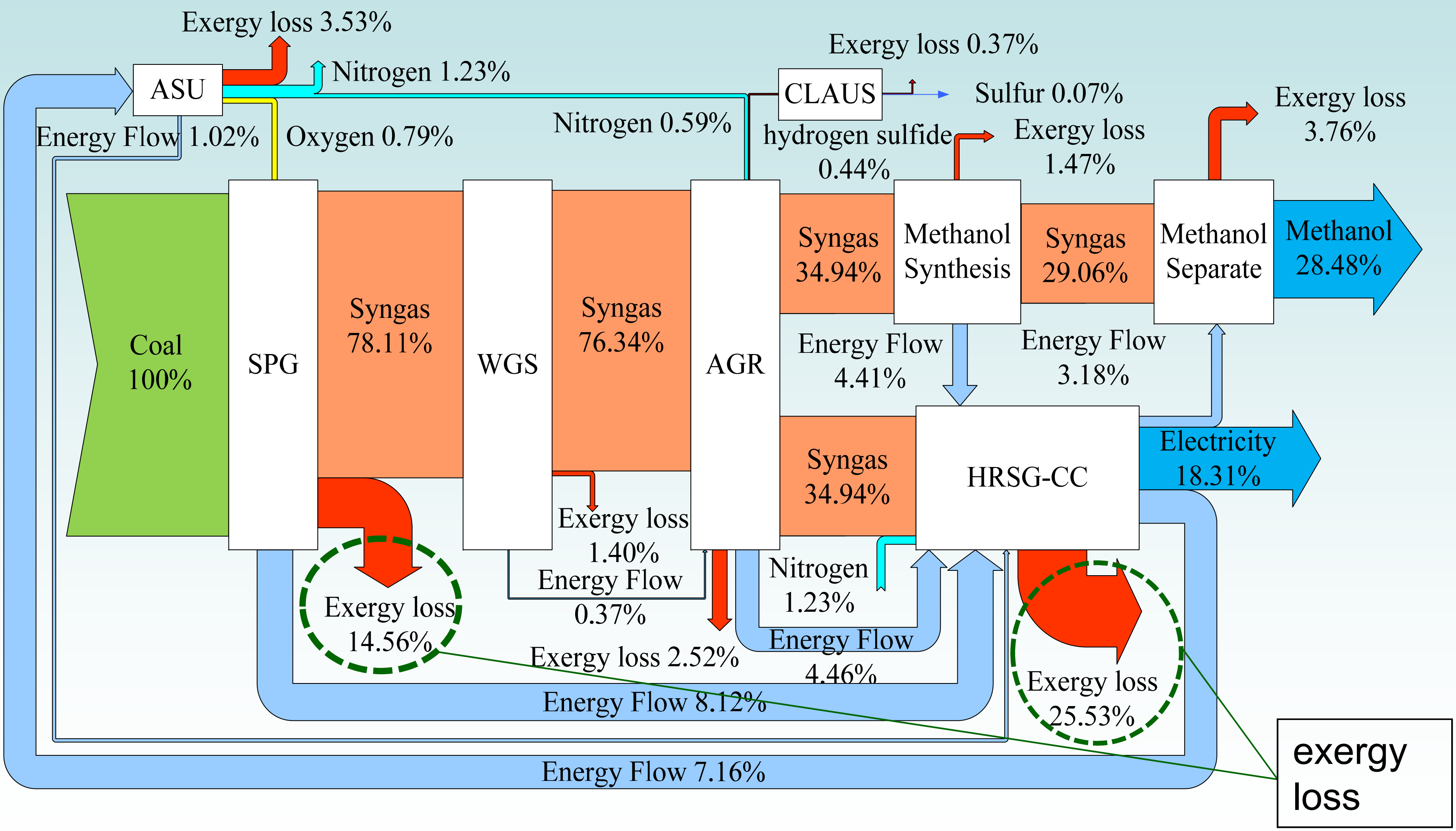


Gasification

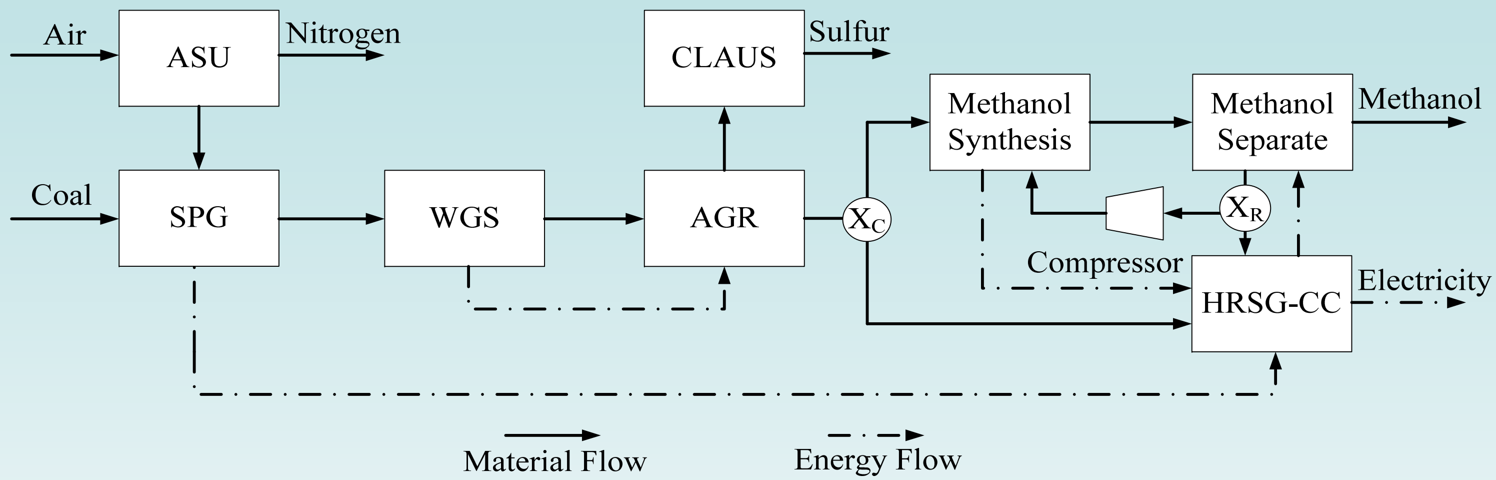
Combined Cycle

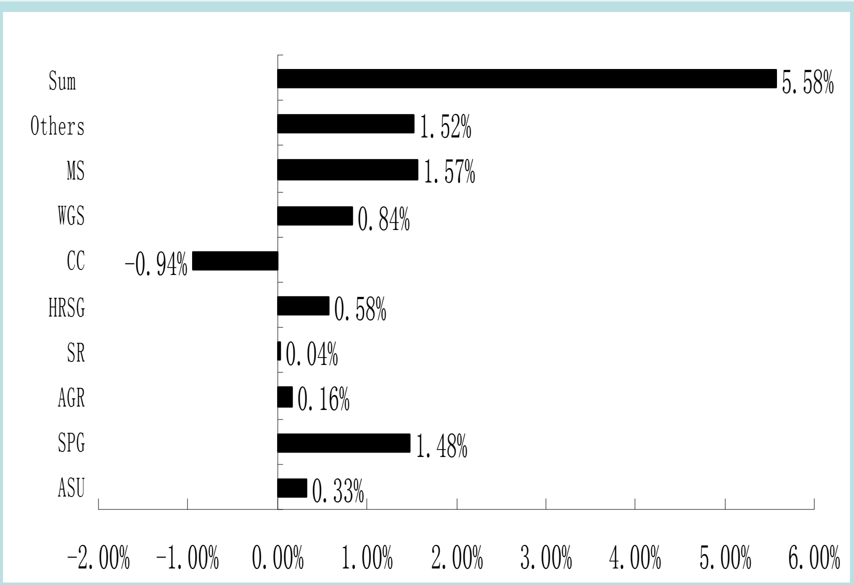
MeOH Synthesis

Exergy efficiency analysis



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;

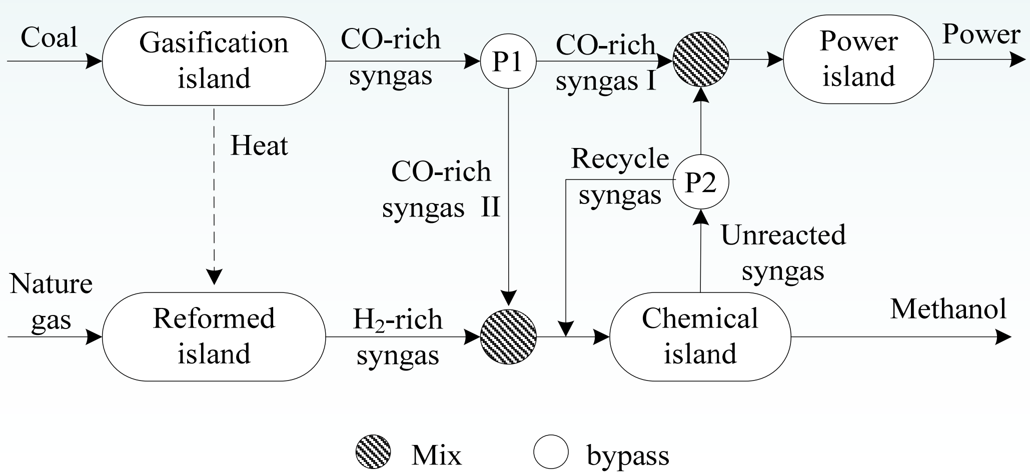
H/C ratio to produce chemicals: 2.

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

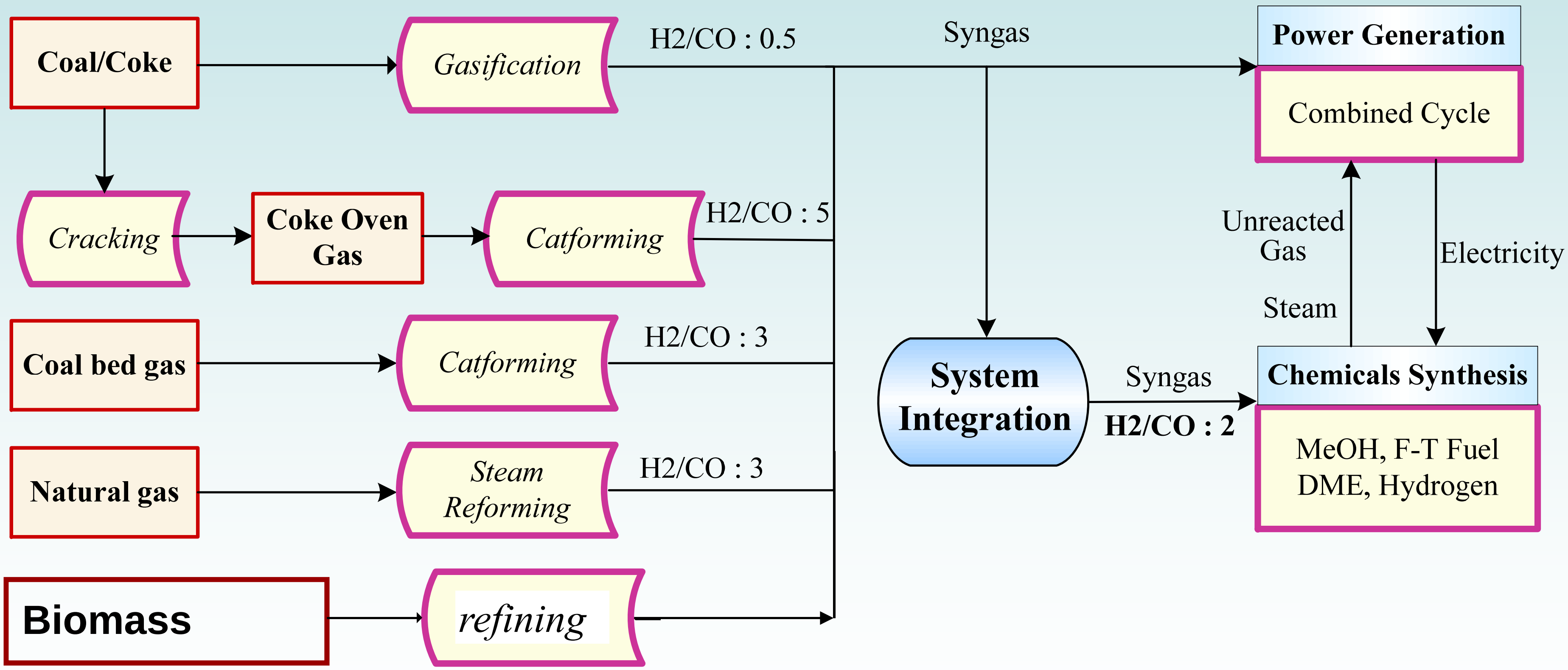


Key structural variables:

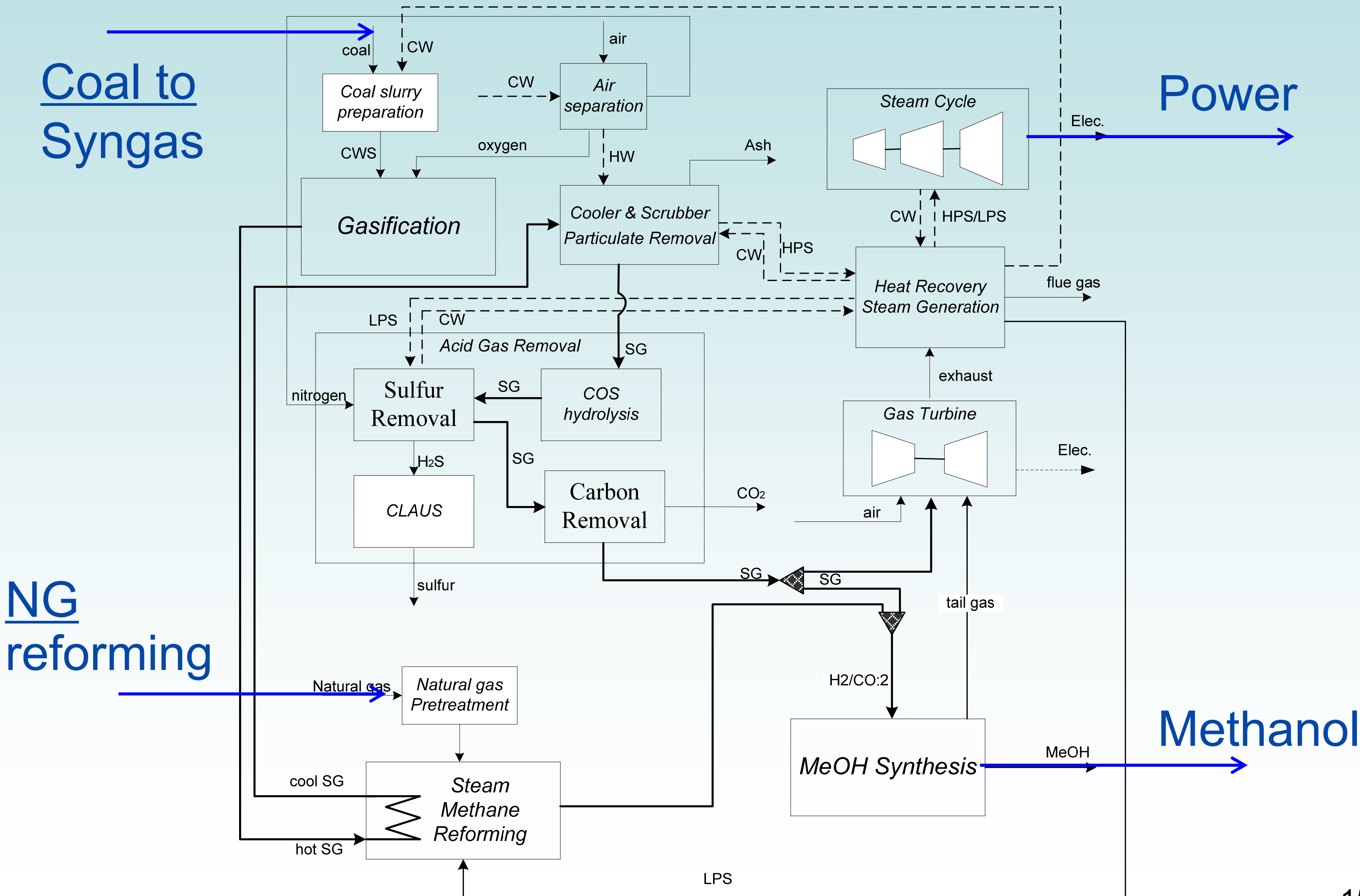
co- feed factor P_1

co-generation factor: P_2

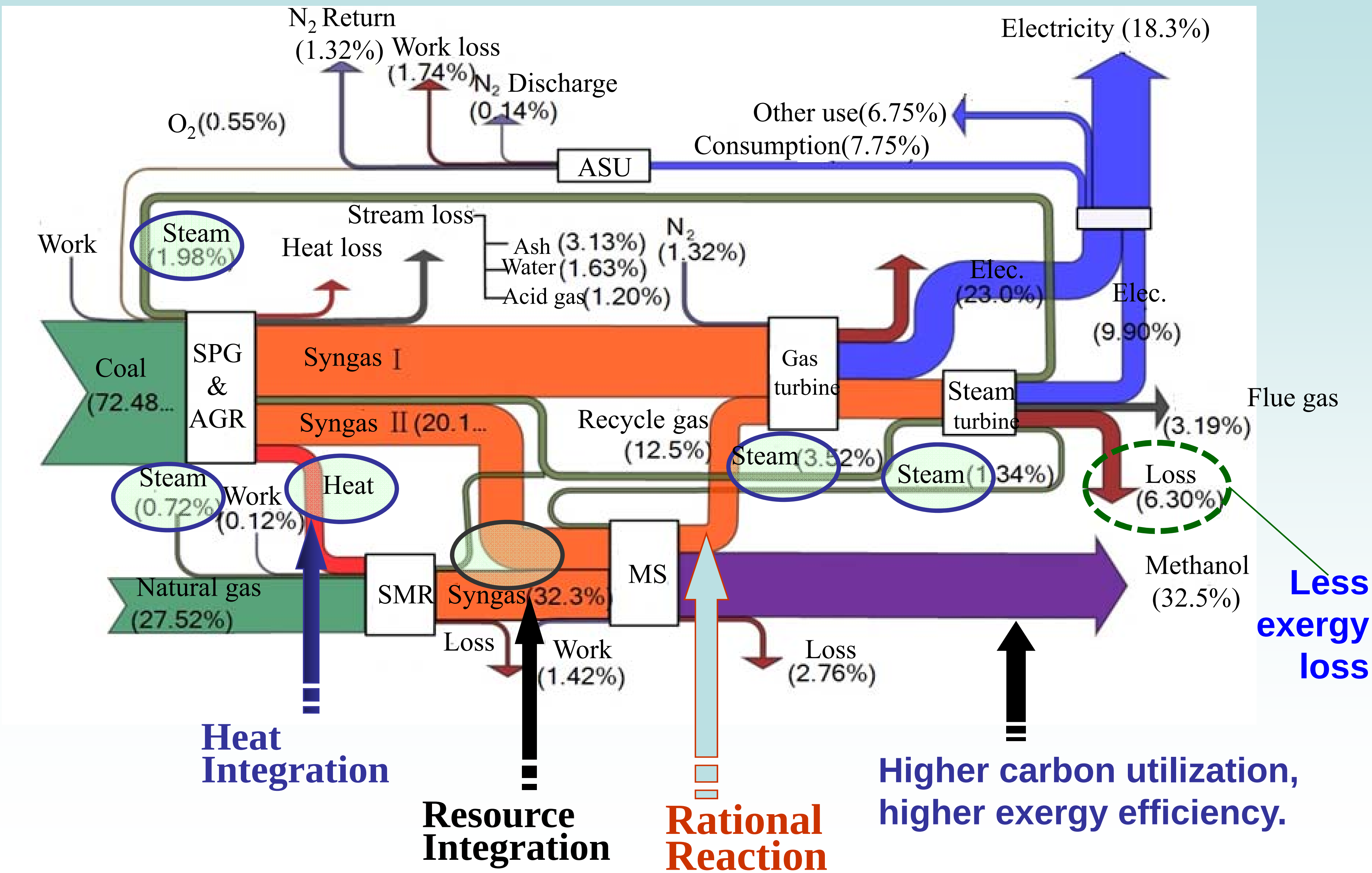
Multi-feed Co-production System



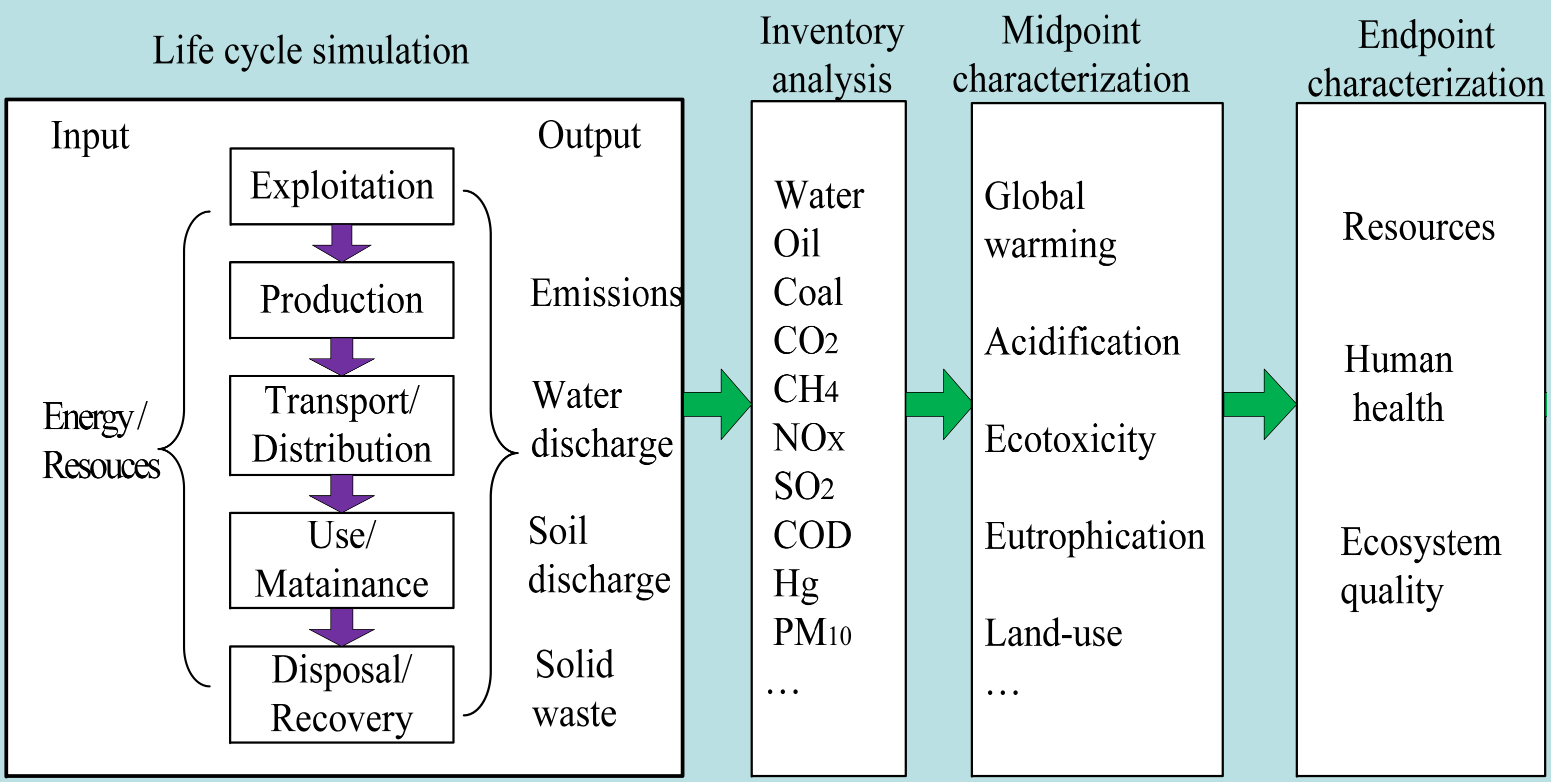
NG-Coal co-feed co-generation process



Mass/exergy flow diagram for integration & optimization



Modeling with Eco-indicator 99

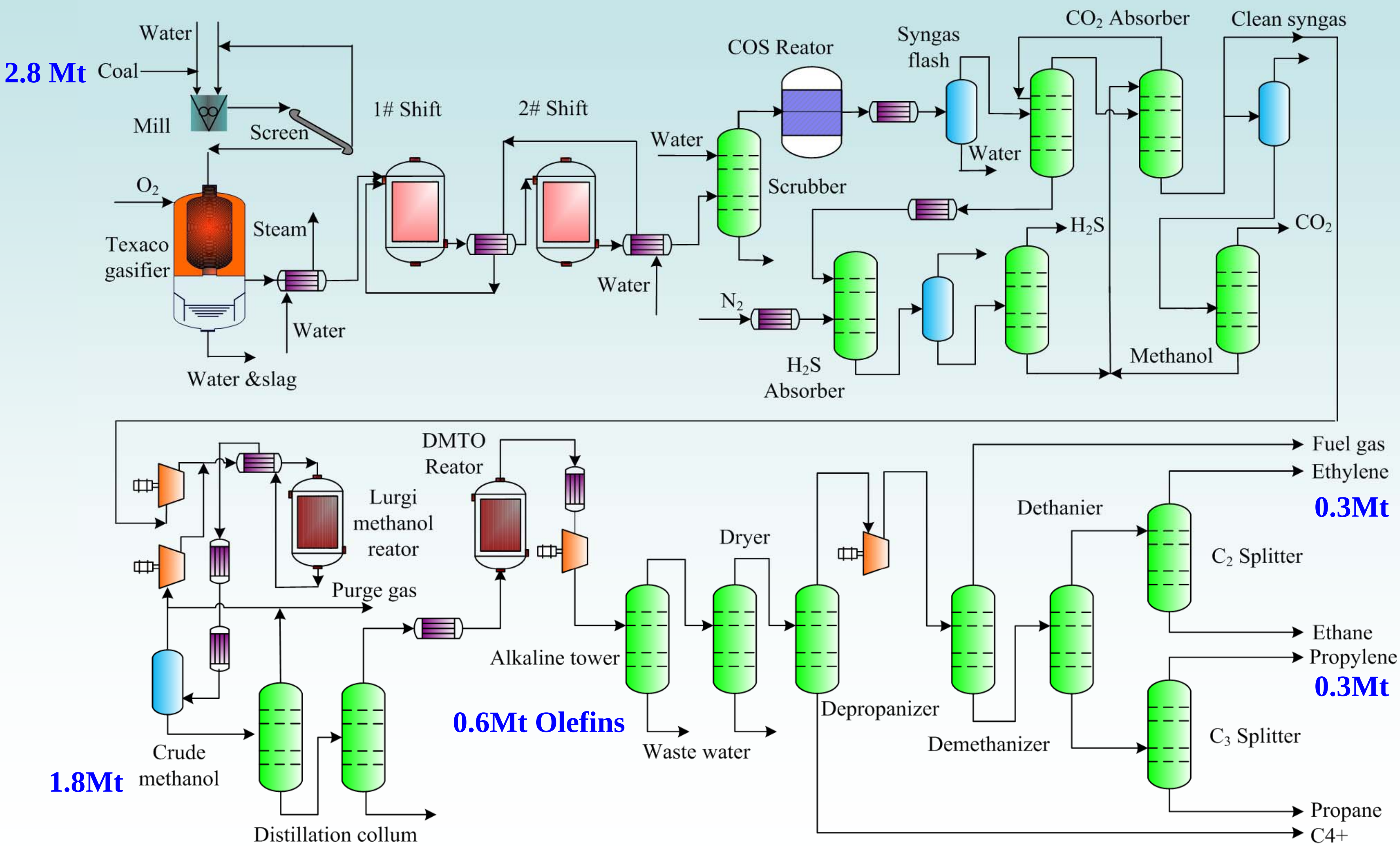


1. Establish LCA model and simulation of the process;
2. Sort out environmental impact factor through inventory analysis;
3. Characterization in several major concerning catalogues.

Eco-indicator 99 manual for designers: a damage oriented method for life cycle impact assessment, 2000

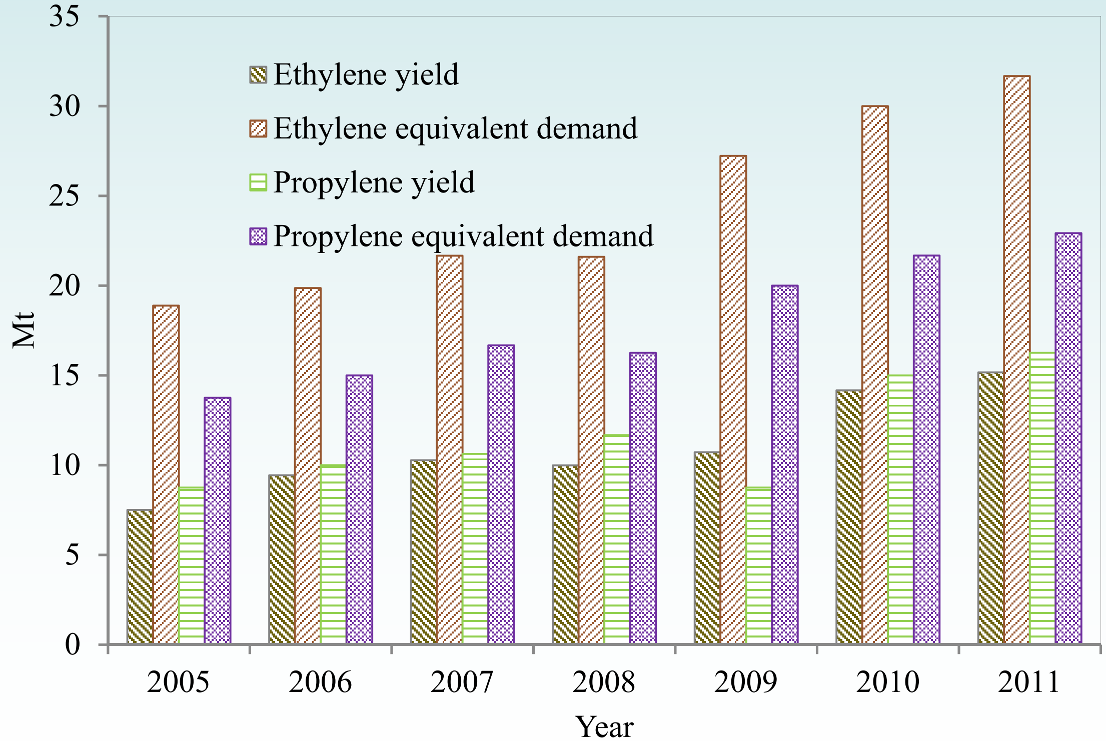
Industrial Case: Coal to Olefins

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.



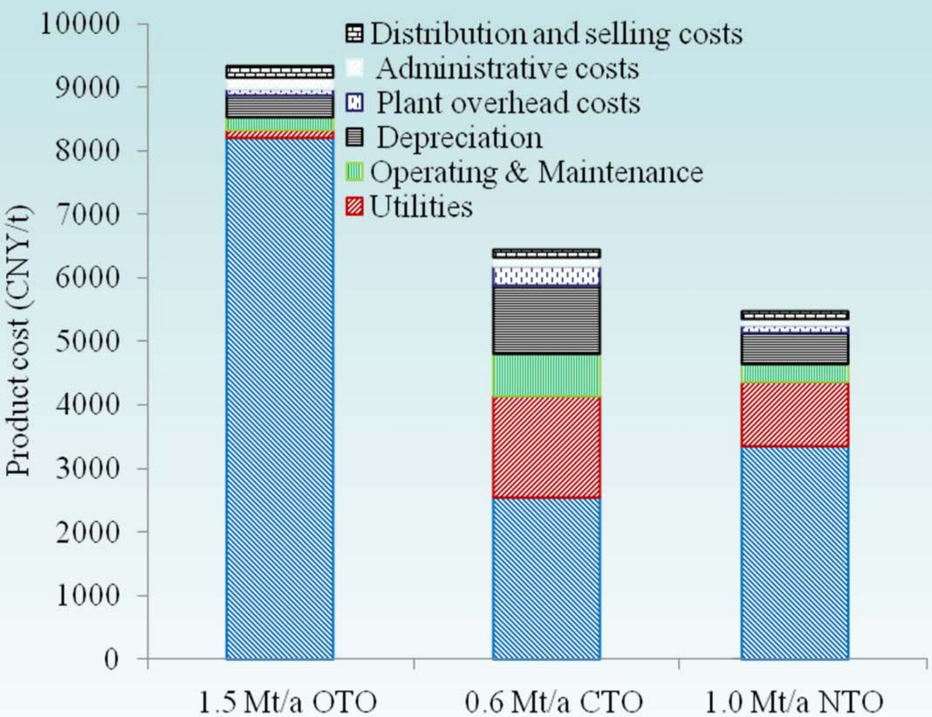
CTO Development Opportunity

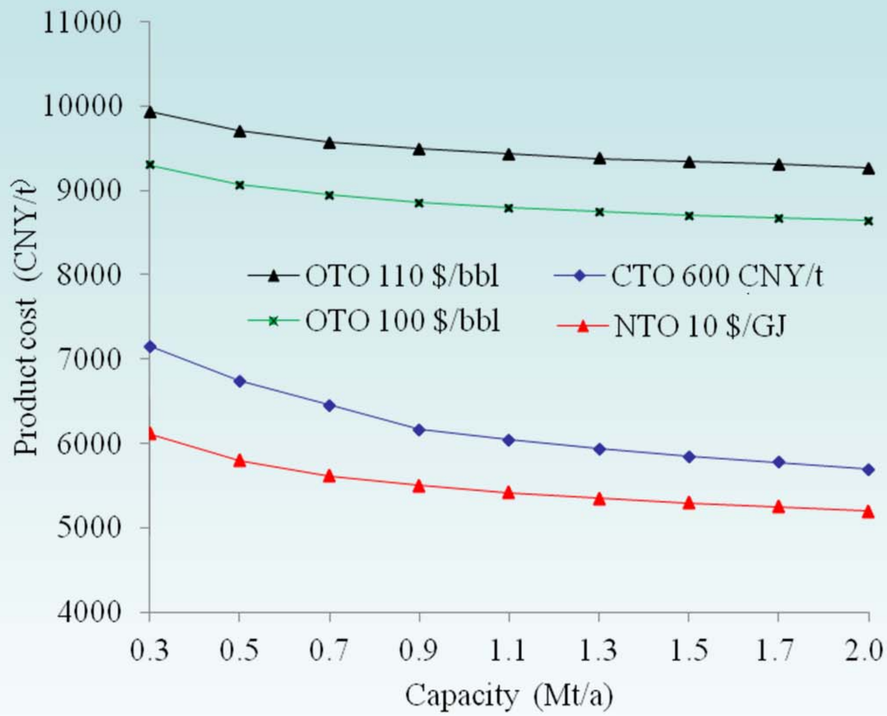
- There is a big gap between olefins demand and production capacity in China. Ethylene and propylene are produced only 50% and 70% of market demand, respectively.
- Coal is relatively abundance and low price in China.



Source: China Energy Statistics Yearbook, 2011. An F, Ming J. Petro Petrochem Today 2012; 20: 18-23.

Cost evaluation of CTO





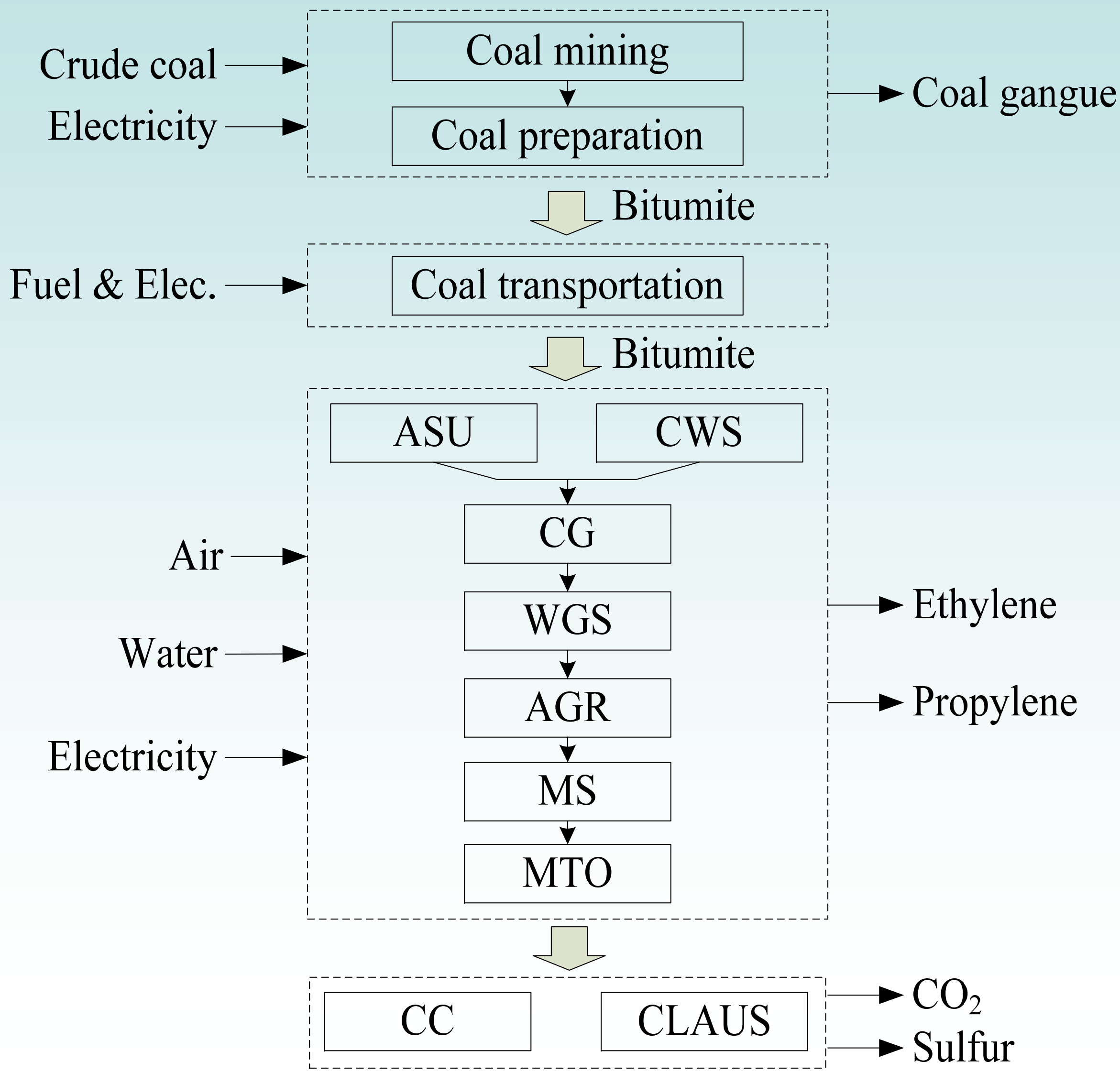
- Coal feedstock cost accounts for 39% of olefins product cost, much lower than 88% of OTO. It may, however, be offset with oil/coal price fluctuation, beside of high utility/investment cost.
- CTO efficiency could be improved with better process integration, utility, operation, equipment.
- On the other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

CTO Energy efficiency, in comparison with OTO

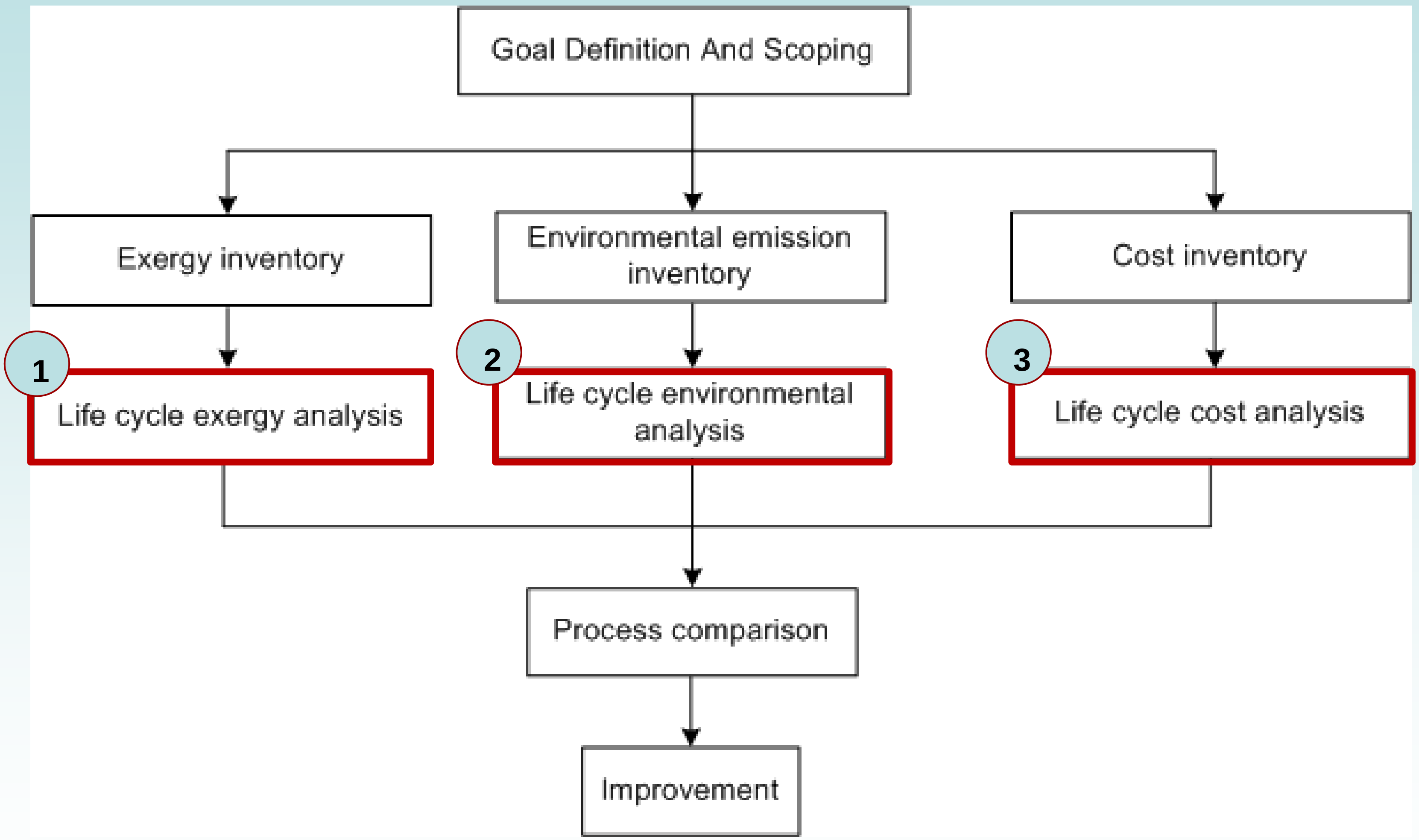
Item	OTO	CTO	LHV
Consumption			
Naphtha (t/t olefins)	1.4	N/A	45000MJ/t
Coal (t/t olefins)	N/A	4.1	28100MJ/t
Water (t/t olefins)	**9**	**30**	2.6 MJ/t
Electricity (kWh/t olefins)	74	1671.0	3.6MJ/KWh
Steam (MJ/t olefins)	1140	8753	
Total E input(GJ/t olefins)	66230	130057	—
Product/output			
Ethylene (t/t olefins)	0.56	0.45	47000MJ/t
Propylene (t/t olefins)	0.26	0.45	47000MJ/t
C_4 (t/t olefins)	0.17	0.10	47000MJ/t
CO_2 (t/t olefins)	**1.3**	**5.8**	—
Product energy (MJ)	47000	47000	—
Energy efficiency (%)	**71.0**	**36.1**	—

We have to explore new process to improve CTO performance.

Life cycle boundary of the CTO process

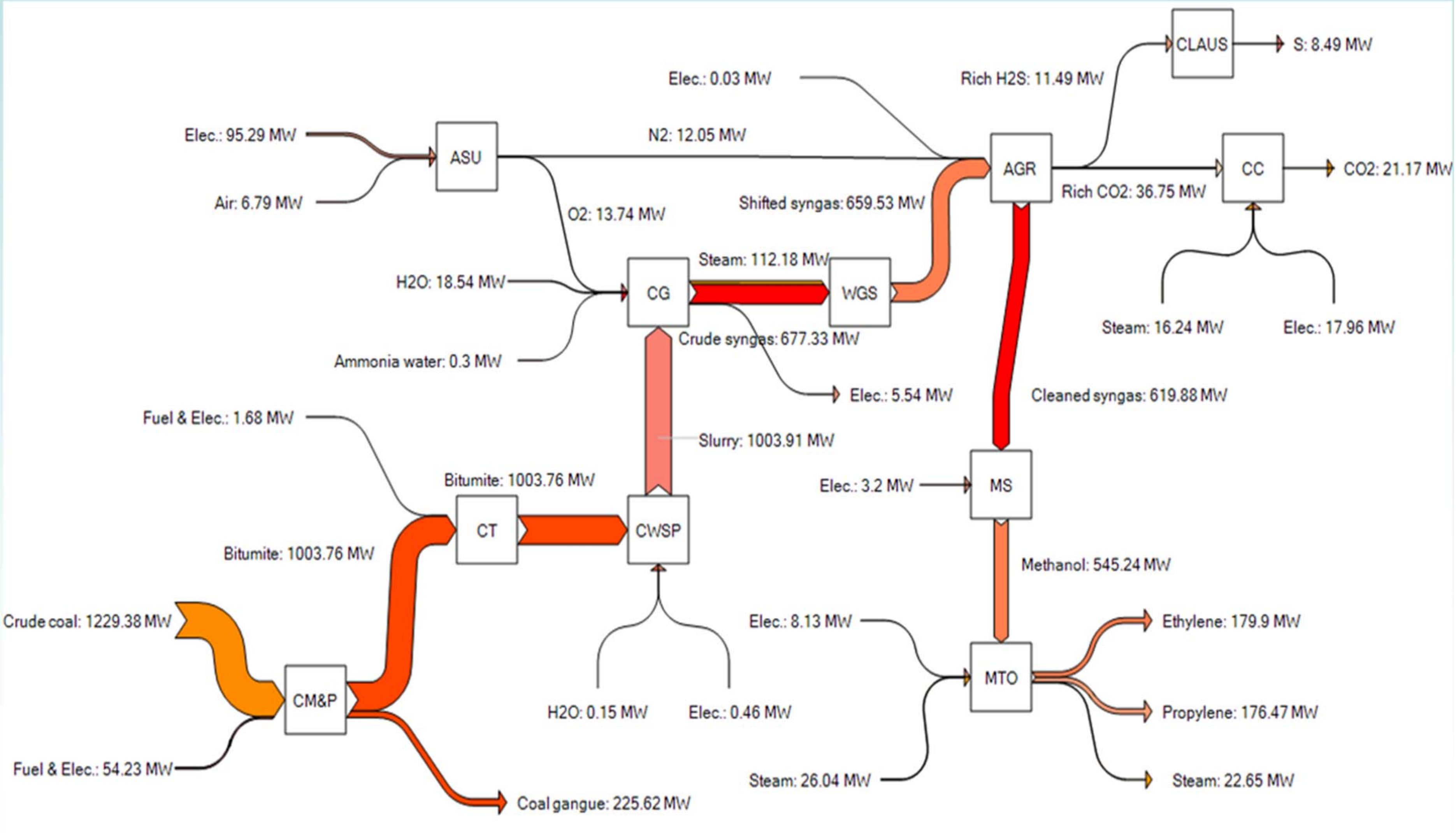


LCA



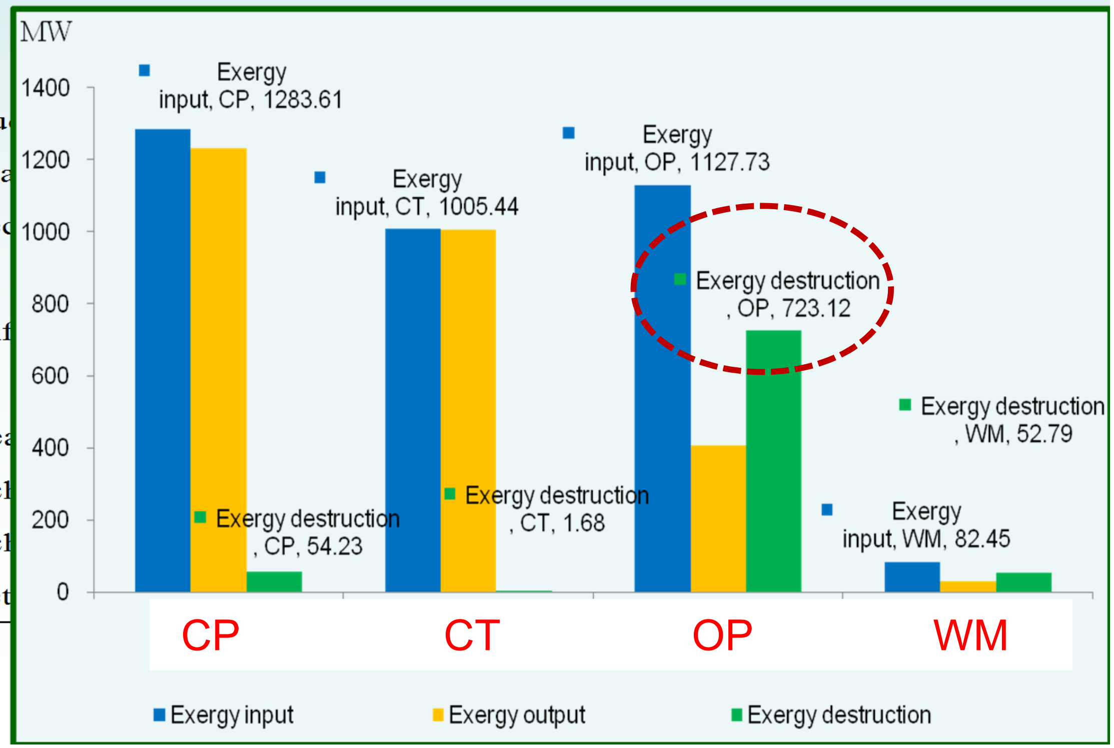
Goal Definition And Scoping
Exergy inventory
Environmental emission inventory
Cost inventory
1
Life cycle exergy analysis
2
Life cycle environmental analysis
3
Life cycle cost analysis
Process comparison
Improvement

Life cycle exergy flow diagram of CTO



Life cycle exergy inventory of CTO

Stage	Unit	Input Item	Input Ex_{flow} (MW)	Output Item	Output Ex_{flow} (MW)	$Ex_{dest.}$ (MW)	η
CP	CM&P	Crude coal	1229.38	Bitumite	1003.76	54.23	95.78%
		Elec. and fuel	54.23	Coal gangue	225.62		
CT	CT	Bitumite	1003.76	Bitumite	1003.76	1.68	99.83%
		Elec. and fuel	1.68				
OP	ASU	Air	6.79	O_2	13.74	69.50	27.06%
		Elec.	95.29	N_2	12.05		
	CWS	Bitumite	1003.76	Slurry	1003.91	0.46	99.95%
		Water	0.15				
		Elec.	0.46				
	CG	Slurry	1003.91	Cru			
		O_2	13.74	Stea			
		Cooling water	18.54	Elec			
		Ammonia water	0.30				
	WGS	Crude syngas	677.33	Shif			
		Steam	112.18				
	AGR	Shifted syngas	659.53	Clea			
		N_2	12.05	Ricl			
		Elec.	0.03	Ricl			
	MSU	Cleaned syngas	619.88	Met			



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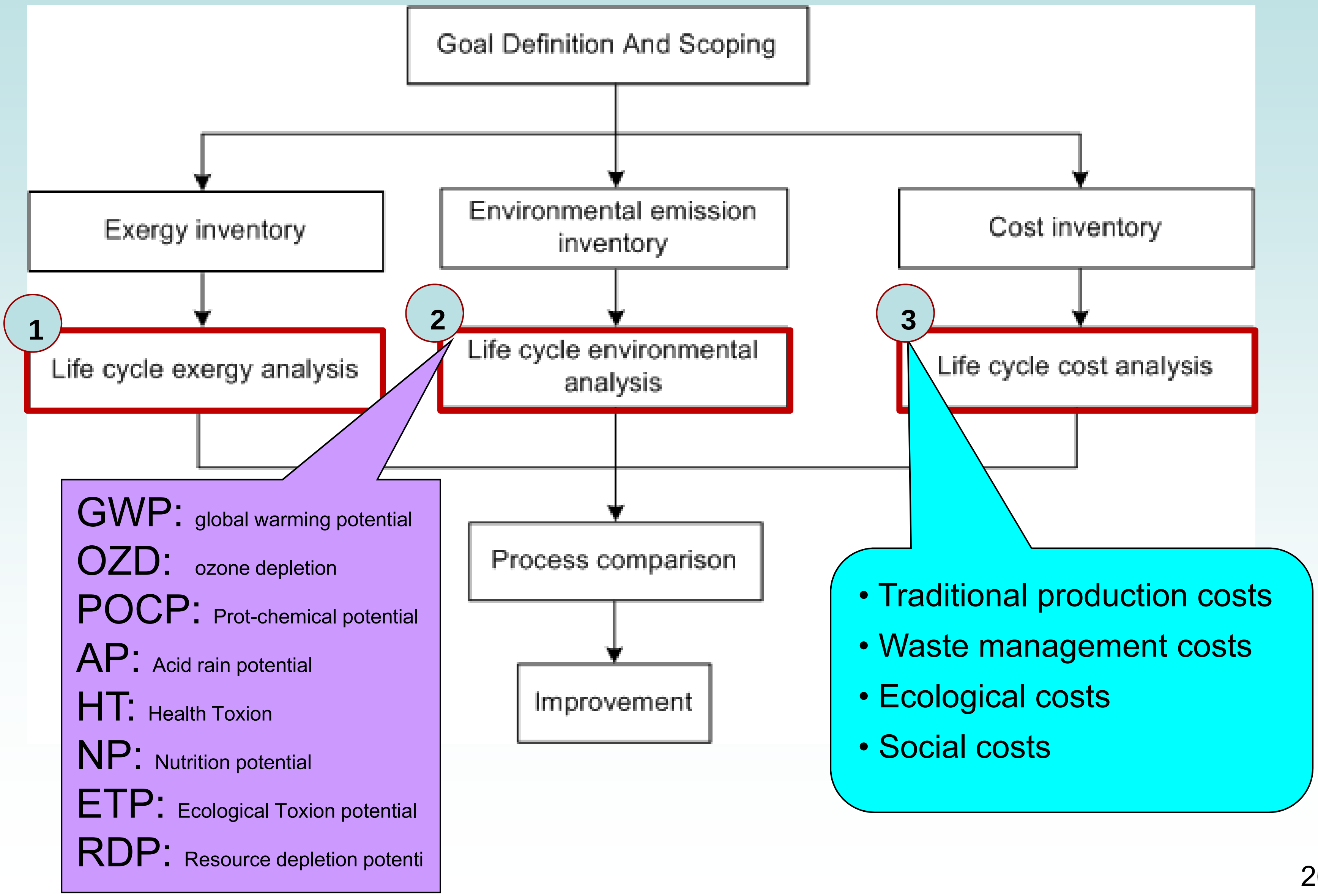
Goal Definition And Scoping
Exergy inventory
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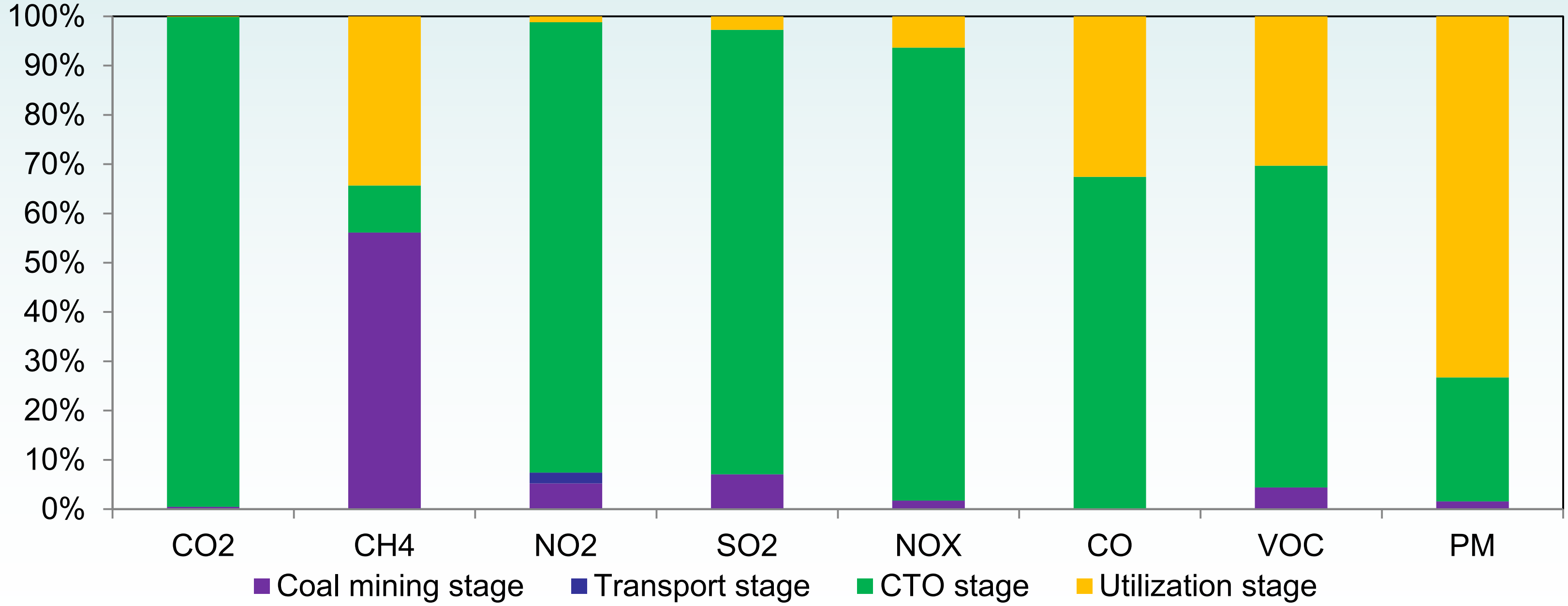
GWP: global warming potential
OZD: ozone depletion
POCP: Prot-chemical potential
AP: Acid rain potential
HT: Health Toxion
NP: Nutrition potential
ETP: Ecological Toxion potential
RDP: Resource depletion potenti
• Traditional production costs
• Waste management costs
• Ecological costs
• Social costs

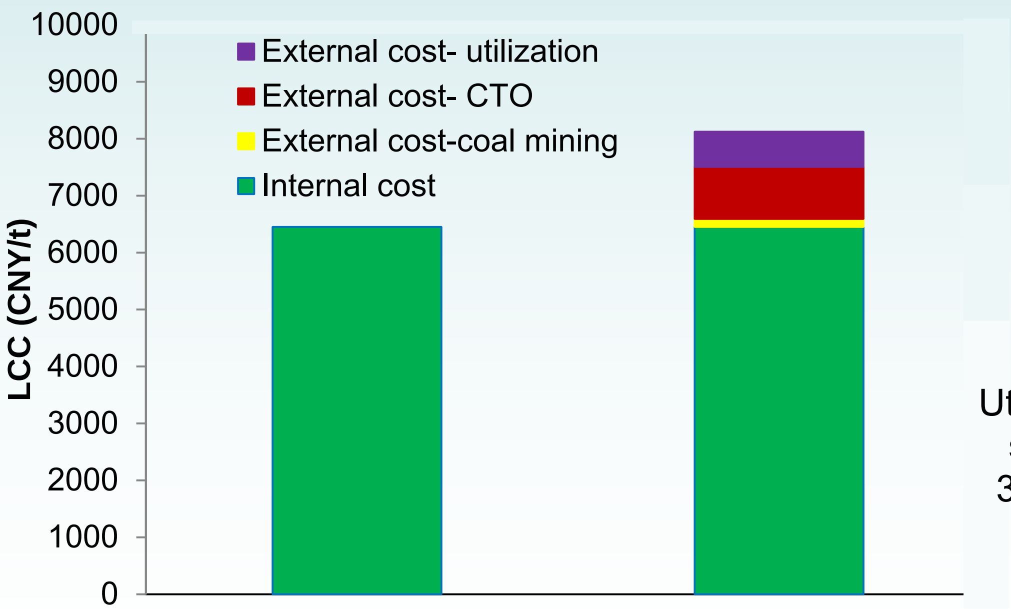
Life cycle environmental inventory of CTO

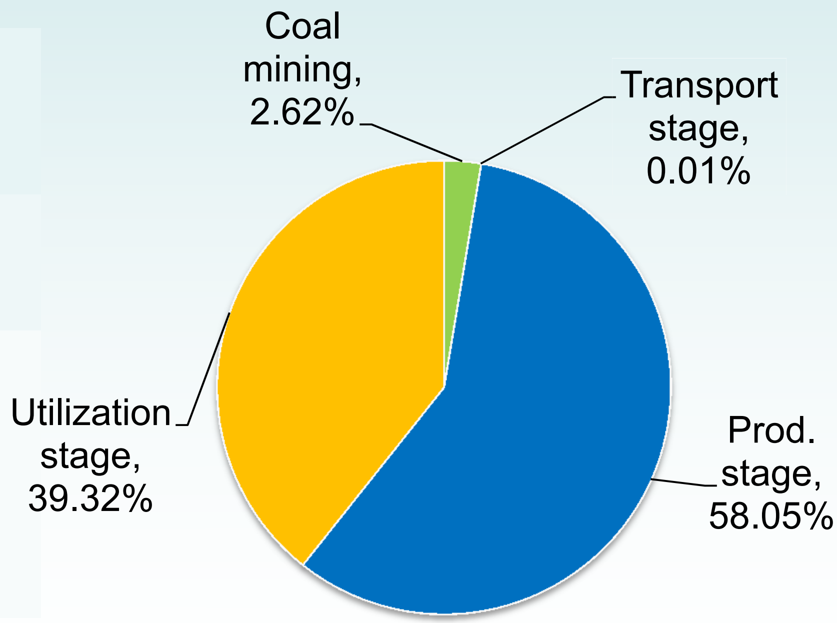
kg/t olefins	CO_2	CH_4	NO_2	SO_2	NOX	CO	VOC	PM
Coal mining stage	42.5	10.94	.003	0.41	0.11	0.01	0.11	0.11
Transport stage	0.1	0.00	.001	0.00	0.00	.000	.000	.000
Production stage	8744.0	1.86	.044	5.31	5.72	9.11	1.60	1.81
Utilization stage	10.9	6.69	.001	0.16	0.39	4.41	0.74	5.28
Total	8797.0	19.50	.048	5.88	6.22	13.53	2.45	7.21



Life cycle cost of CTO

CNY/t olefins	CO_2	CH_4	NO_2	SO_2	NOX	CO	VOC	PM	Total
Coal mining stage	2.1	9.83	0.02	13.3	1.7	0.00	1.6	12.8	41
Transport stage	0.0	0.00	0.01	0.0	0.1	0.00	0.0	.01	0.1
Production stage	424.4	1.67	0.34	170.5	90.3	0.66	22.9	202.4	913
Utilization stage	0.5	6.01	0.00	5.2	6.2	0.32	10.6	589.7	618
Total	427.0	17.51	0.37	189.0	98.3	0.99	35.1	804.9	1573





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

Life cycle cost of CTO

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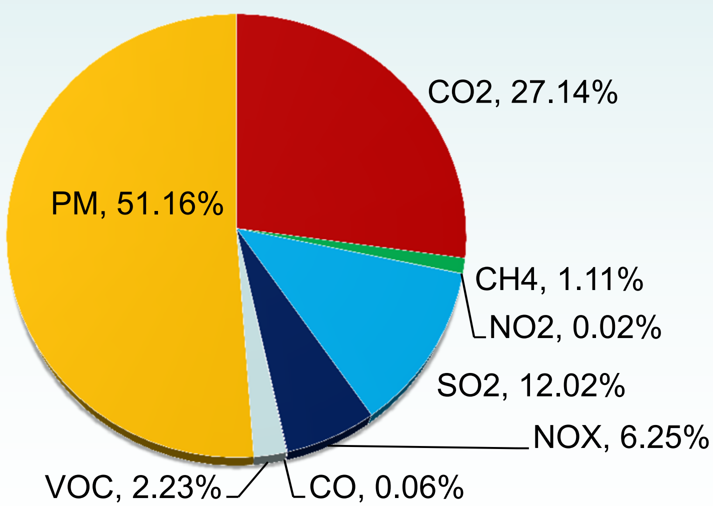


In LCC of CTO,

PM treatment is the largest external cost.

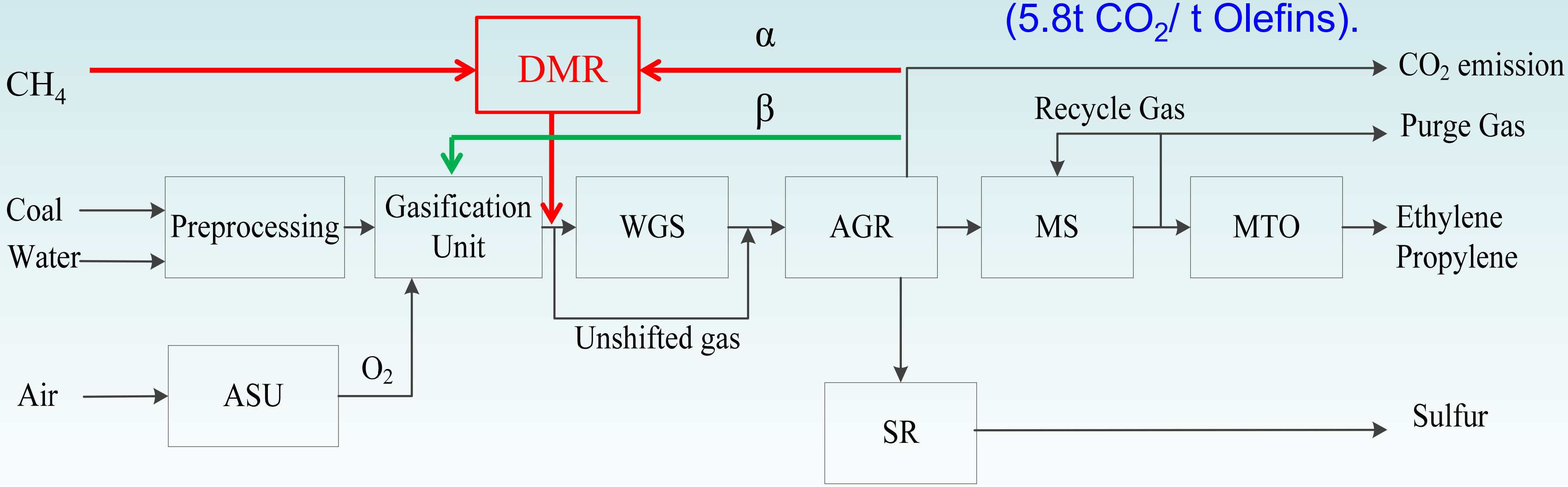
CCS cost is the second.

How to improve the sustainability of CTO? Process innovation.

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

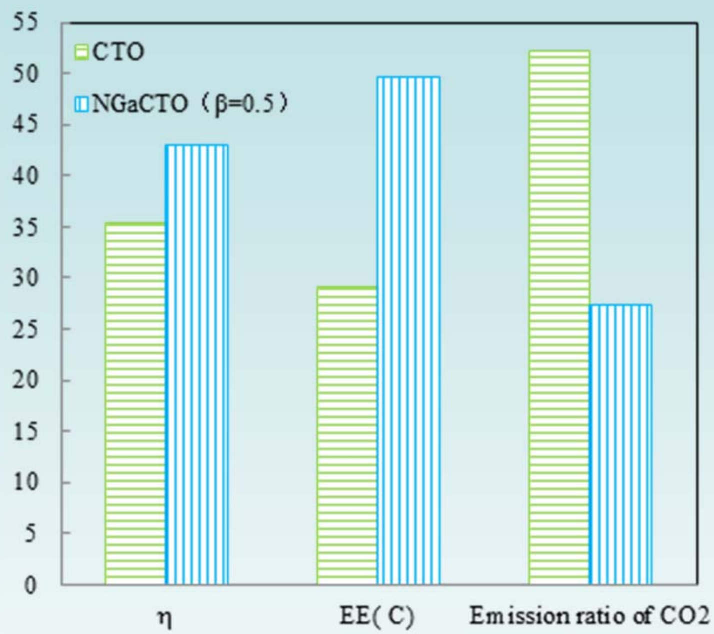
(1) CH_4 introduced to a dry reformer with recycled CO_2. The syngas H_2/CO ratio 1:1, to improve mixed syngas H/C ratio.

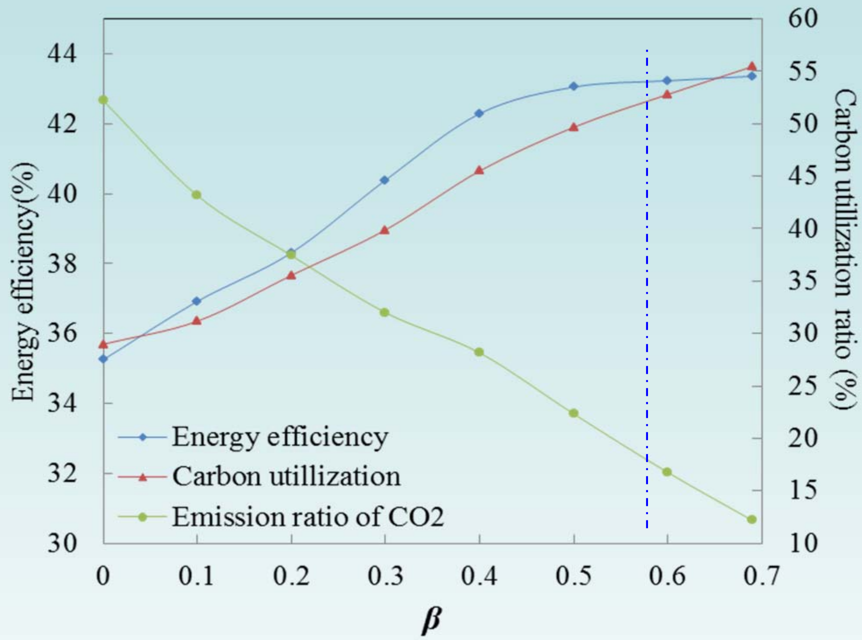
Huge CO_2 emission (5.8t CO_2/ t Olefins).



(2) A part of pressurized hot CO_2 is recycled to the gasifier, as a gasification agent, to increase syngas production.

Mass and Energy Efficiency Improvement



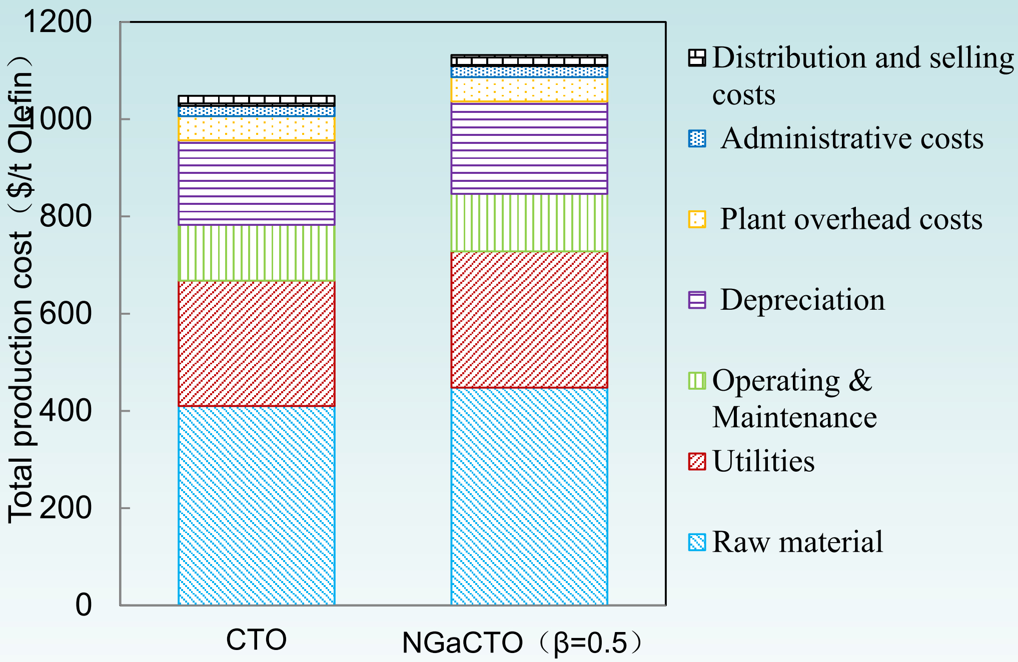


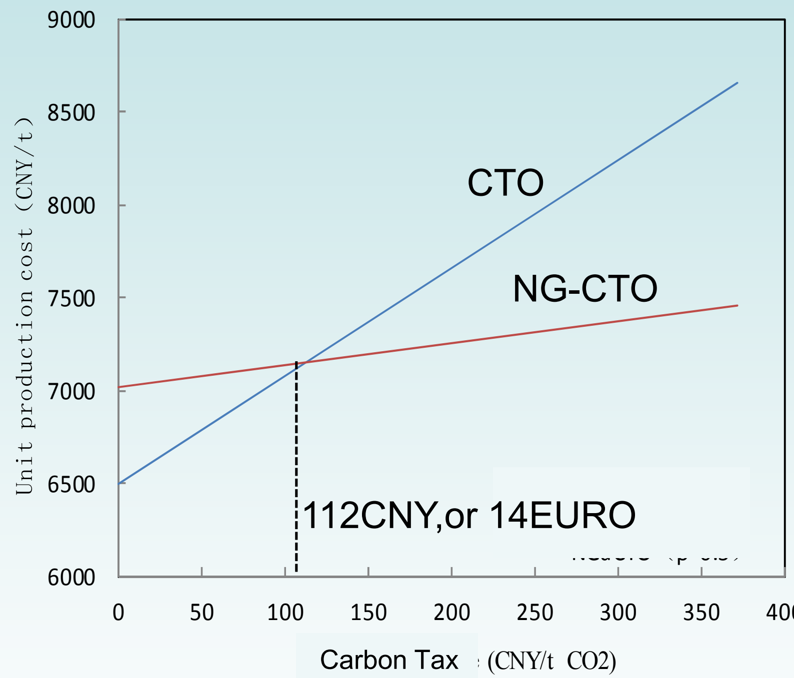
NG-CTO efficiency for material, energy, and CO_2 emission.

As CO_2 recycle, Carbon element and energy efficiency increase, while CO_2 emission is reduced.

Methane dry reforming reaction is strongly endothermic. It is important to select CO_2 recycle rate for a rational energy integration.

Economic performance of CTO



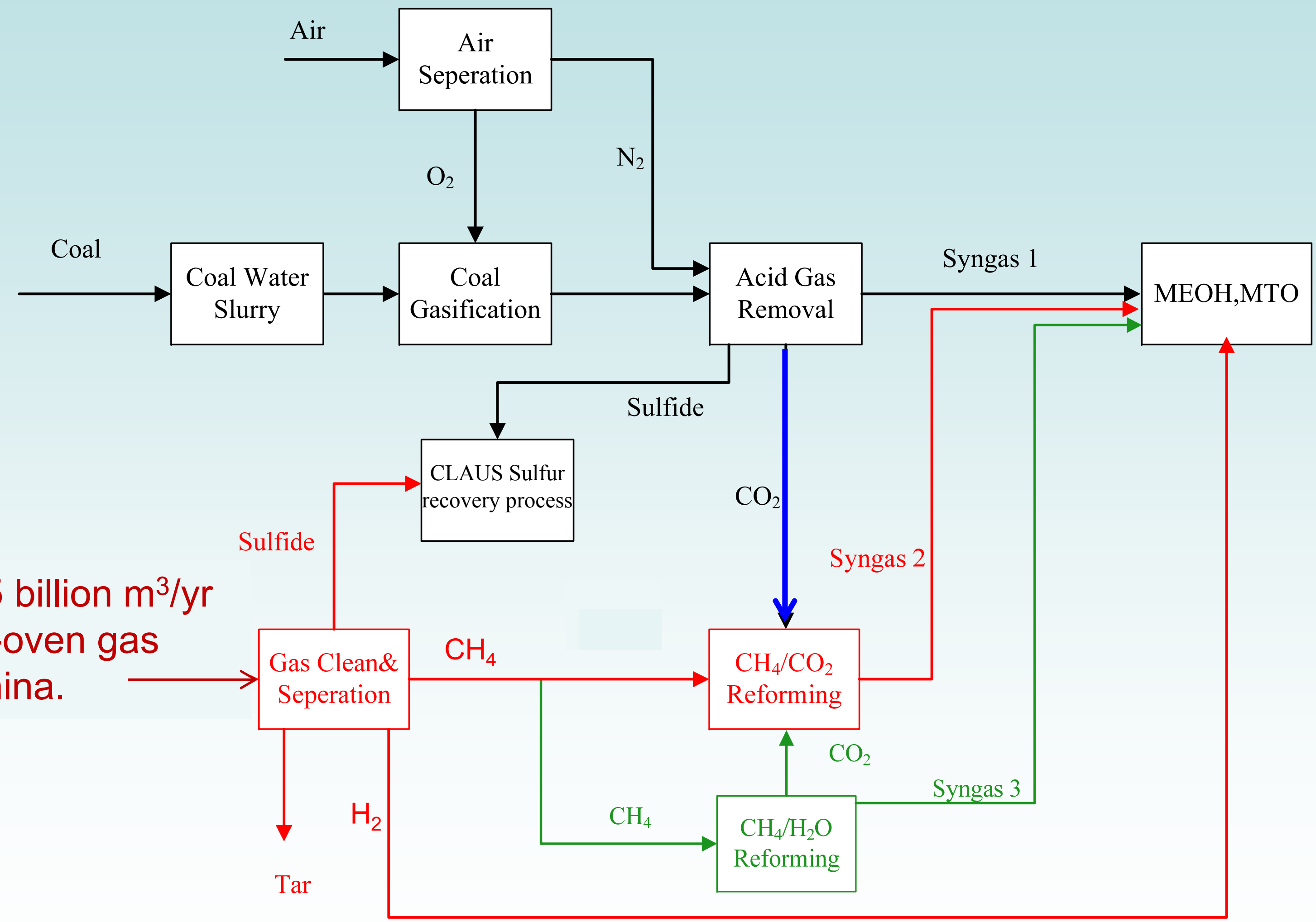


NG-CTO production cost 7020 CNY/t, slightly higher than CTO 6500 CNY/t.

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)

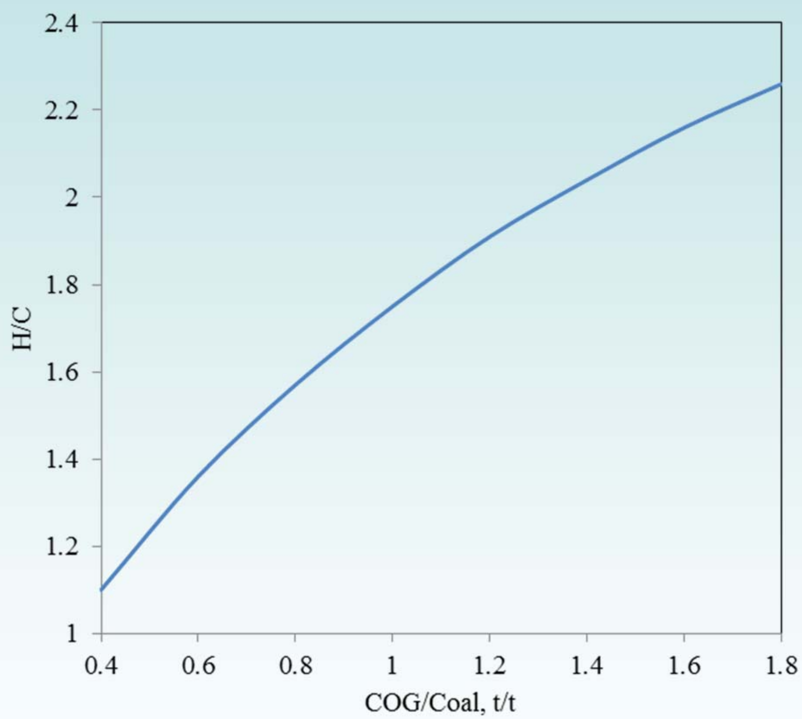


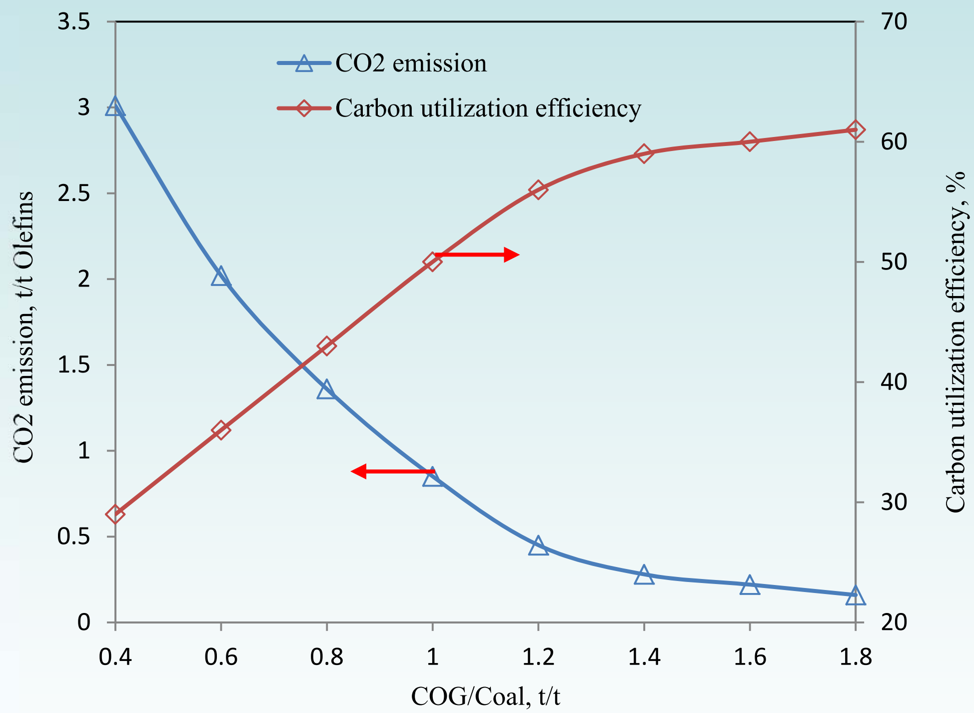
There are 35 billion m³/yr H_2 rich coke-oven gas burned in China.

- H_2 -rich coke-oven gas fed, CH_4/CO_2 reforming raise H/C ratio to 1.

CH_4/H_2O reforming raise H/C further to 2

Material and Environmental performance of GCTO





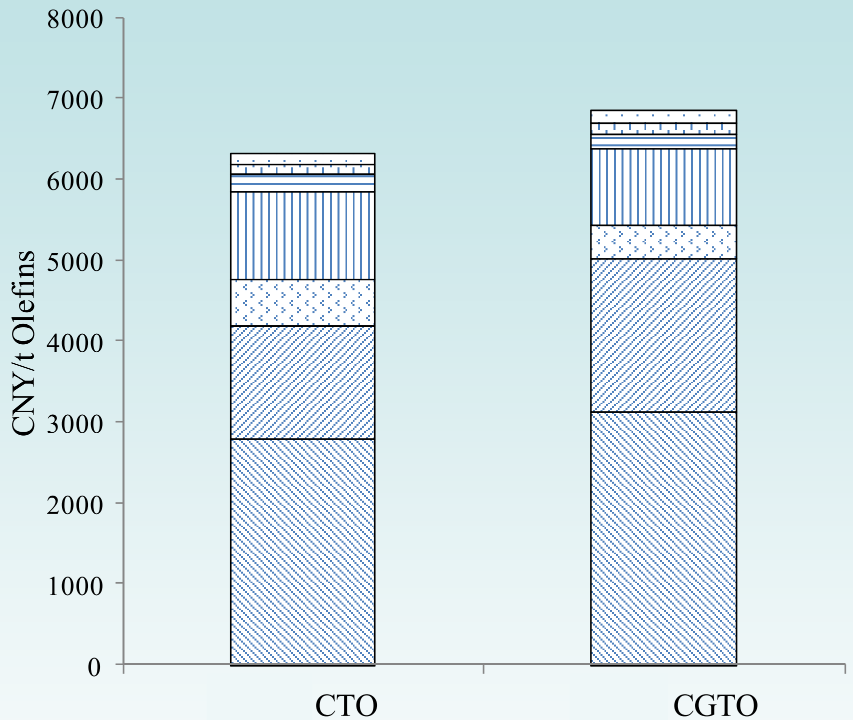
H/C increases with the introduce of coke-oven gas

As introduce of coke oven gas, C utilization efficiency rises, while CO_2 emission decreases.

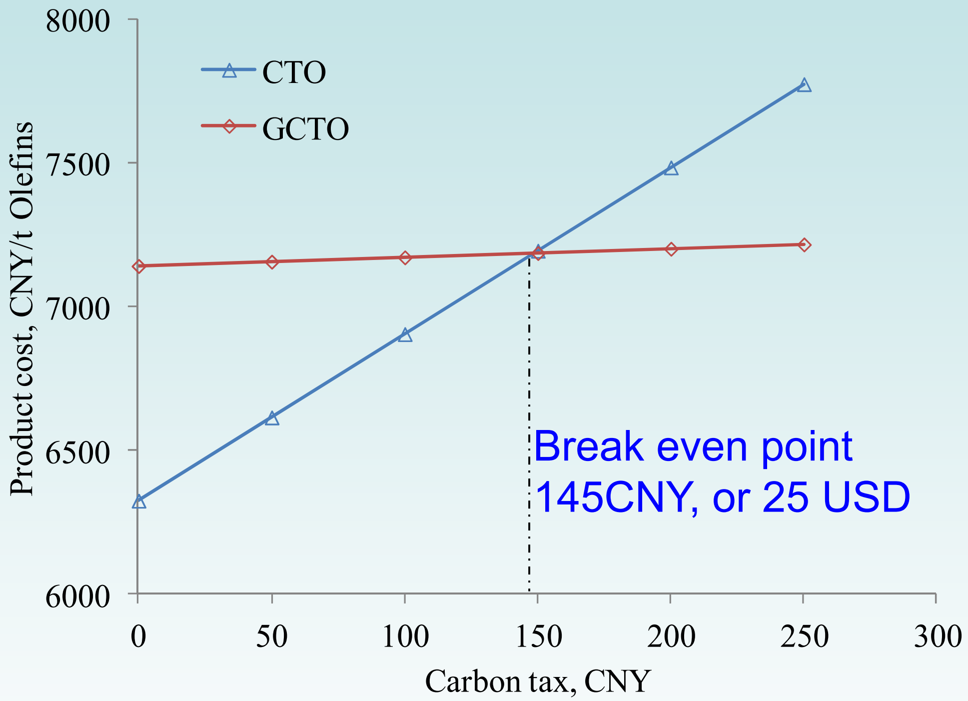
Energy efficiency and CO_2 release of GCTO

Item	CTO	CGTO	LHV
Consumption			
Coal (t/t olefins)	4.10	0.97	28100.0 MJ/t
Coke-oven gas (m^3/t olefins)	N/A	3288	17.4 MJ/m^3
Water (t/t olefins)	**30.00**	**48.00**	2.6 MJ/t
Electricity(kWh/t olefins)	1671	2064	3.6 MJ/kWh
Steam (MJ/t olefins)	8753	12498	—
Total energy input (MJ)	130056	104521	—
Products output			
Ethylene (t/t olefins)	0.45	0.45	47000.0 MJ/t
Propylene (t/t olefins)	0.45	0.45	47000.0 MJ/t
C_4^+ (t/t olefins)	0.10	0.10	47000.0 MJ/t
CO_2 emission(t/t olefins)	**5.80**	**0.30**	—
Olefins energy (MJ)	47000	47000	—
Energy efficiency (%)	**36.10**	**50.70**	—

Economic analysis of GCTO - Product cost



Product costs comparison



Product cost of GCTO vs CTO when carbon tax is applied

* Feedstock: 620 CNY/t coal, 0.8 CNY/m^3 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

2014: Techno-economic analysis of the coal-to-olefins process in comparison with the oil-to-olefins process, ***Applied Energy***, 113, 639-647(2014).

2014 Sustainability assessment of the coal/biomass to Fischer−Tropsch fuel processes, ***Sustainable Chem. Eng.,*** 2(1) 80-87, 2014.

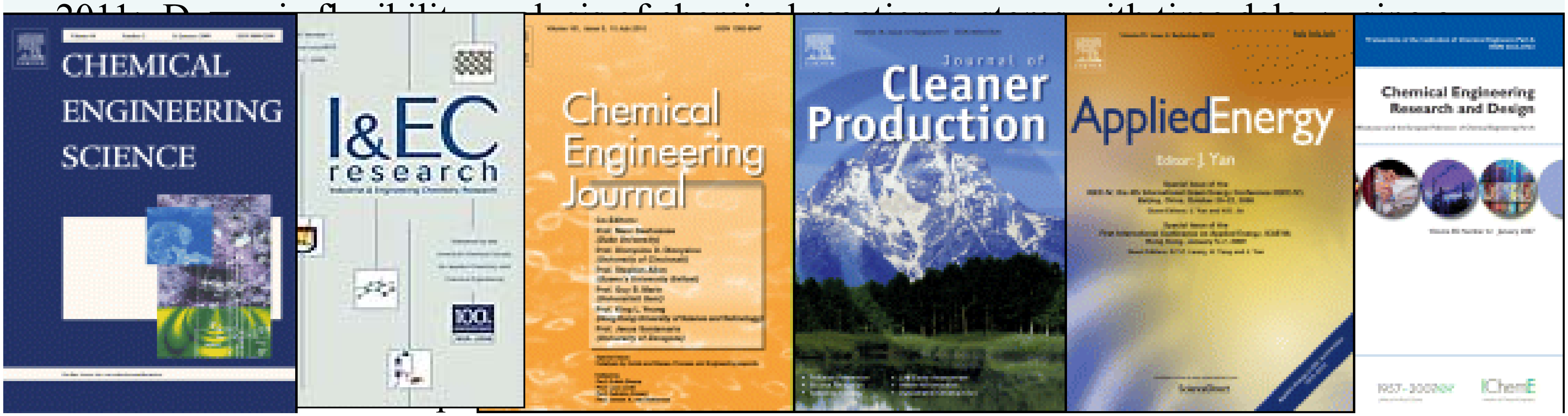
2014 Techno-economics of the CTO process with CCS, ***Chem Eng J***., 240, 45-54(2014).

2013: A revision and extension of Eco-LCA metrics for sustainability assessment of chemical processes, ***Environ. Sci. Technol***., 47(24) 14450–14458, 2013.

2013: A composite efficiency metrics for resource utilization, ***Energy***.61, 455-462 (2013)

2013: Conceptual design and analysis of a nature gas assisted coal-to-olefins process for CO2 reuse, ***Ind. Eng. Chem. Res***., 52, 14406-14414(2013).

2012: Integrated modeling, synthesis, & optimization of coal gasification based energy and chemical processes, ***Ind. Eng. Chem. Res.*** 51: 15763-15777, 2012.



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Questions and comments please.

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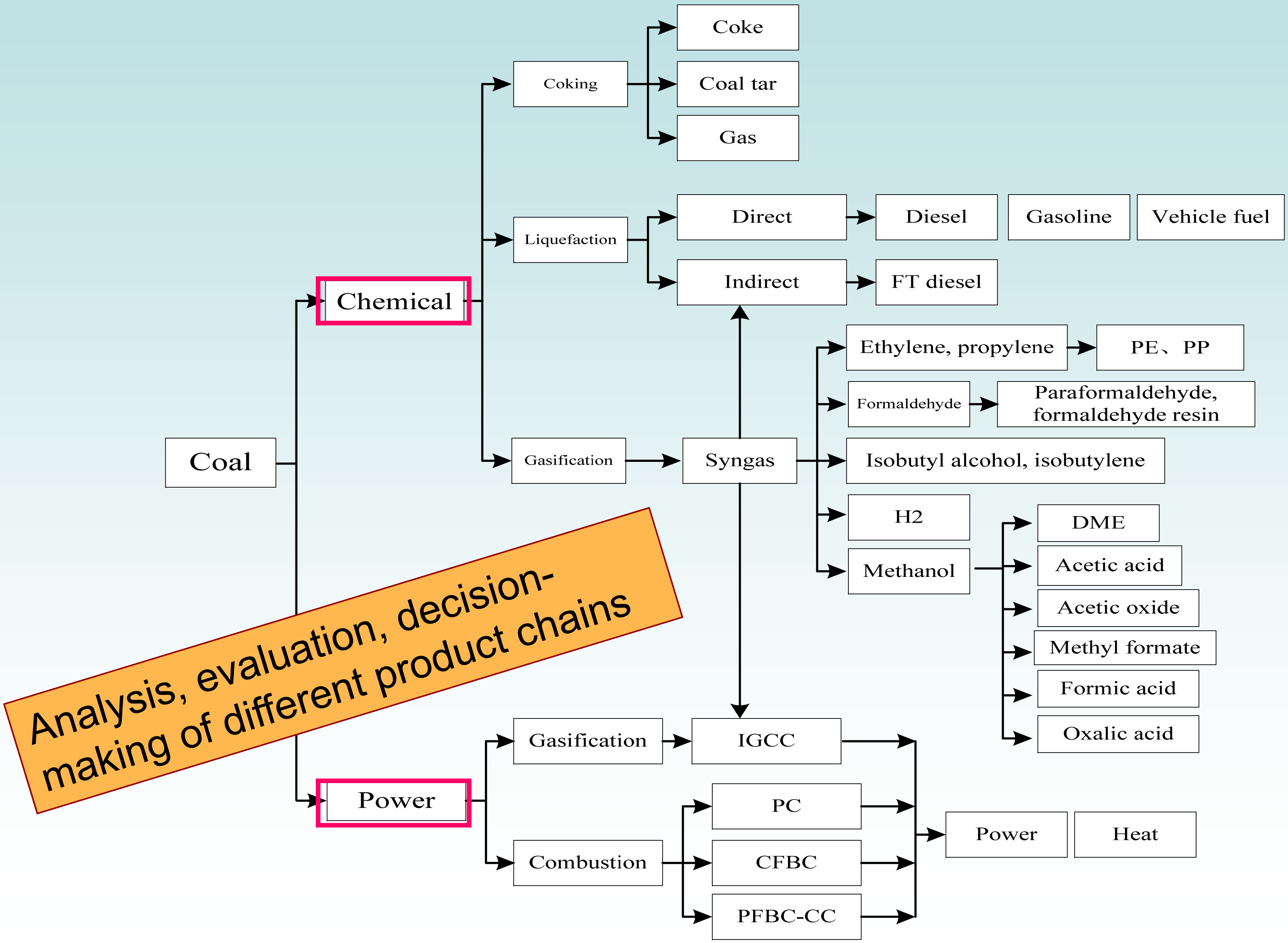
Outline

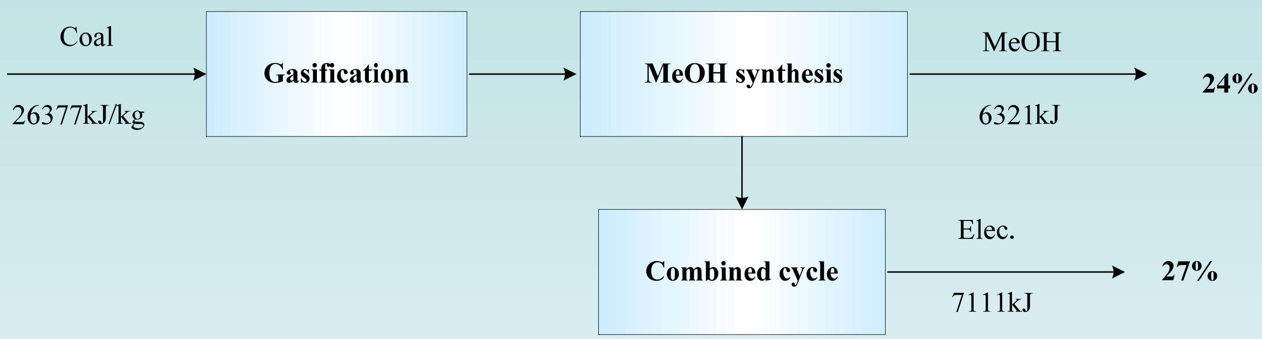
- Background
- Objectives and approaches of sustainability analysis
- Energy efficiency analysis and process integration
- Sustainability analysis
  - Industrial Case: coal to olefins
- Concluding remarks

Coal-based Energy and Chemical Product Chains



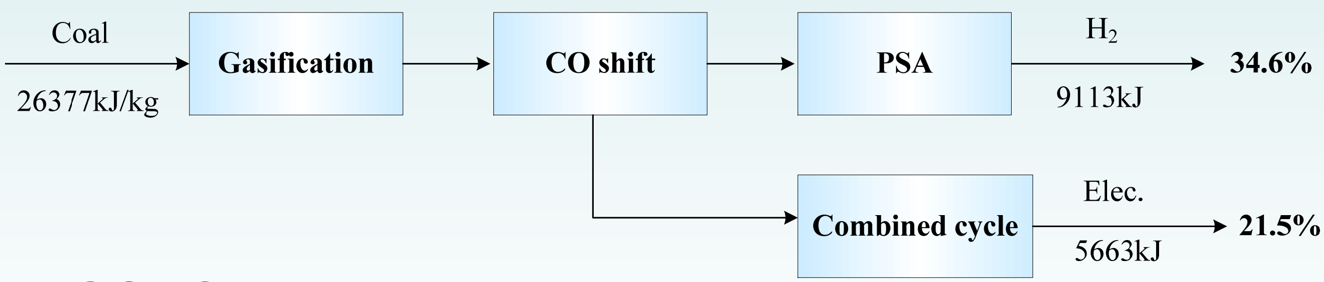
Alternative Co-production processes

Methanol-Power Co-production



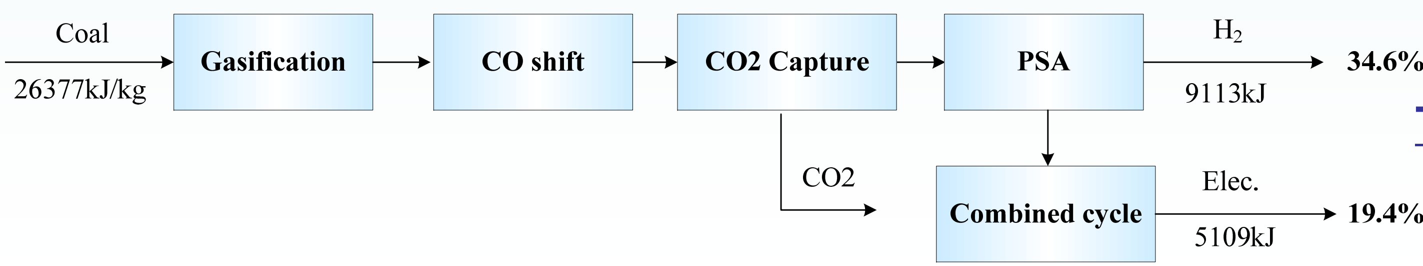
Total: 51%

Hydrogen-Power Co-generation



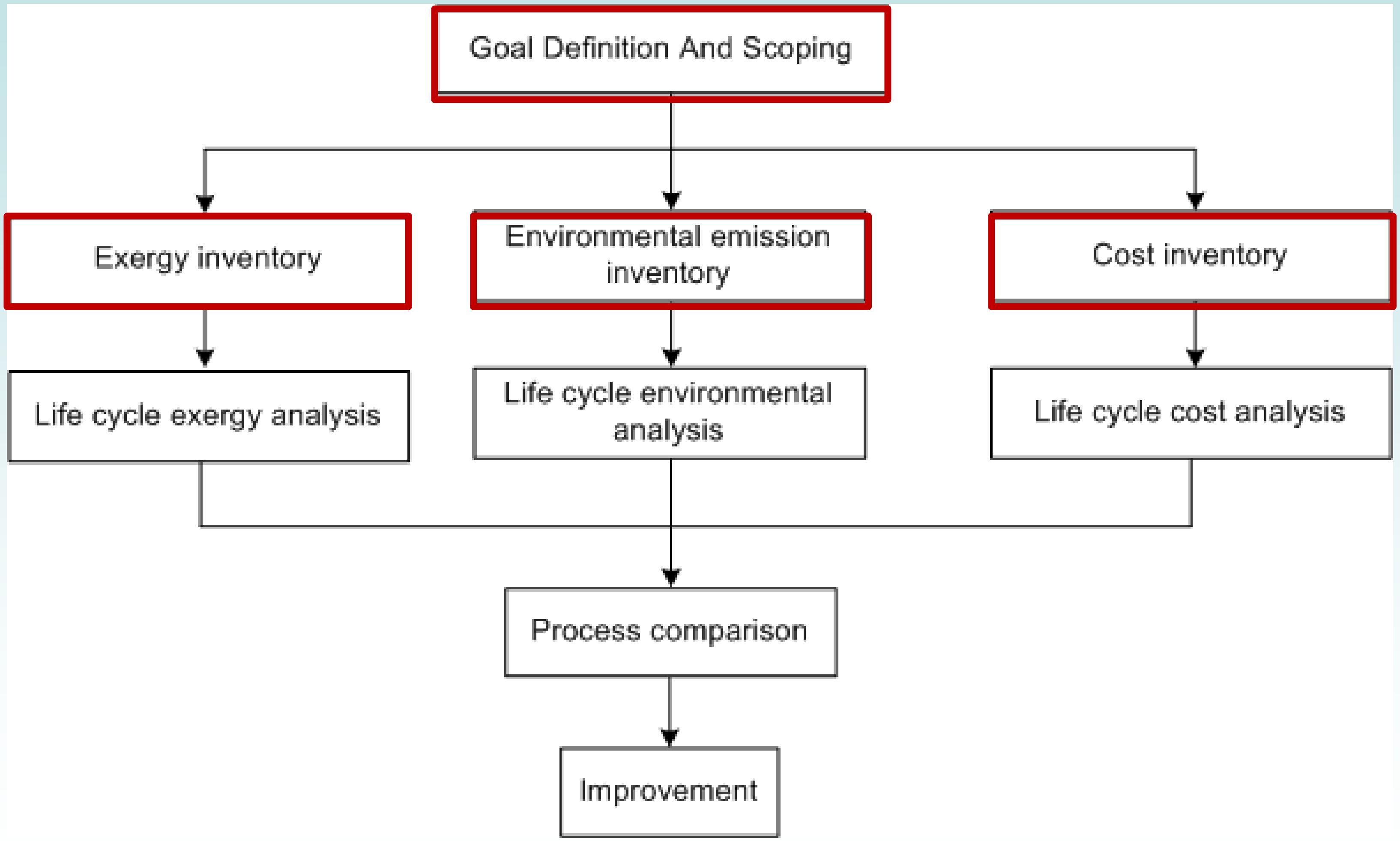
Total: 56%

With CO_2 Capture

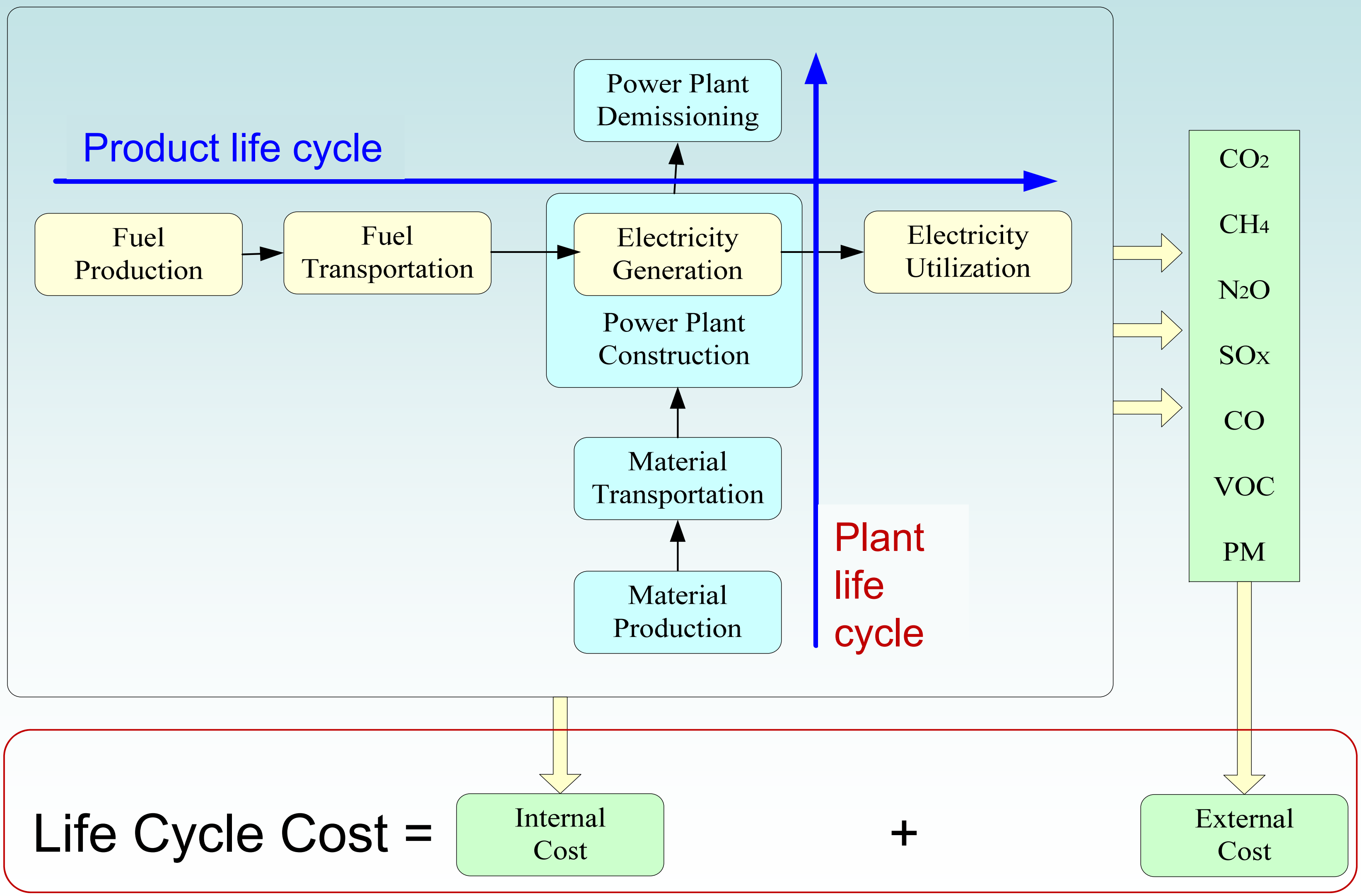


Total: 54%

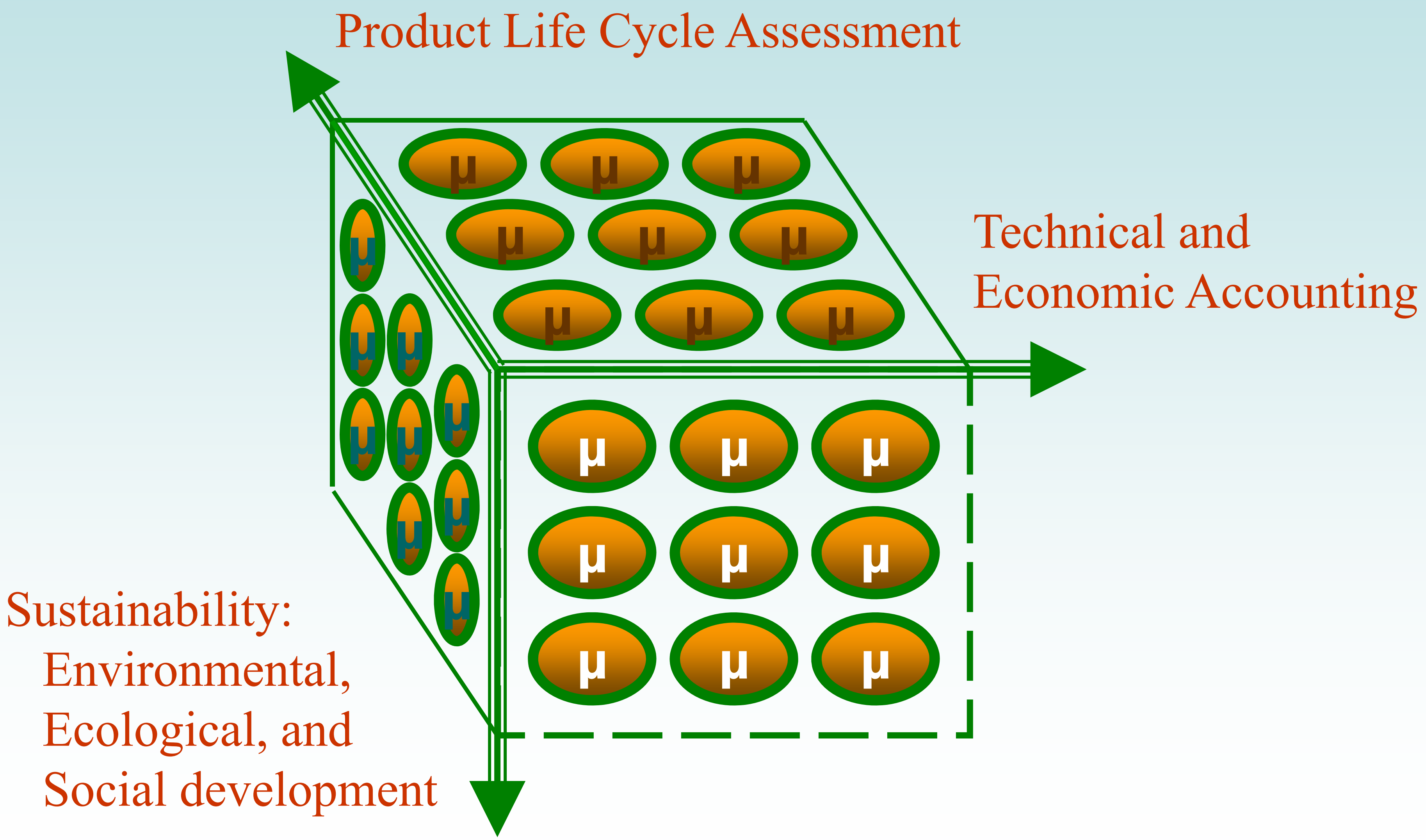
LCA Approach



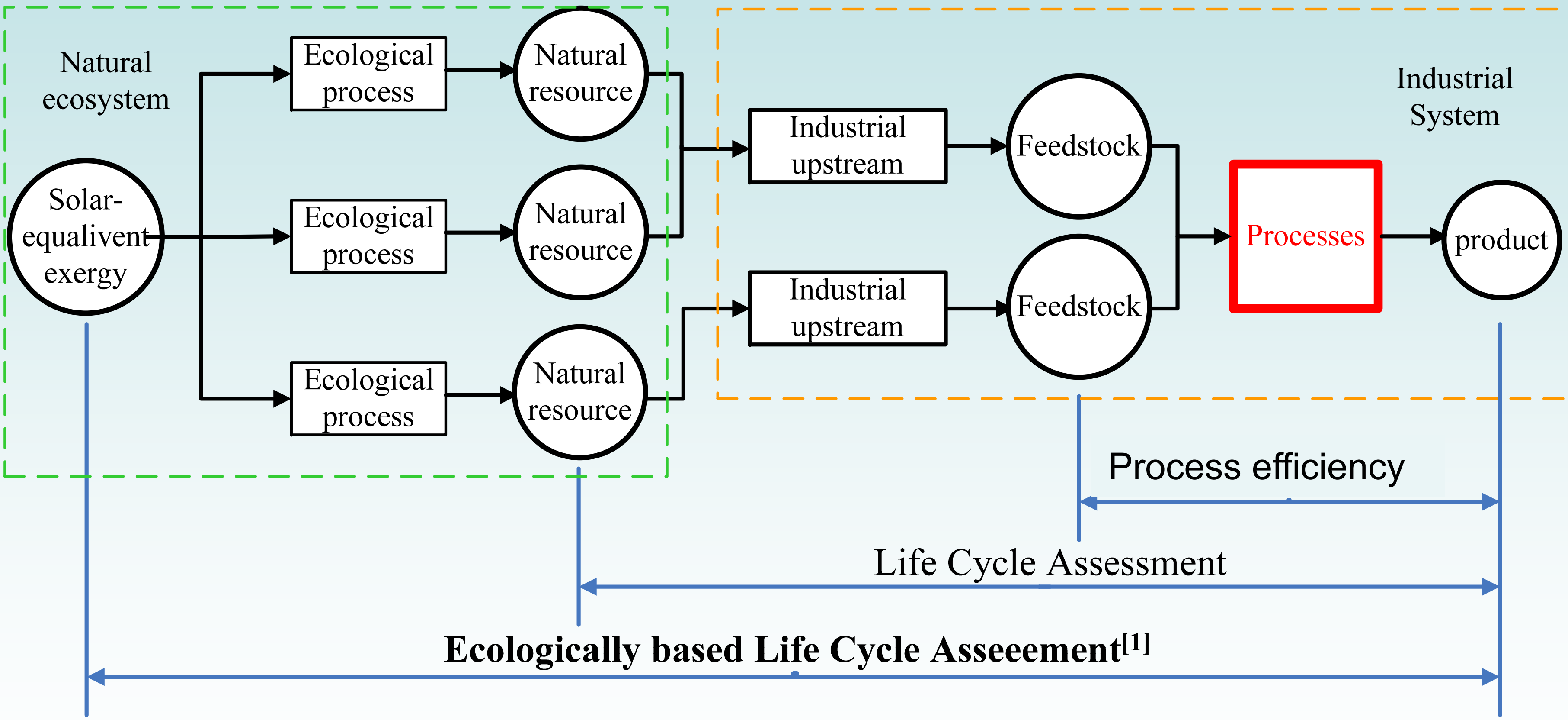
Life Cycle Boundary and Scope



Life Cycle Assessment (LCA) and Sustainability Analysis

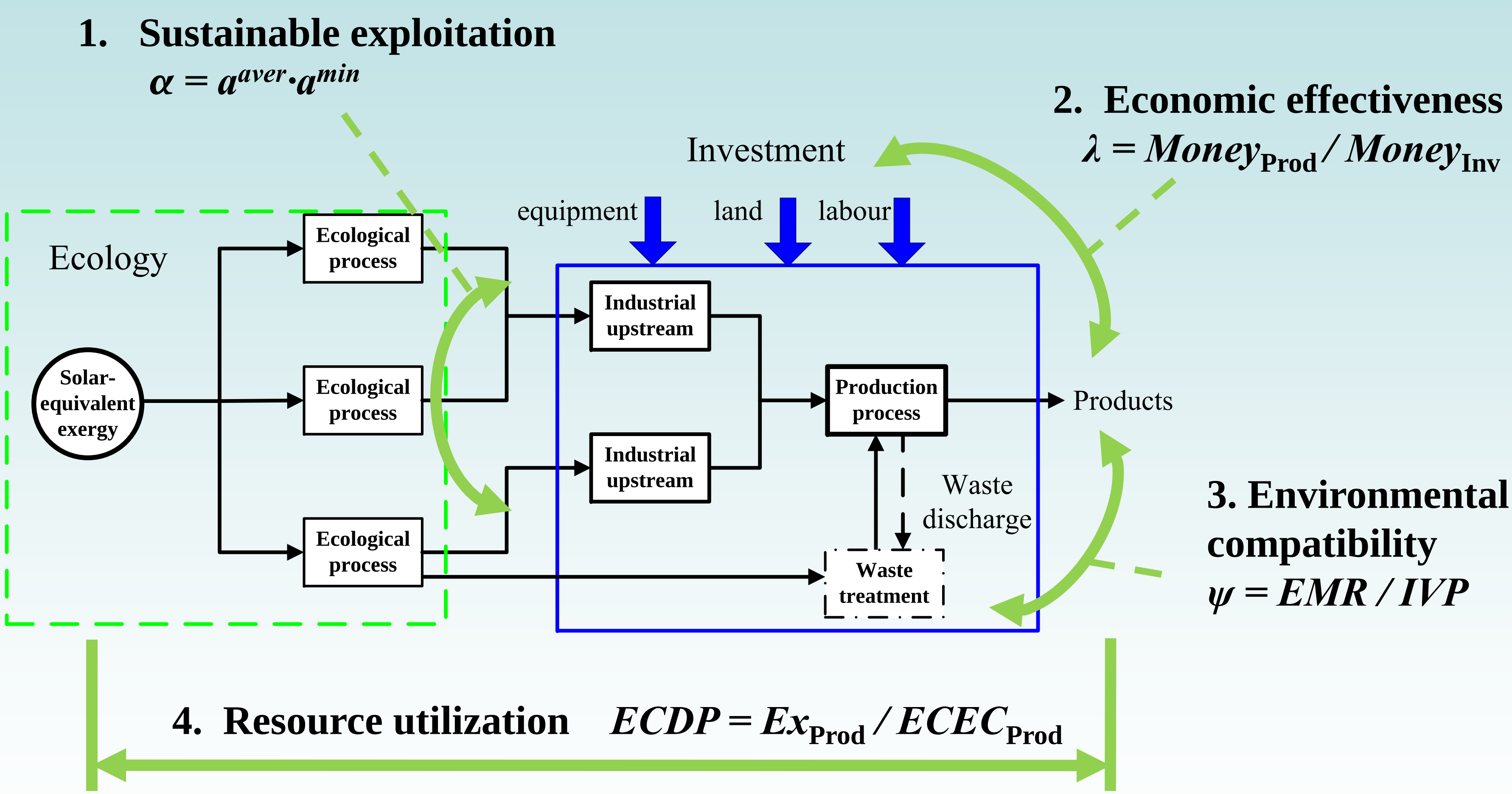


Eco-LCA Framework



[1] Zhang, Y.; Baral, A.; Bakshi, B.R. Accounting for ecosystem services in life cycle assessment, part II: toward an ecologically based LCA. *Environ. Sci. Technol.* **2010**, 44, 2624-2631.

Multi-attribute Eco-LCA Metrics

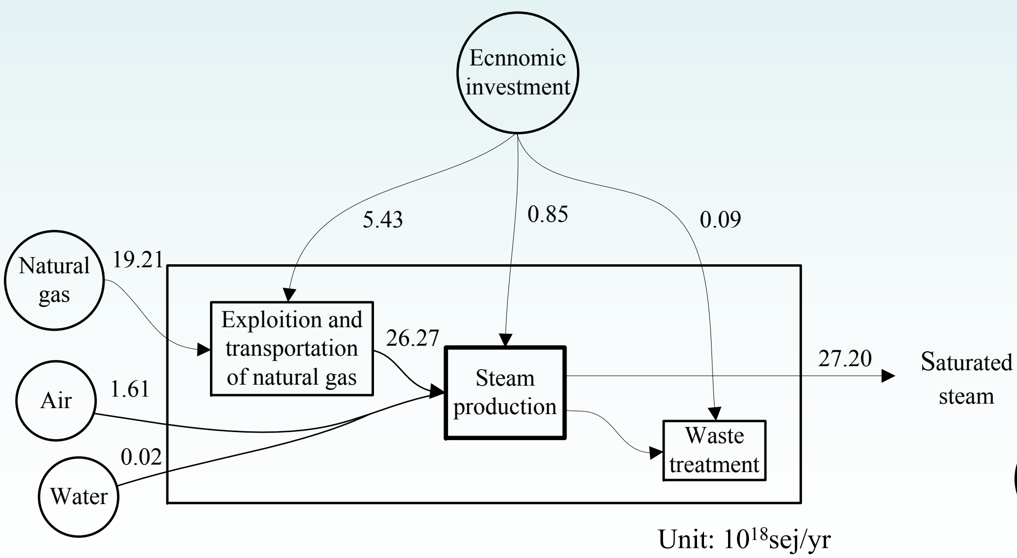


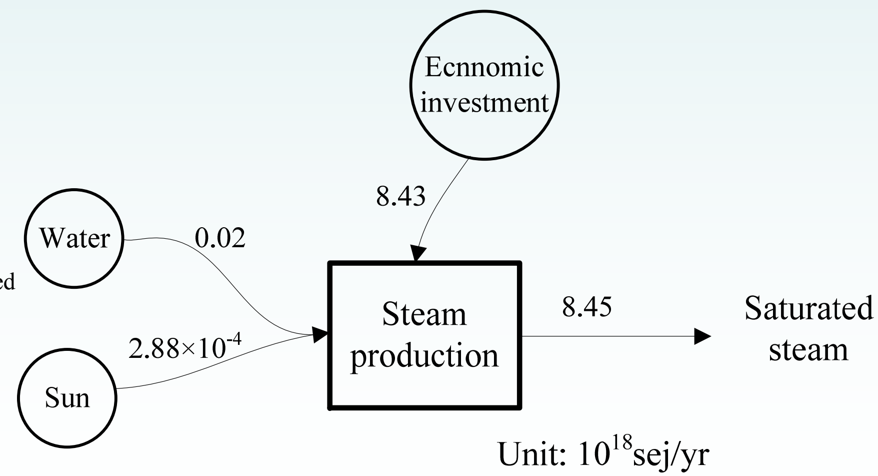
1. Resource abundant factor：Lems, S.; de Swaan Arons, J. The sustainability of resource utilization. *Green Chem.* **2002**, 4, 308-313.
2. *EMR* is the overall *ECEC*/*Money* Ratio, *IVP* is the *ECEC* per unit of economic output. $\boldsymbol{\psi = EMR / (ECEC_{Prod} / Money_{Prod})}$

Eco-LCA of Steam Production

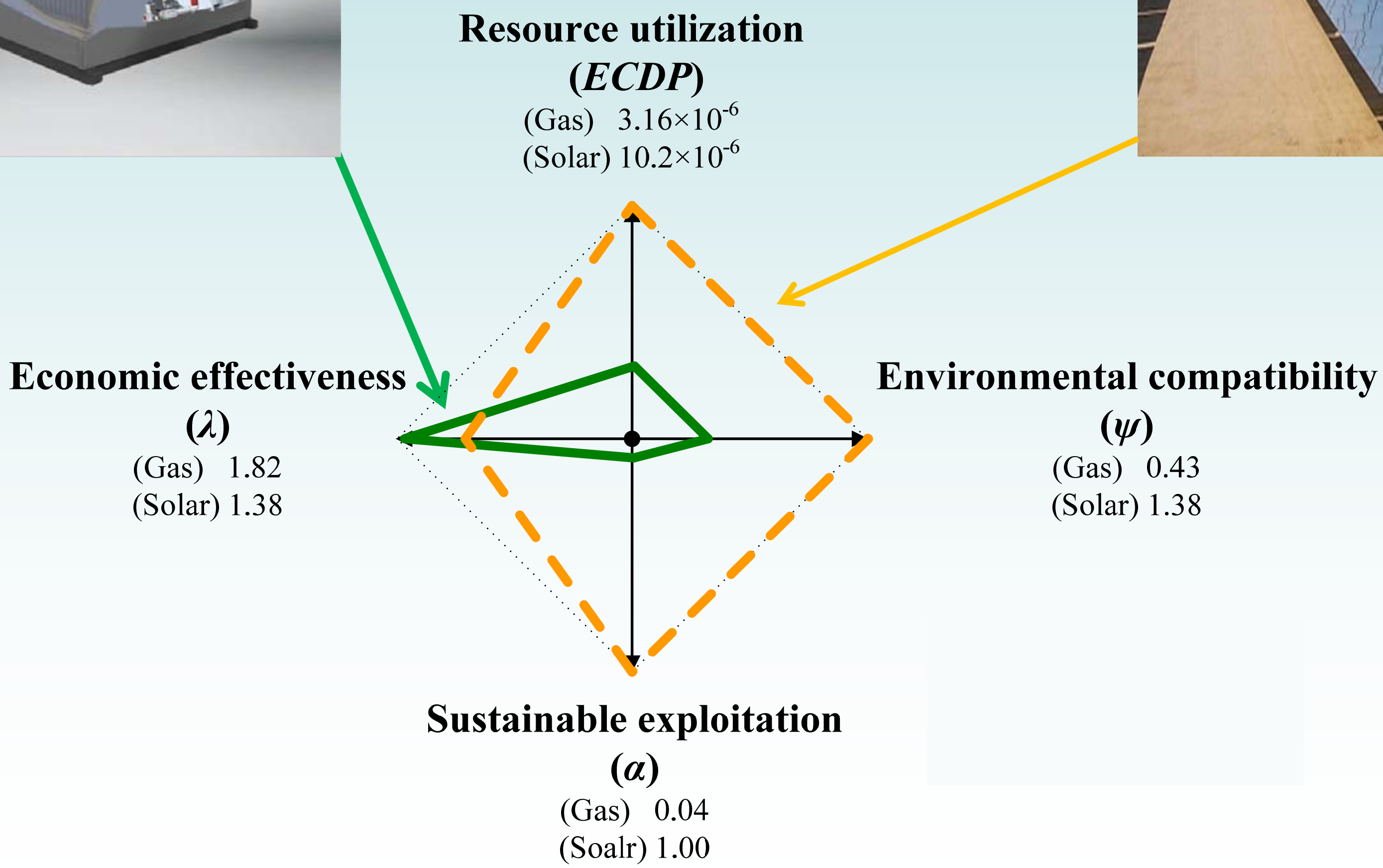
the **functional unit** produces 80 kt/yr of 3.5MPa saturated steam.

<u>**Gas boiler** v.s. **Solar boiler**</u>





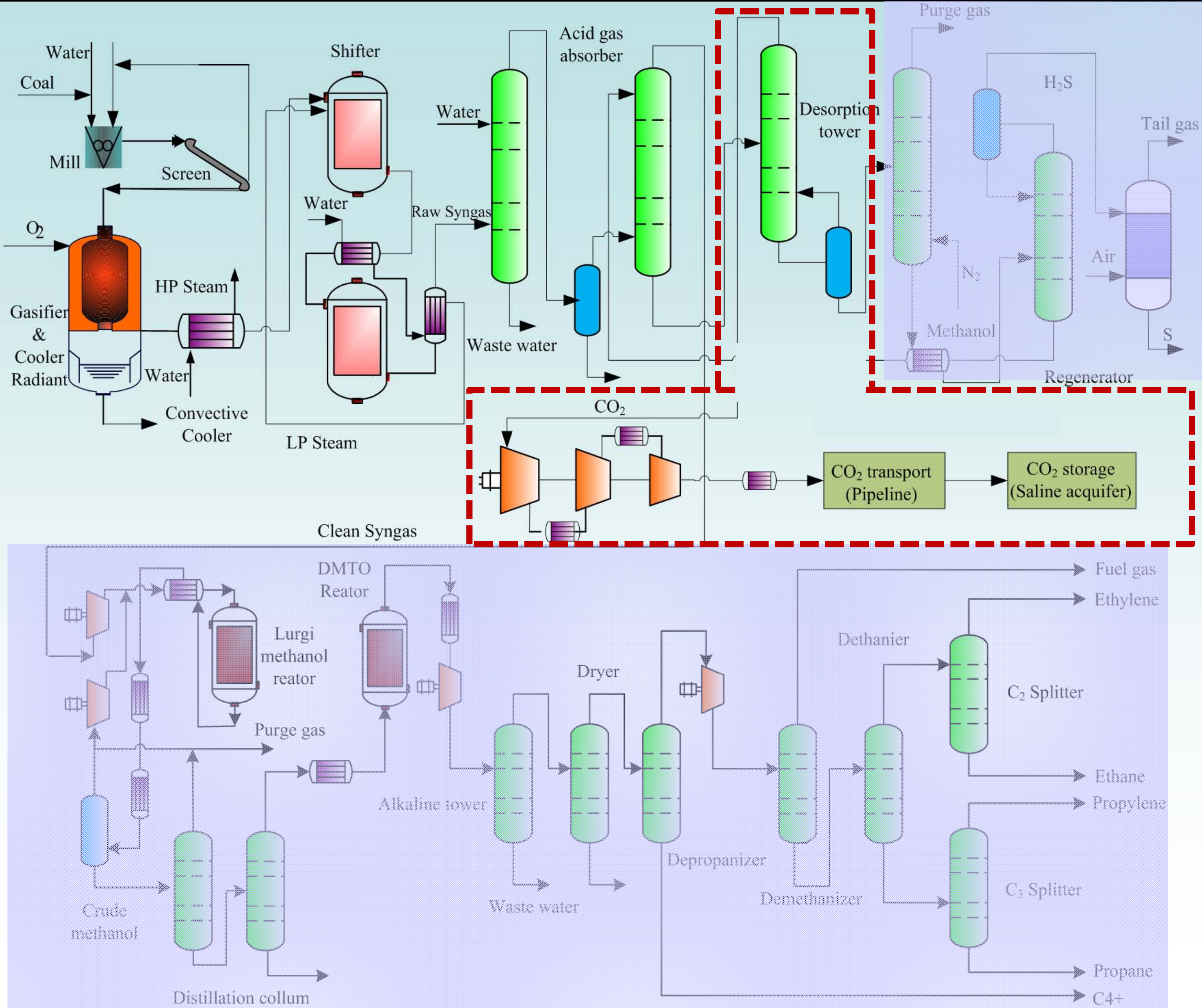
Eco-LCA of Steam Production



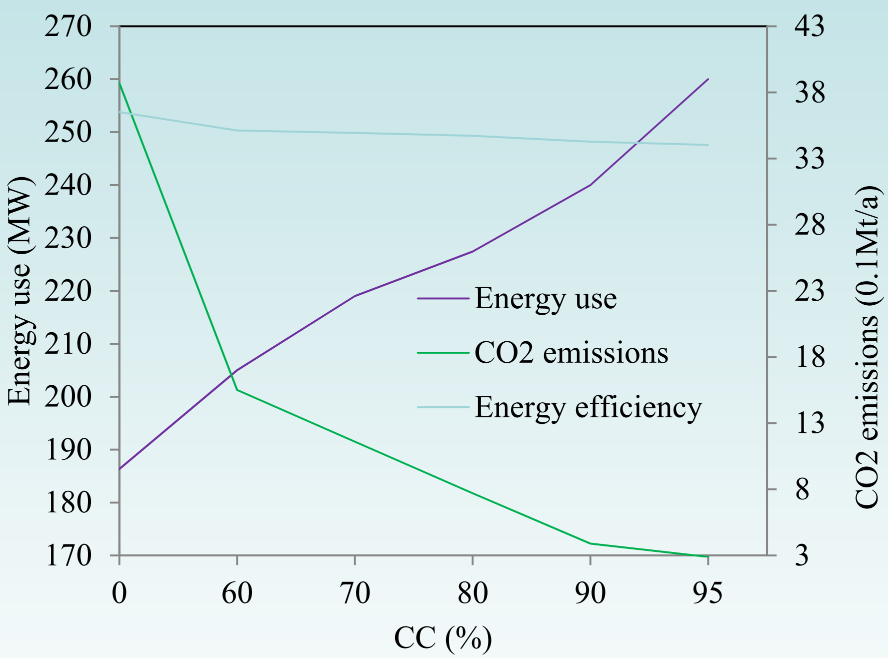
Sustainability analysis on resource, energy, environment, and economy

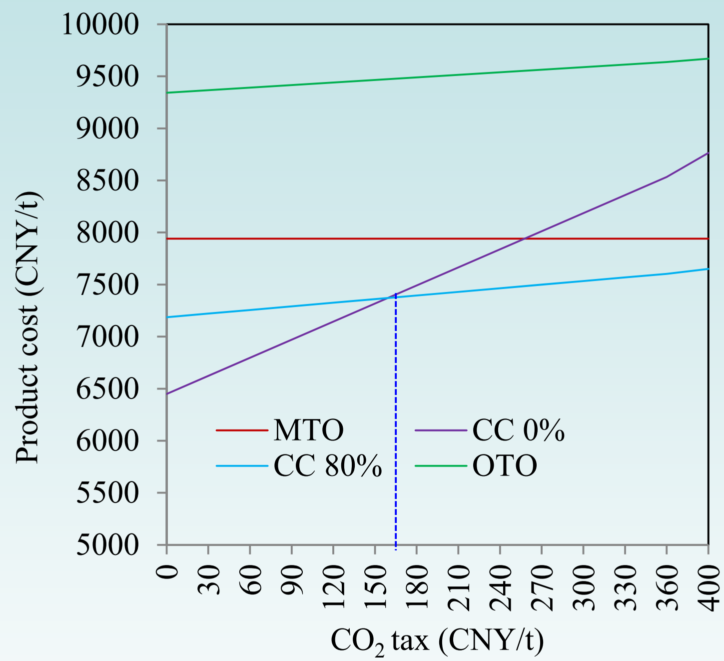
Generic	No.	Indicators	Metric
Resource	1	Mass productivity（*MP*）	kg/kg
	2	Renewability material index（RI_M）	kg/kg
Energy	3	Energy efficiency（η）	kJ/kJ
	4	Exergy efficiency（ψ）	kJ/kJ
Environment	5	Global warming portential（*GWP*）	kg/kg
	6	Atmospheric acidification potential(*AP*)	kg/kg
	7	Environmental loading ratio（*ELR*）	kSej/kSej
Economy	8	Payback period（*PBP*）	yr
	9	Equivalent annual cost（c_{eq}）	$

Case 4: Coal based process with CCS



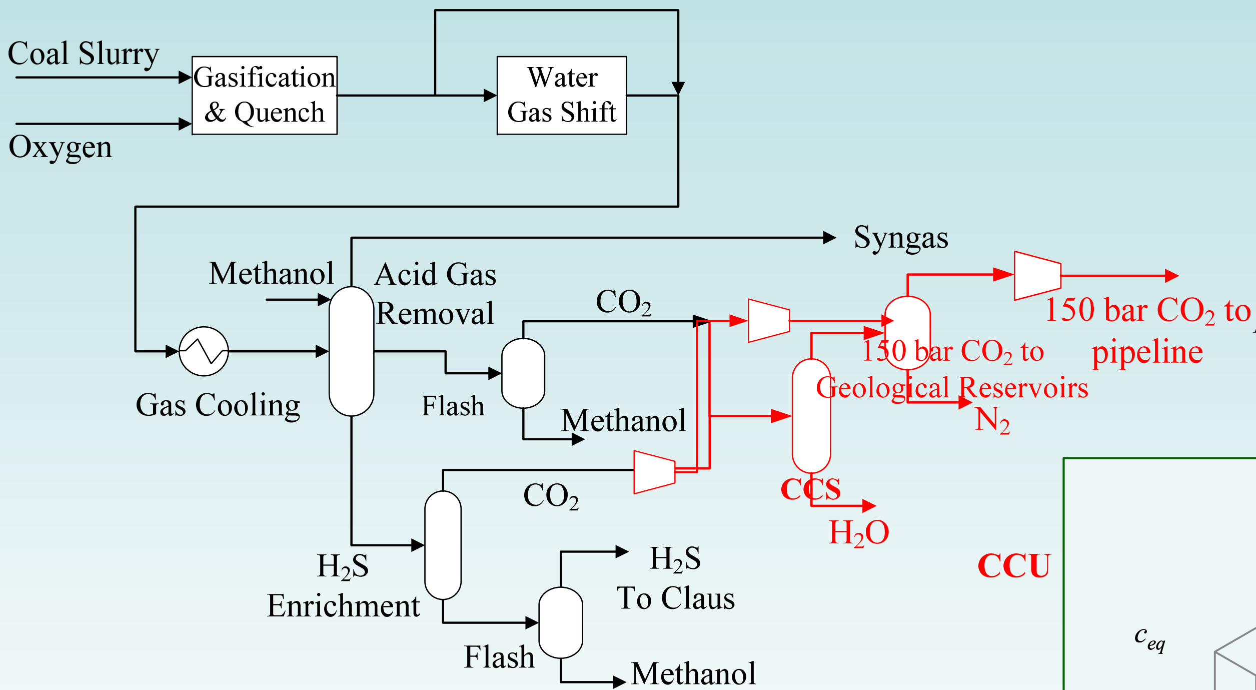
Energy consumption, economic and environmental performance with CC rate

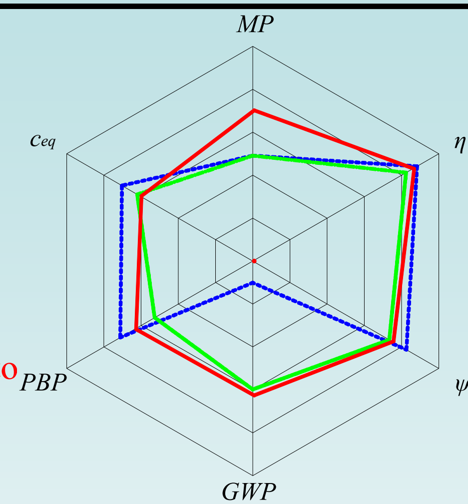


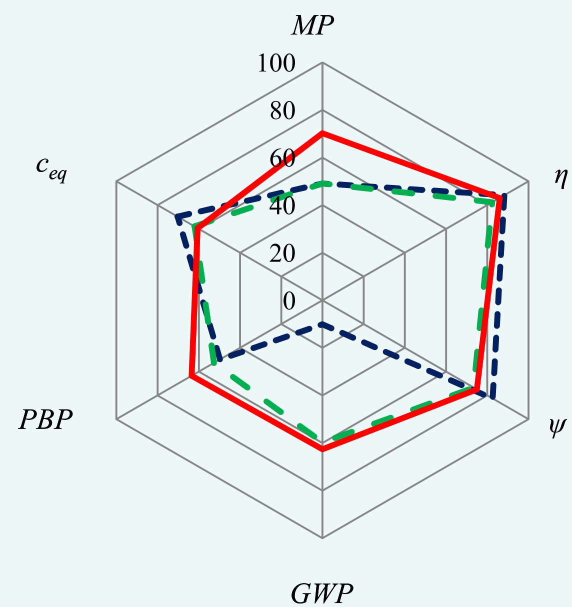


In considering carbon tax (at 20Euro), CTO with 80% CCR is economically attractive than OTO, MTO, or CTO without CC.

Coal gasification with CCS or CCU?



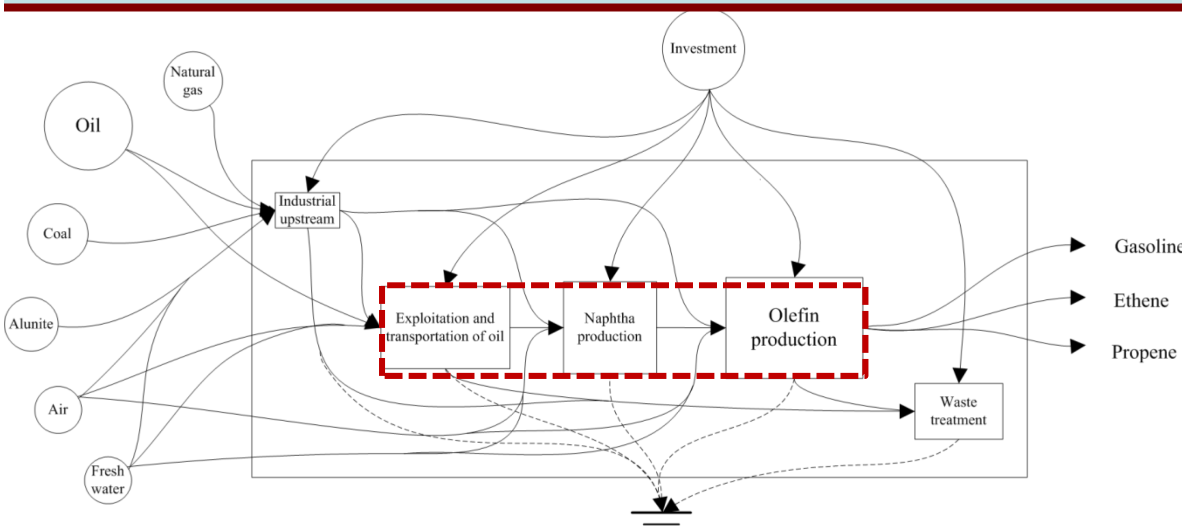




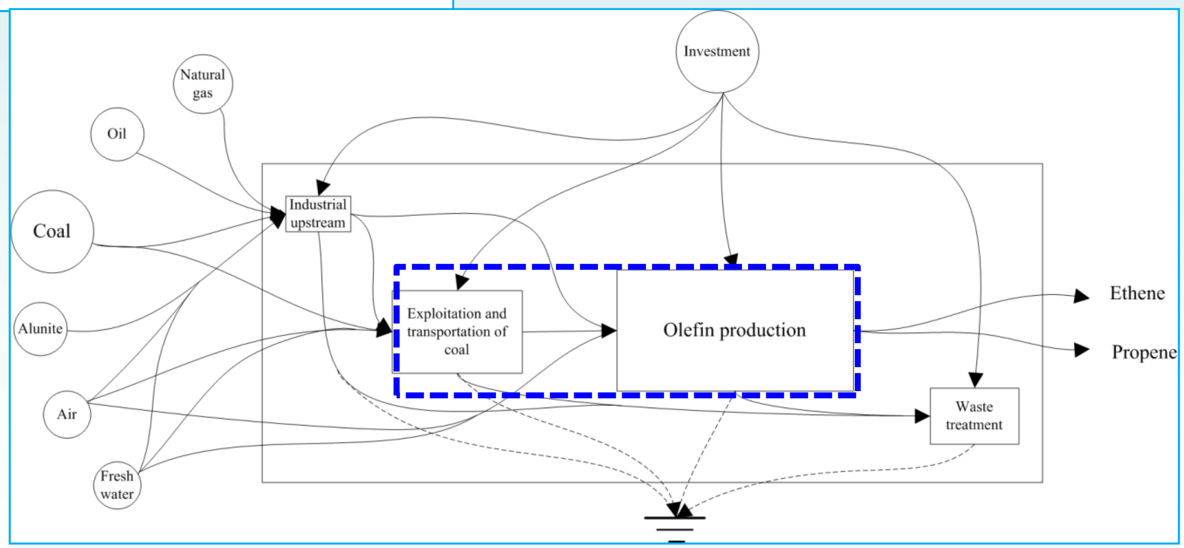
Carbon tax = \$20 USD/t equivalentCO_2

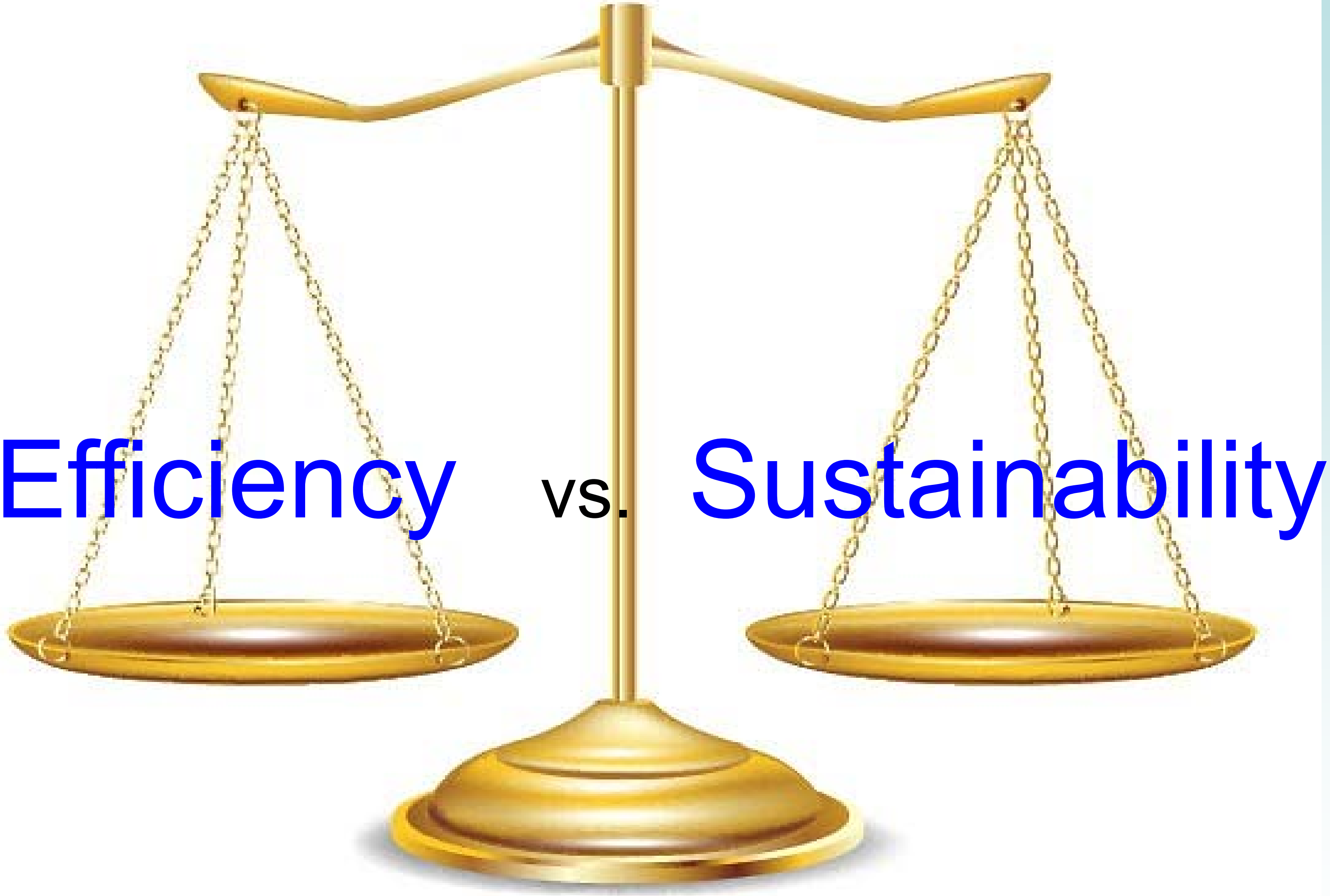
- As shown in the chart, although GWP reduced, CC (90%) for oil extraction/geo-storage are of higher
- On the other side, CO_2 enriched to higher concent better for resource utilization and economic perfo
- Quantitative sustainability analysis helps rational decision making on CCUS approaches.

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

Tools

simulator
ASPEN Plus
LCA software
SimPro
Optimizer
GAMS

Main models

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

outport

- sustainability performance
- Process Improvement and innovation

Process integration, and Innovation