

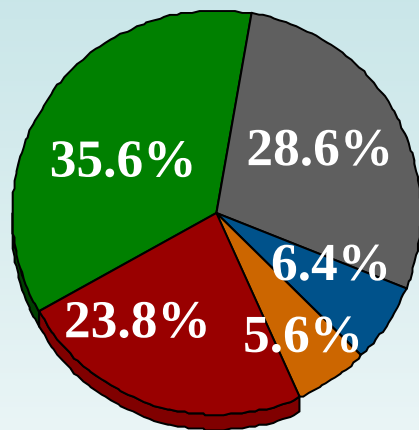
Sustainability Assessment of Coal based Energy and Chemical Processes

Yu Qian

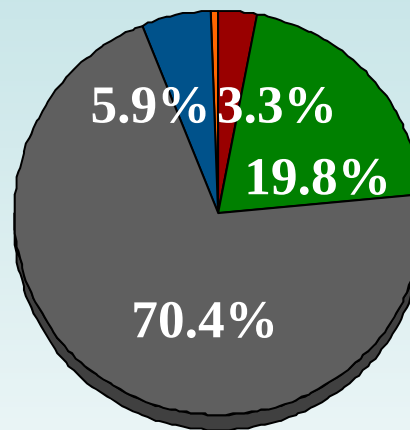
South China University of Technology
Guangzhou, China



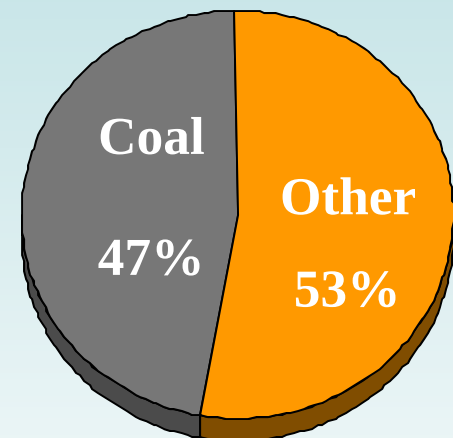
Energy usage spectrum: the world and China



World



Total Consumption



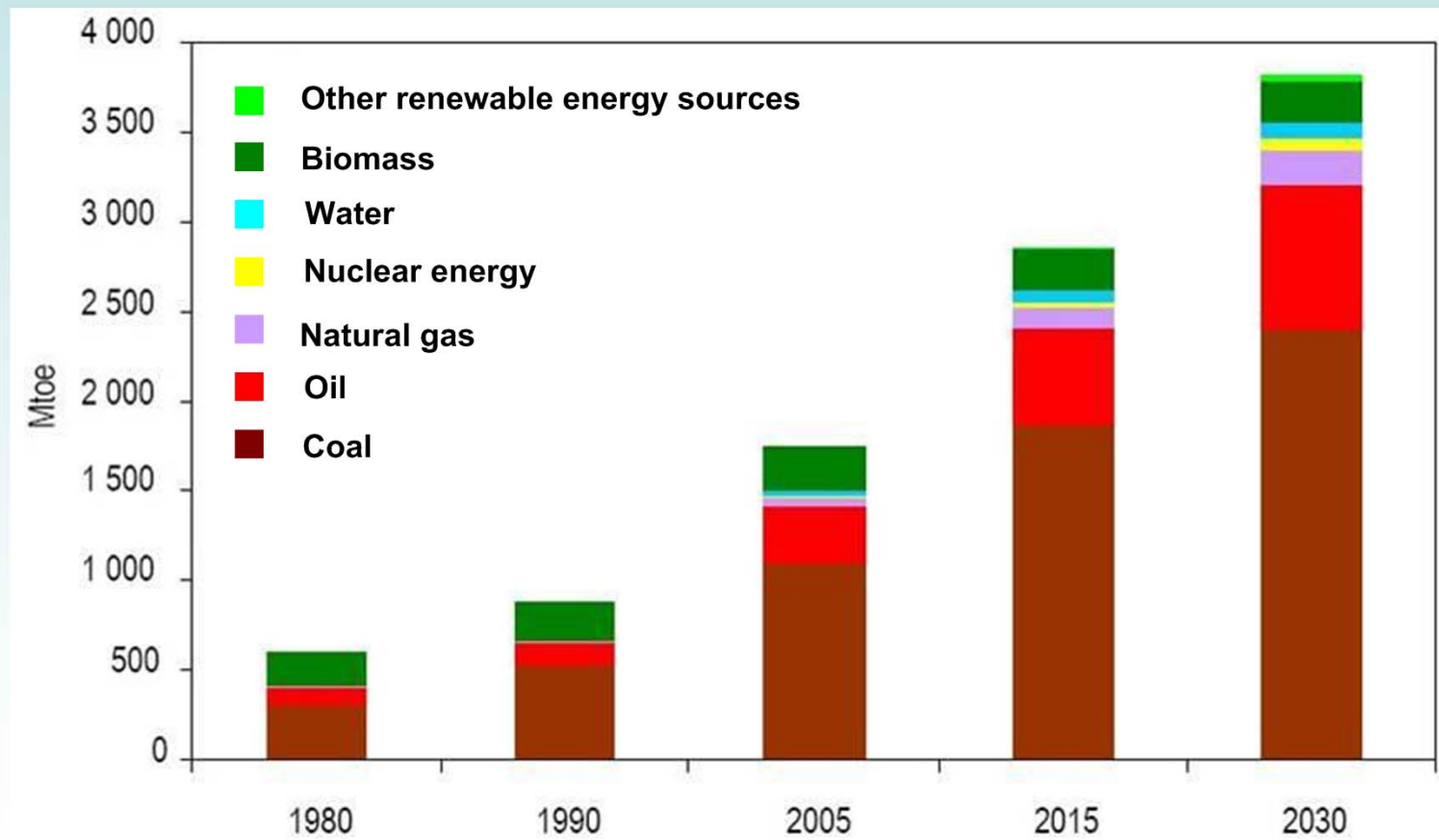
in CPI

China

-  Coal
-  Hydroelectric
-  Nuclear
-  Natural gas
-  Oil

coal usage in CPI includes coking and gasification

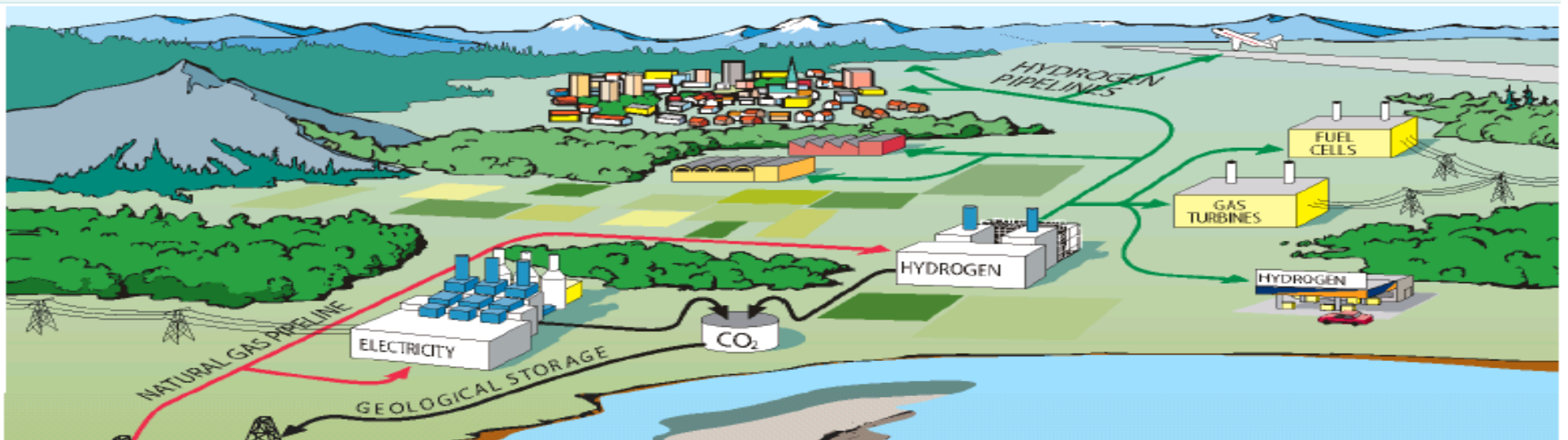
In the next 20 years, half demand growth of China's primary energy/resources supply will remain depending on coal.



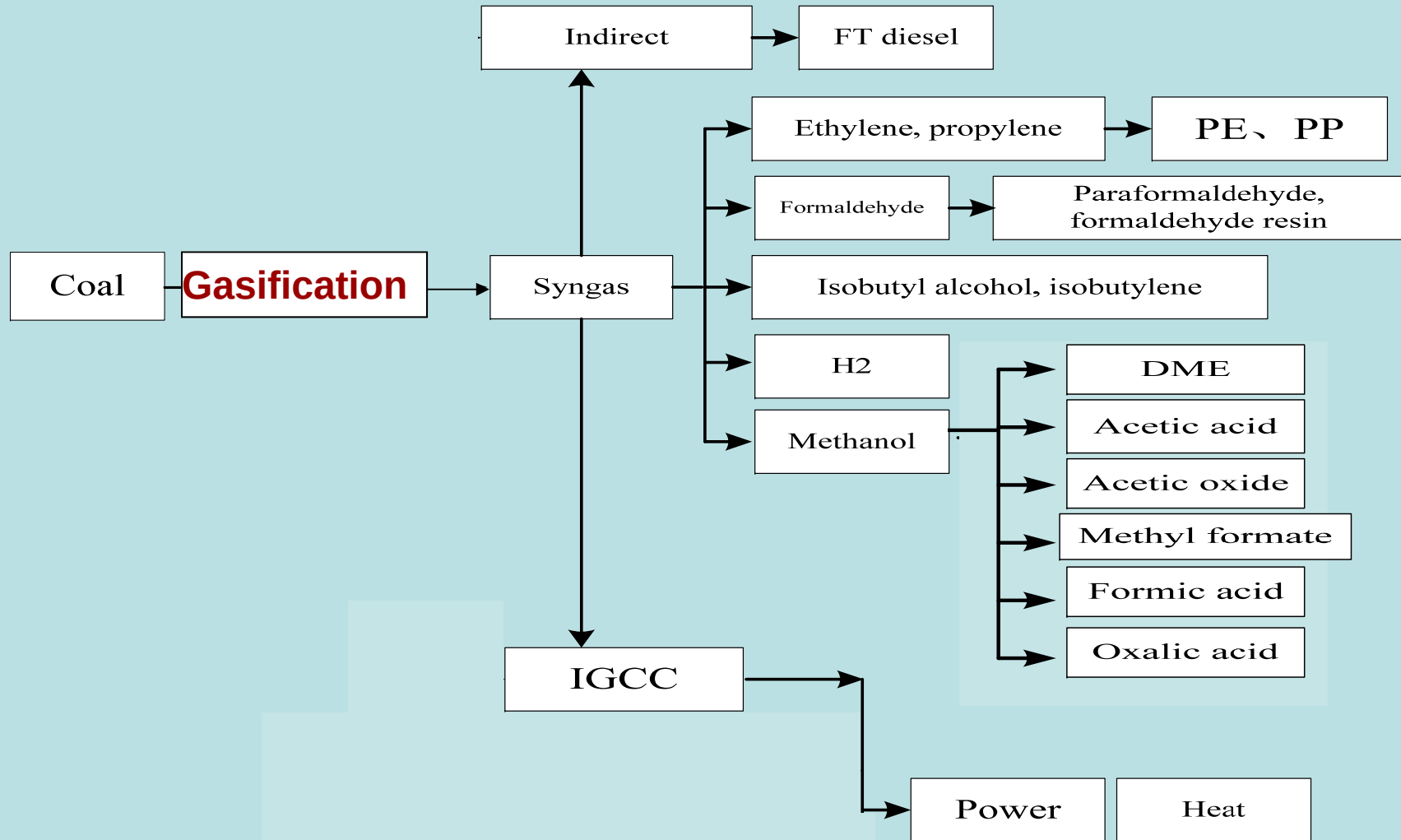
Source: International Energy Agency (IEA, 2010)

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

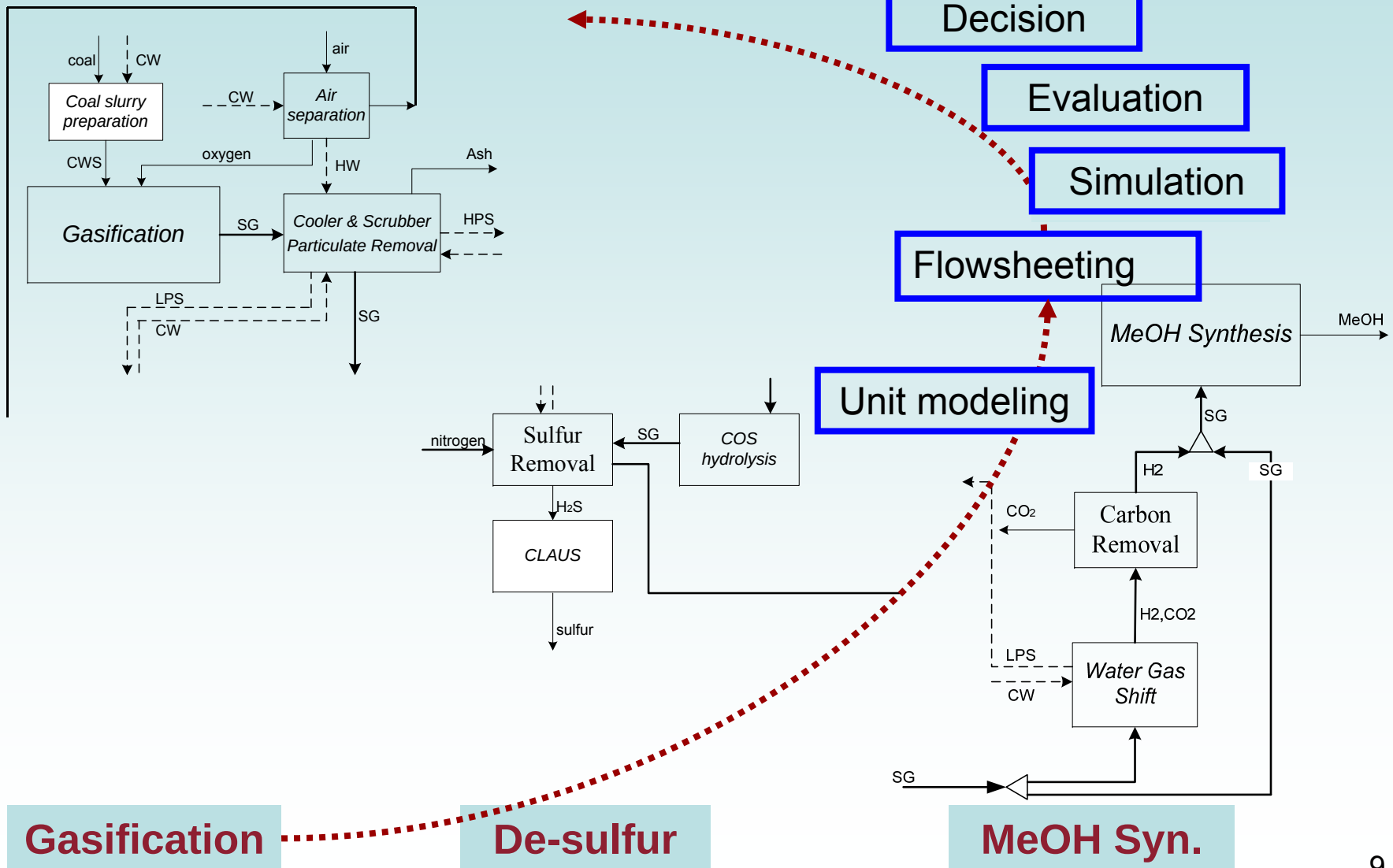
Life cycle costing

Emergy analysis (ecological analysis)

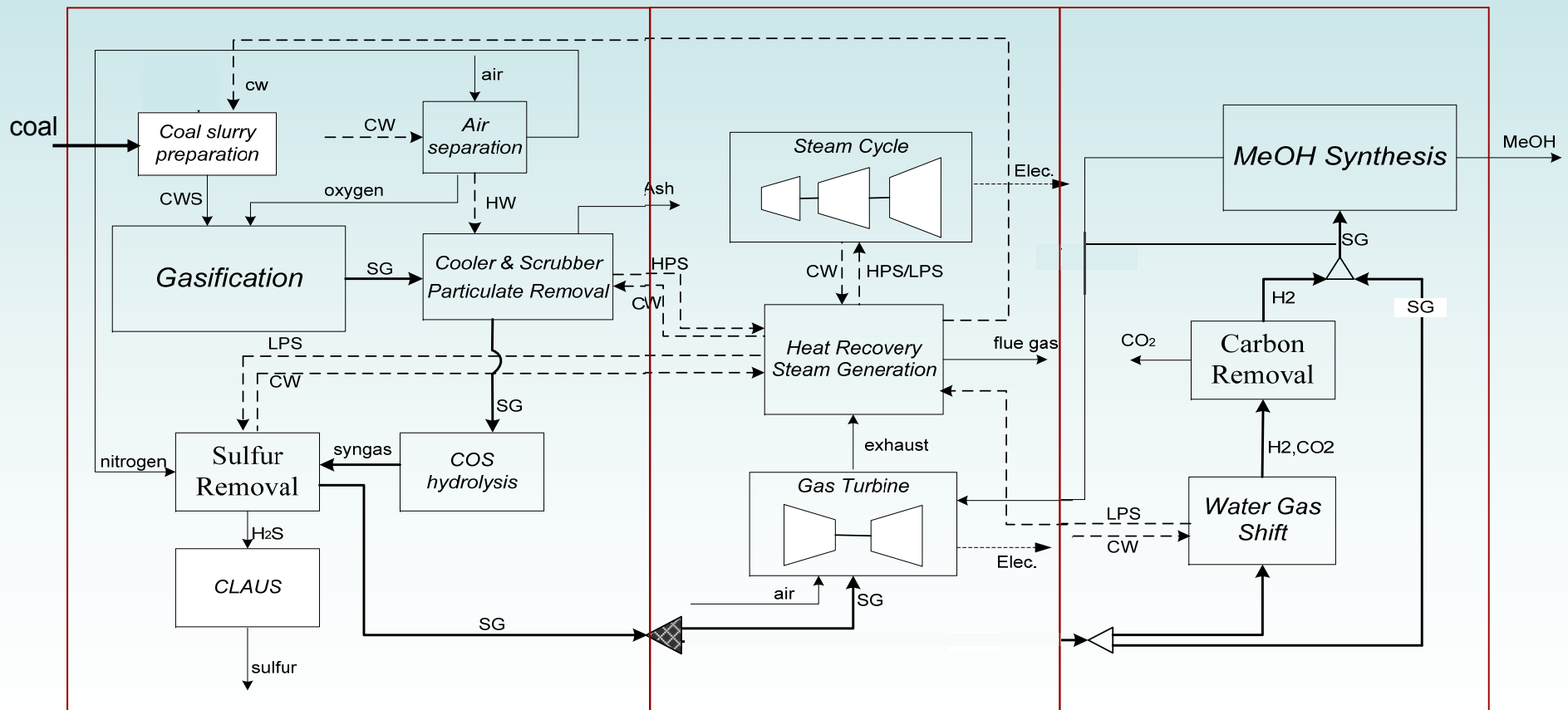
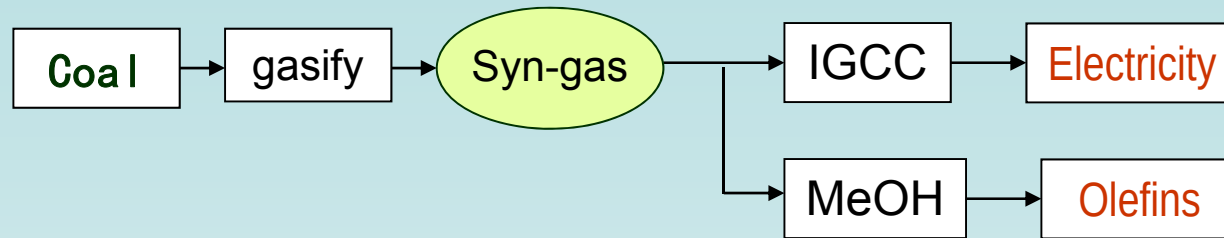
Tech-economic–environ–social: multi-objective coordination

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

Coal to Methanol



coal to IGCC/methanol co-production

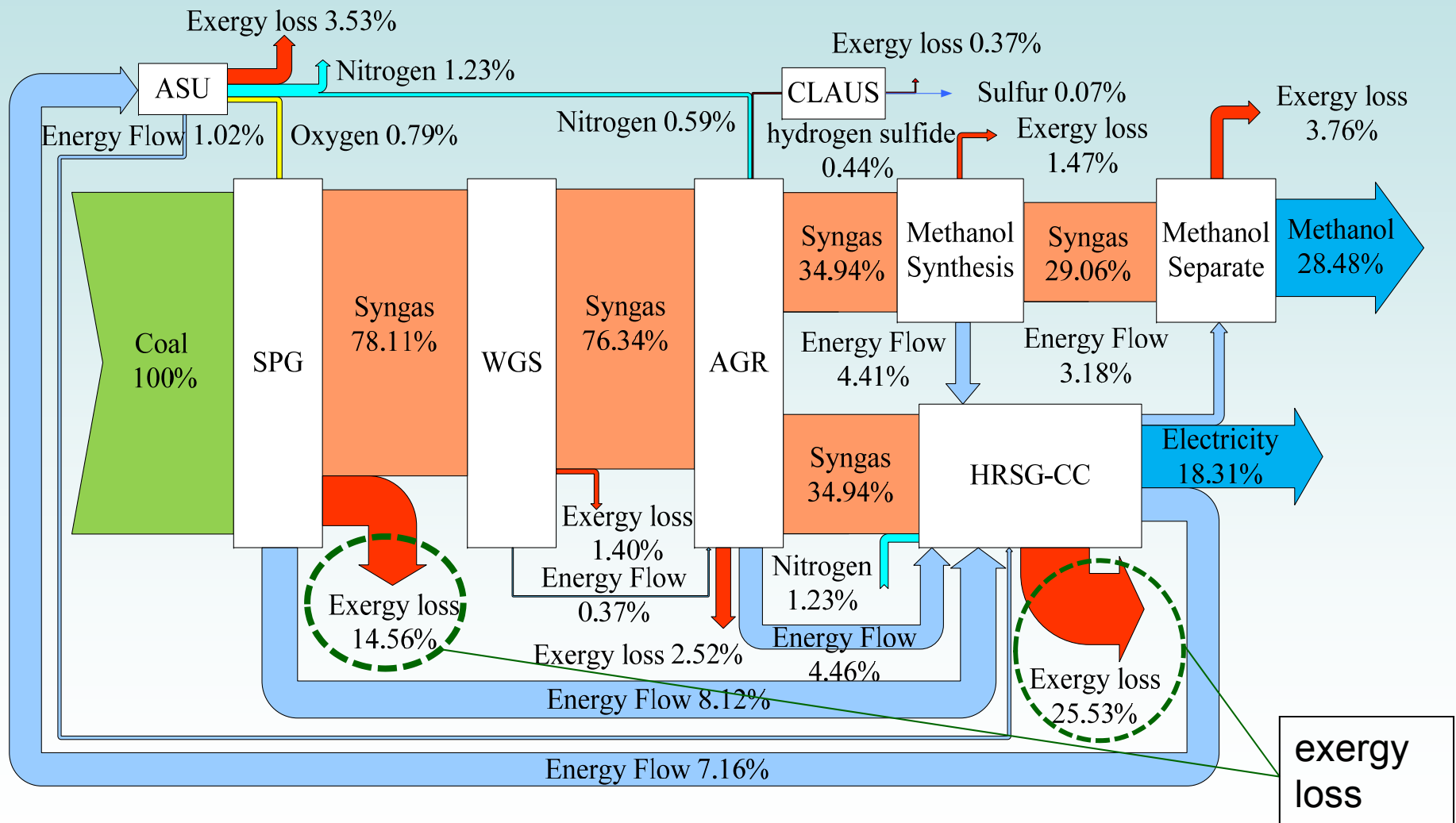


Gasification

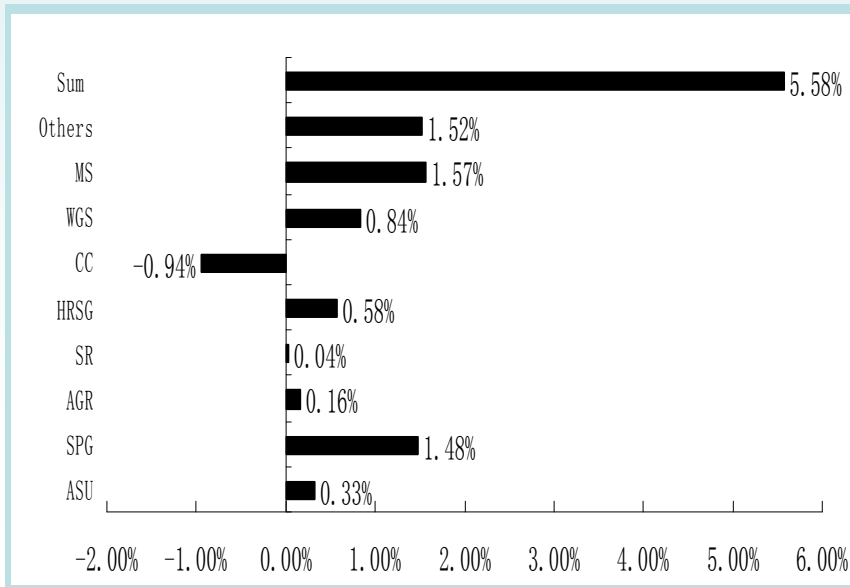
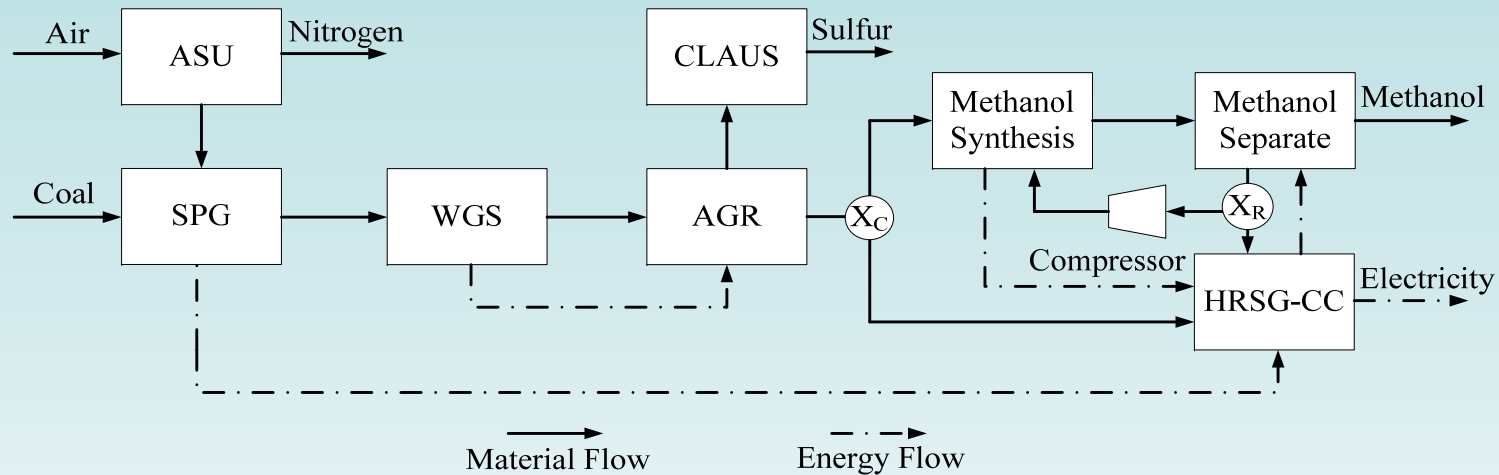
Combined Cycle

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;

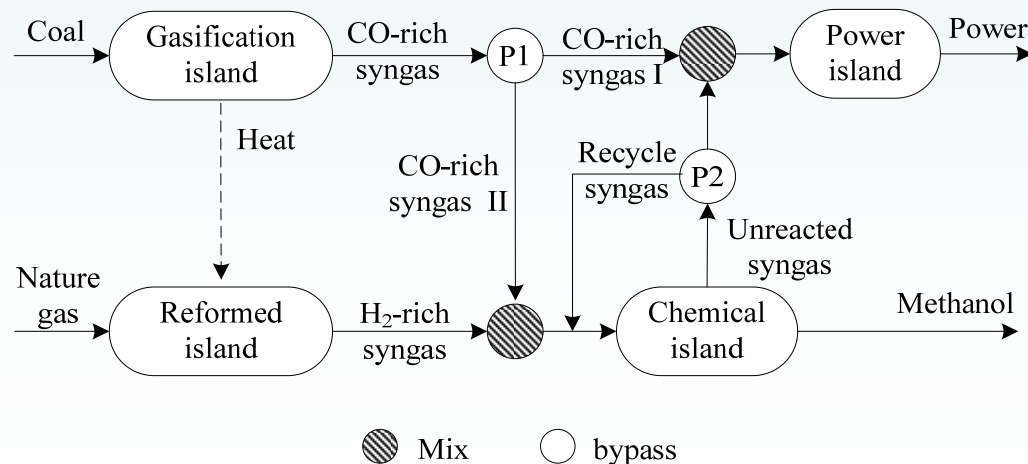
H/C ratio to produce chemicals: 2.

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

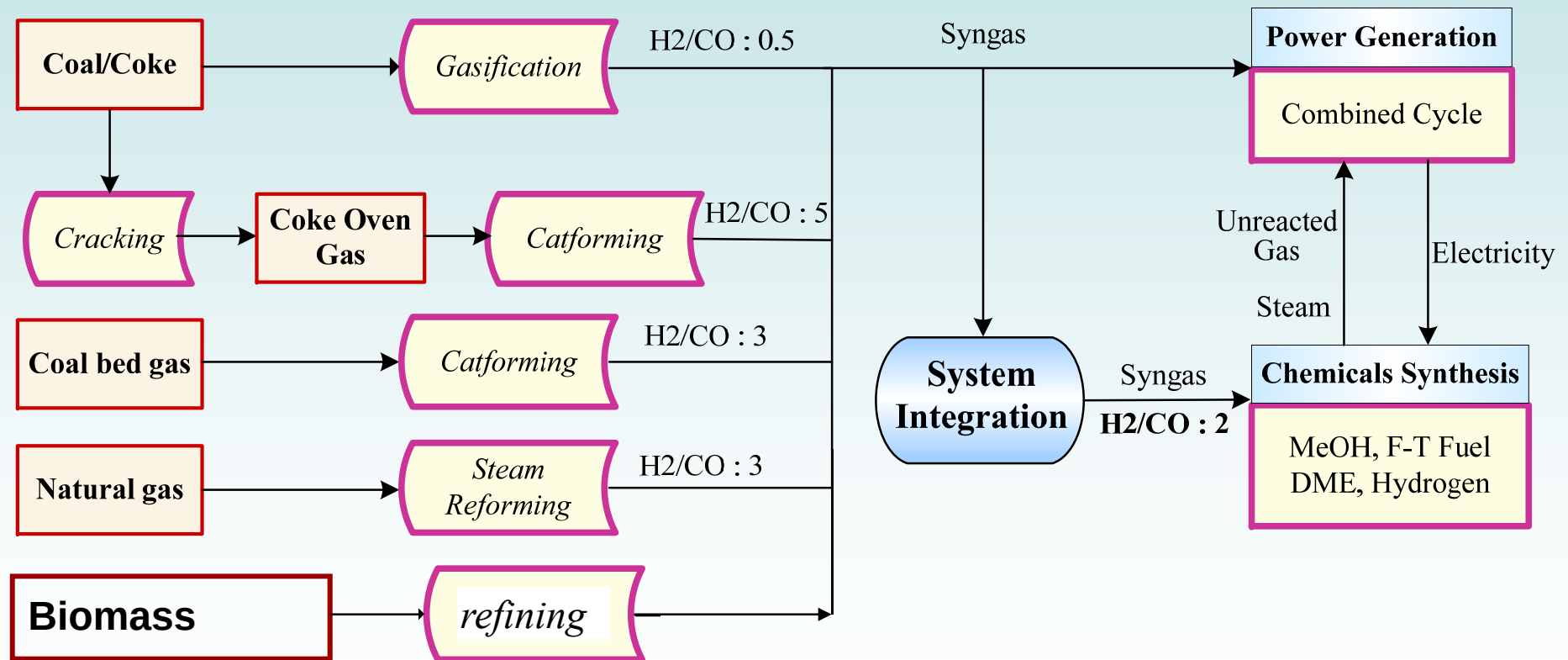


Key structural variables:

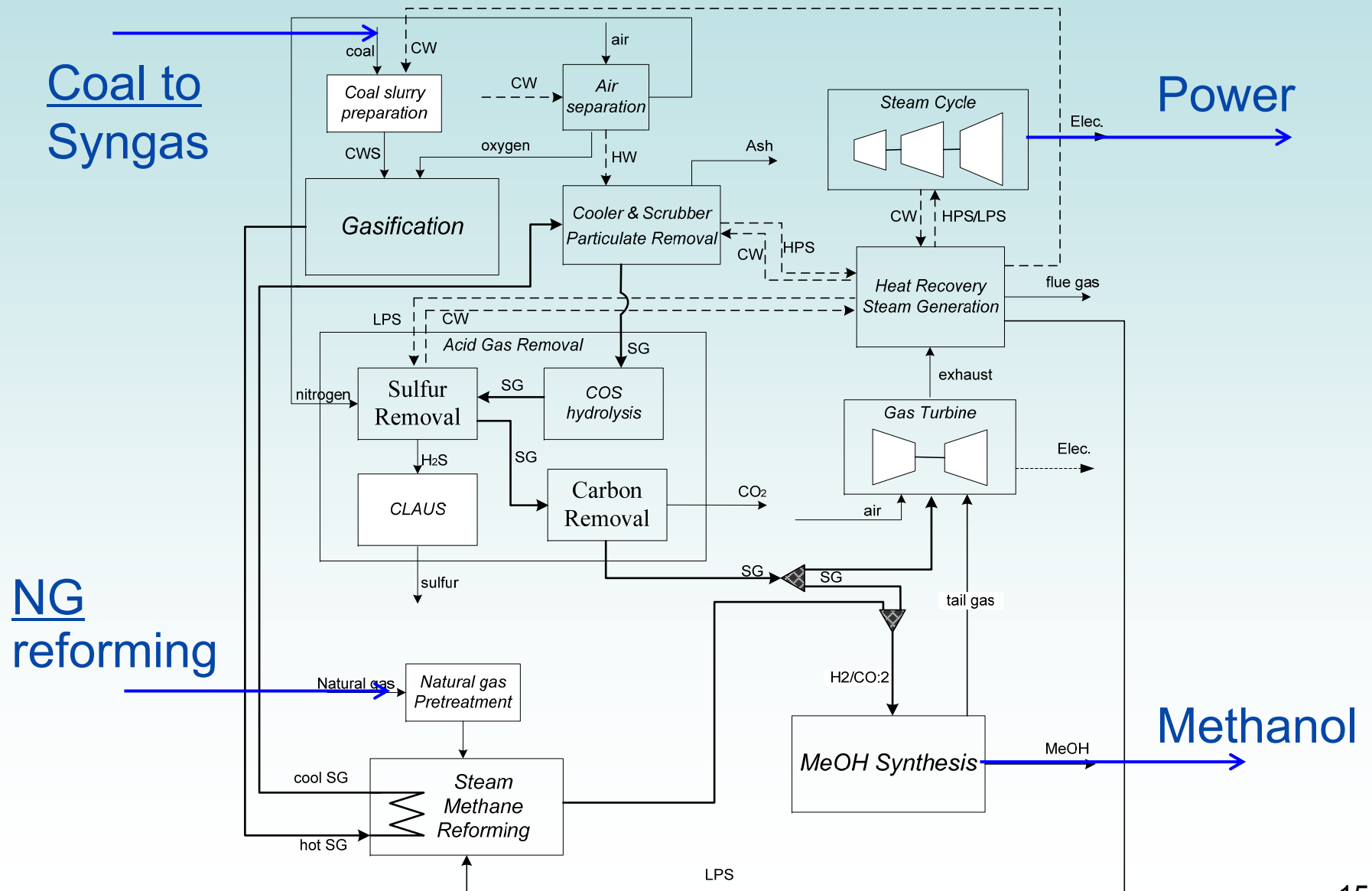
co- feed factor P_1

co-generation factor: P_2

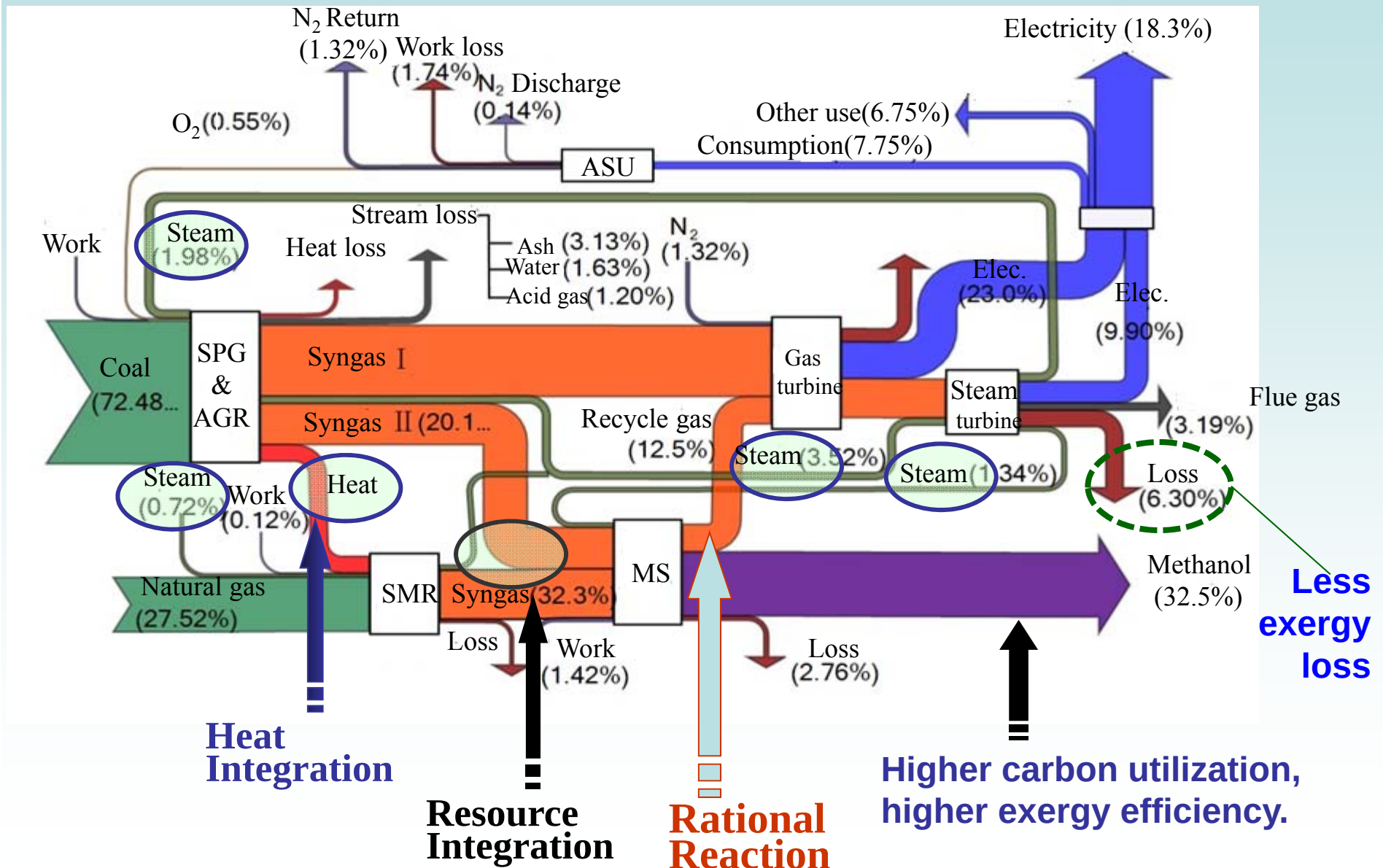
Multi-feed Co-production System



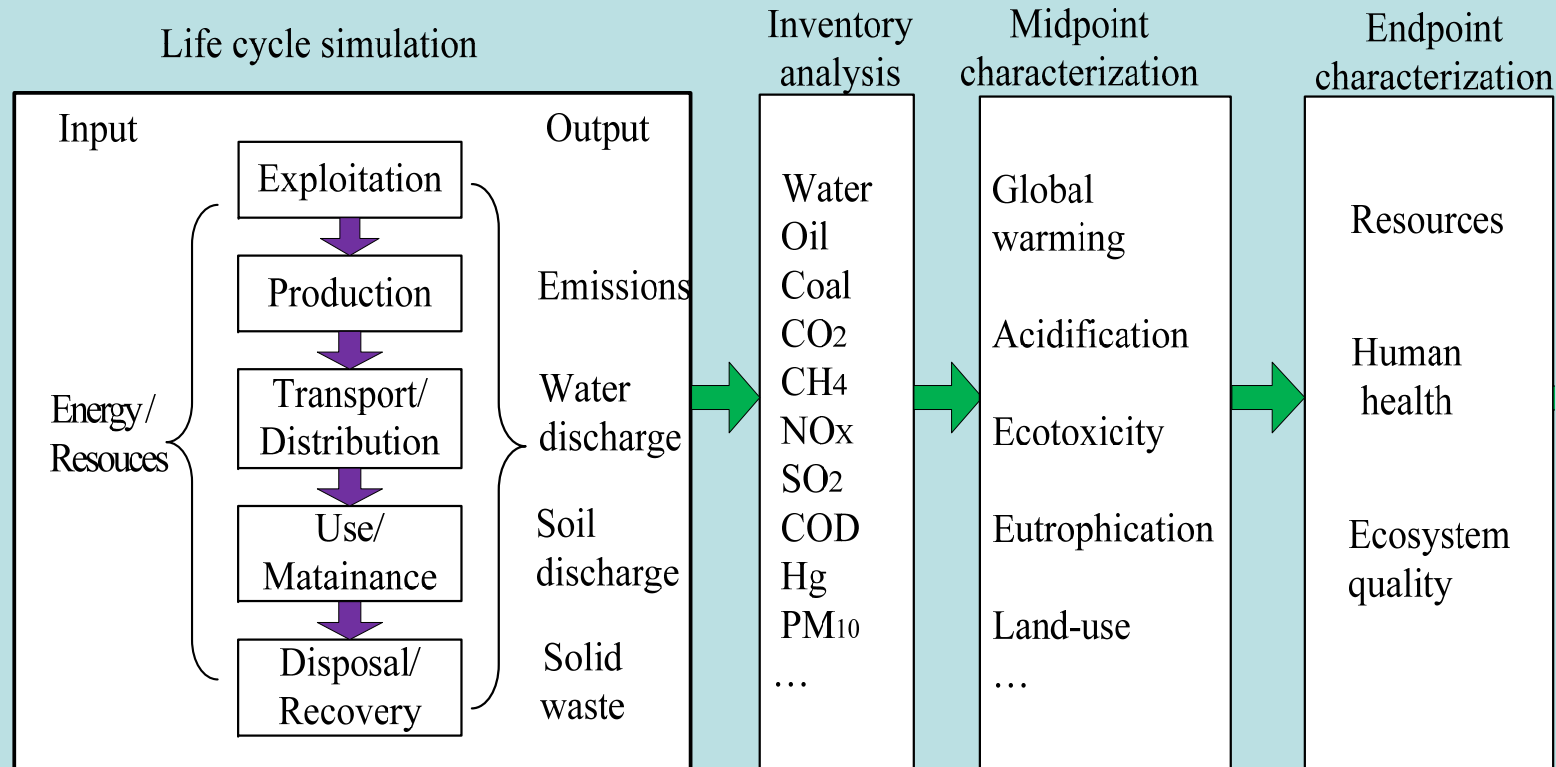
NG-Coal co-feed co-generation process



Mass/exergy flow diagram for integration & optimization



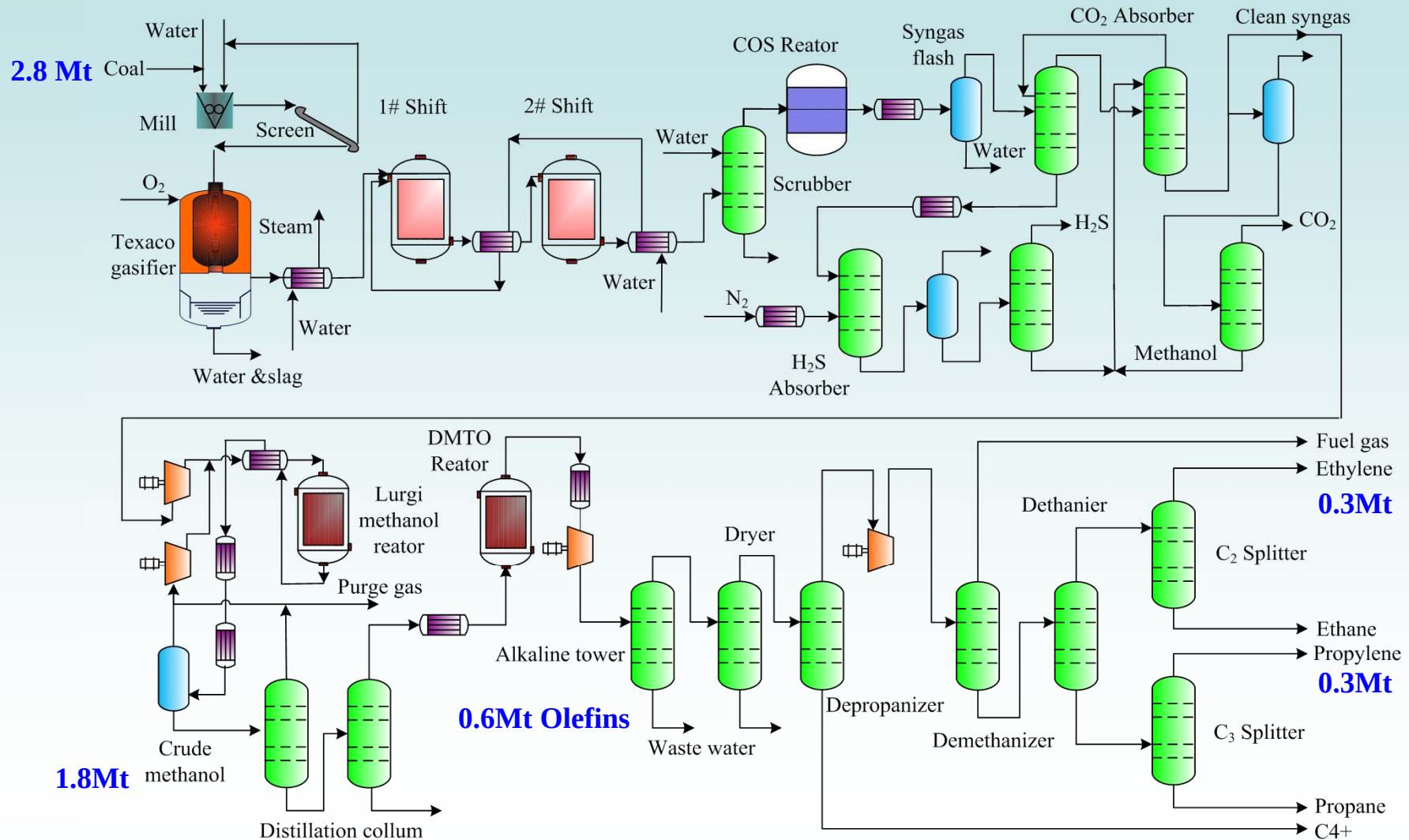
Modeling with Eco-indicator 99



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.

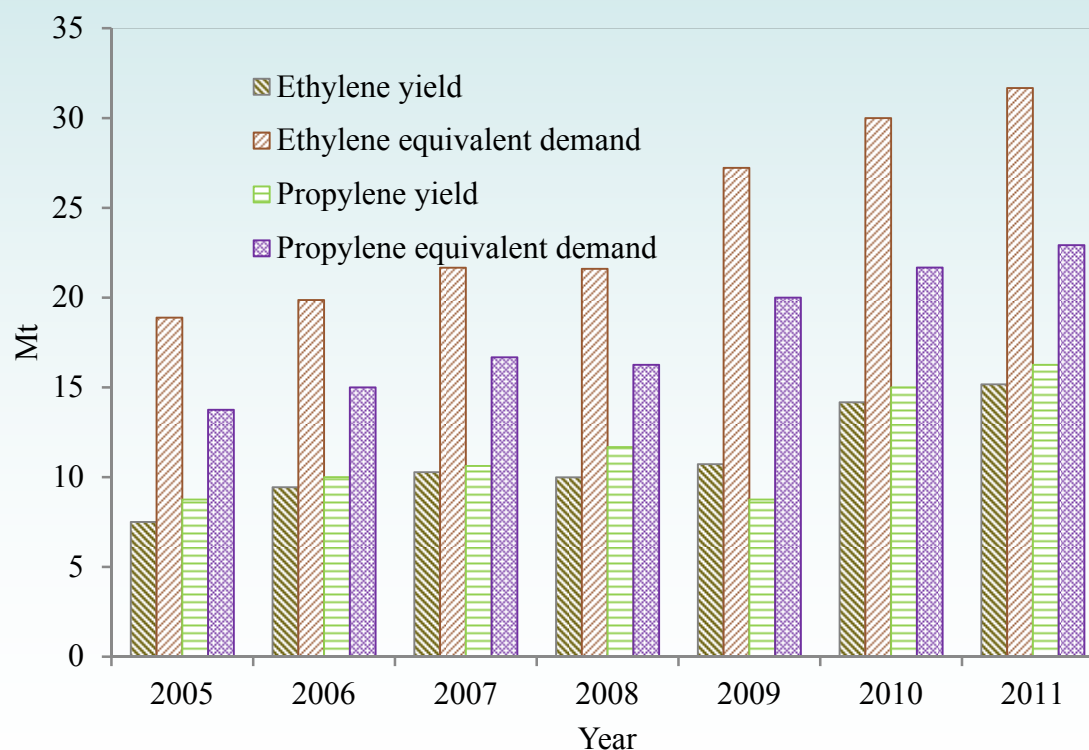
Industrial Case: Coal to Olefins

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.



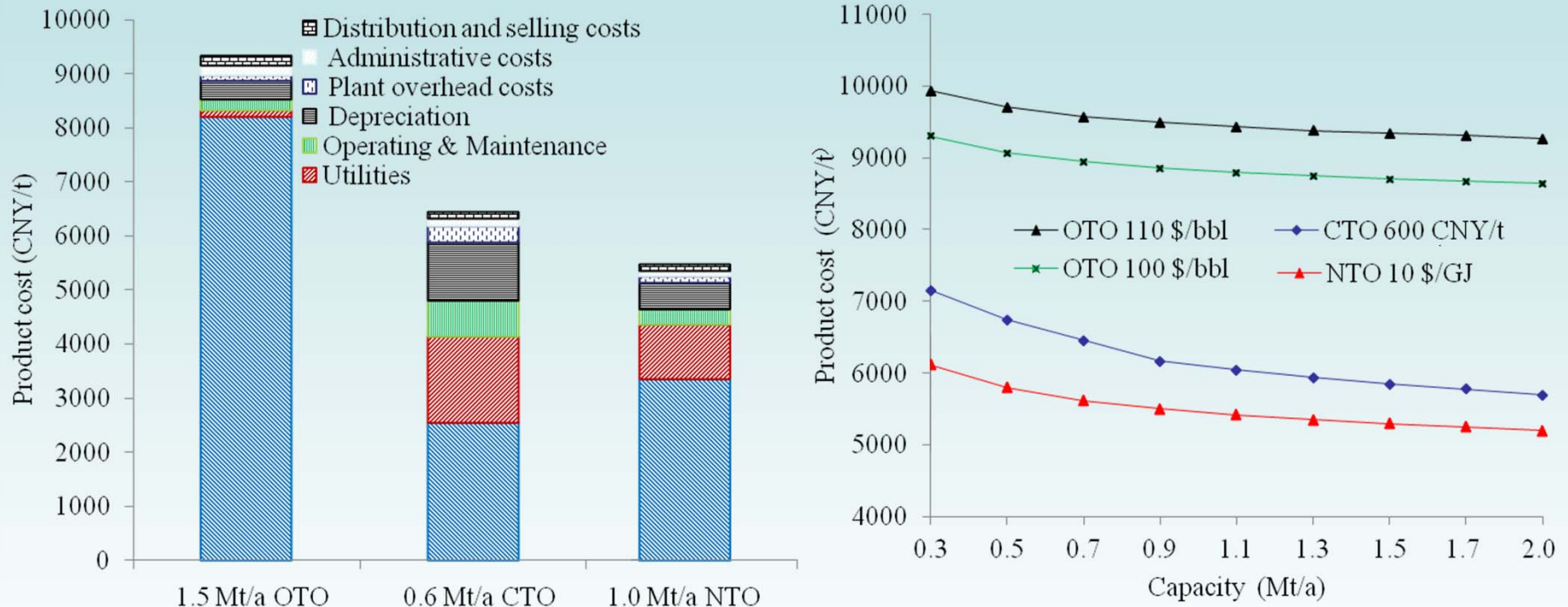
CTO Development Opportunity

- 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



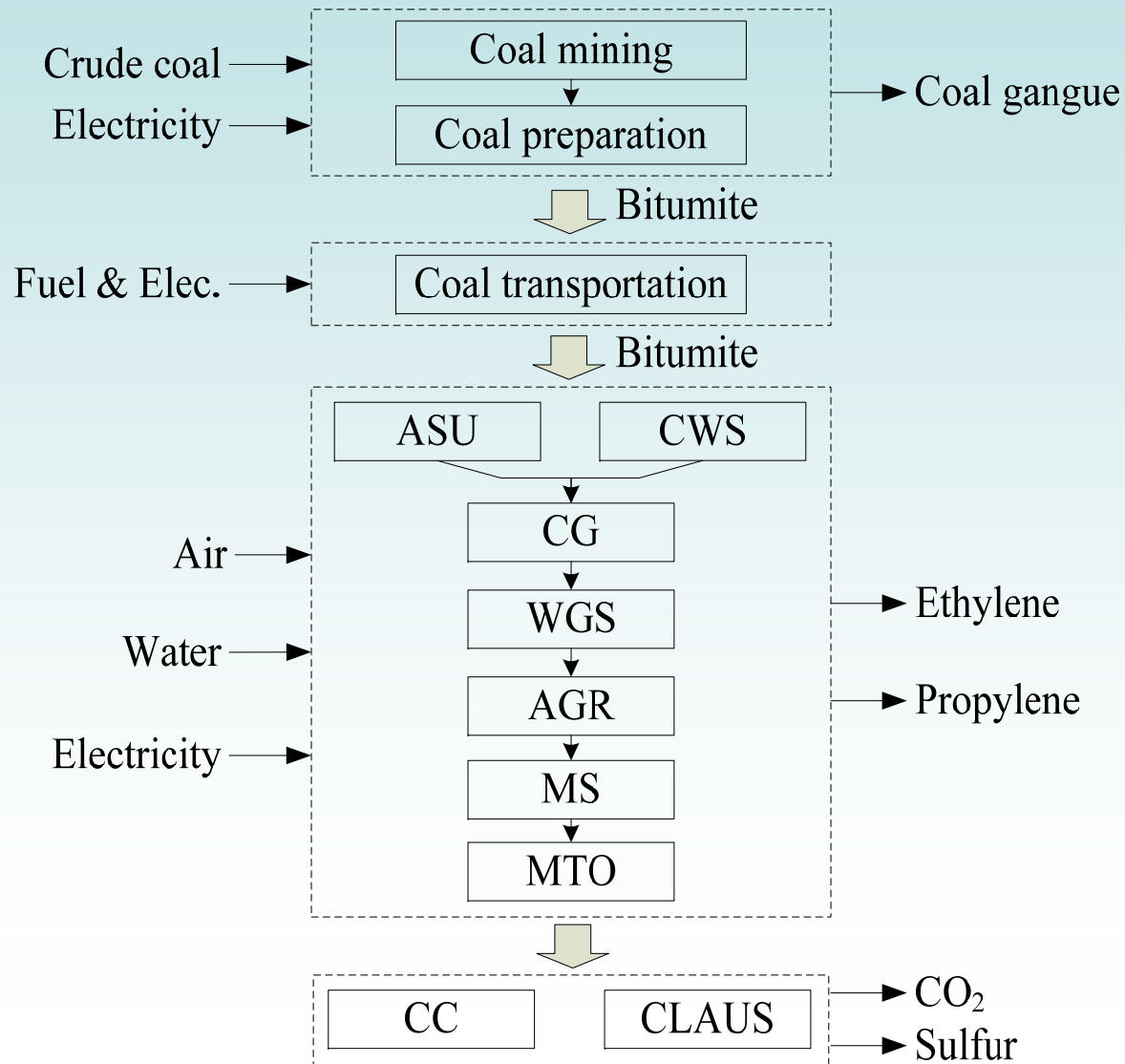
- Coal feedstock cost accounts for 39% of olefins product cost, much lower than 88% of OTO. It may, however, be offset with oil/coal price fluctuation, beside of high utility/investment cost.
- CTO efficiency could be improved with better process integration, utility, operation, equipment.
- On the other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

CTO Energy efficiency, in comparison with OTO

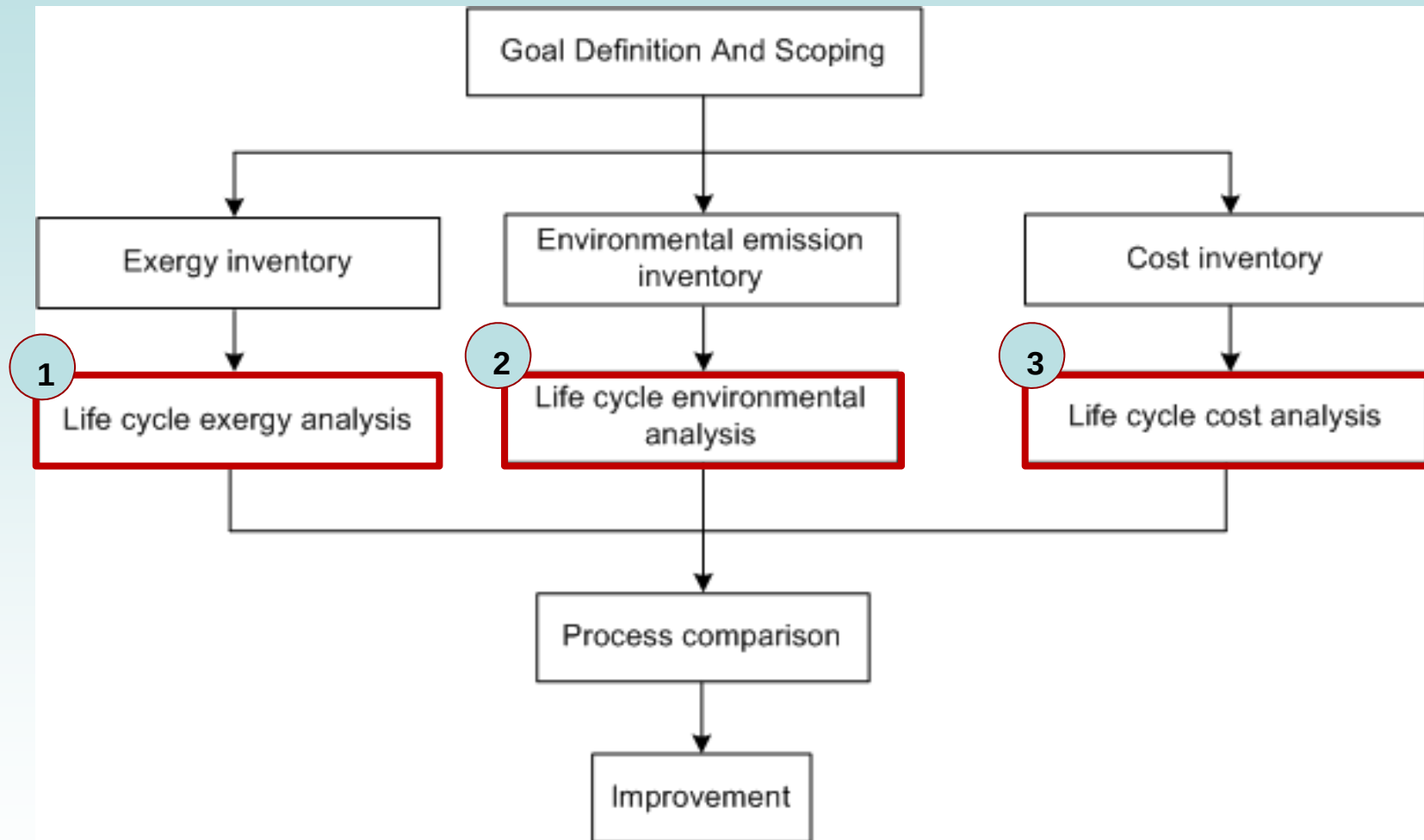
Item	OTO	CTO	LHV
Consumption			
Naphtha (t/t olefins)	1.4	N/A	45000MJ/t
Coal (t/t olefins)	N/A	4.1	28100MJ/t
Water (t/t olefins)	9	30	2.6 MJ/t
Electricity (kWh/t olefins)	74	1671.0	3.6MJ/KWh
Steam (MJ/t olefins)	1140	8753	
Total E input(GJ/t olefins)	66230	130057	—
Product/output			
Ethylene (t/t olefins)	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.

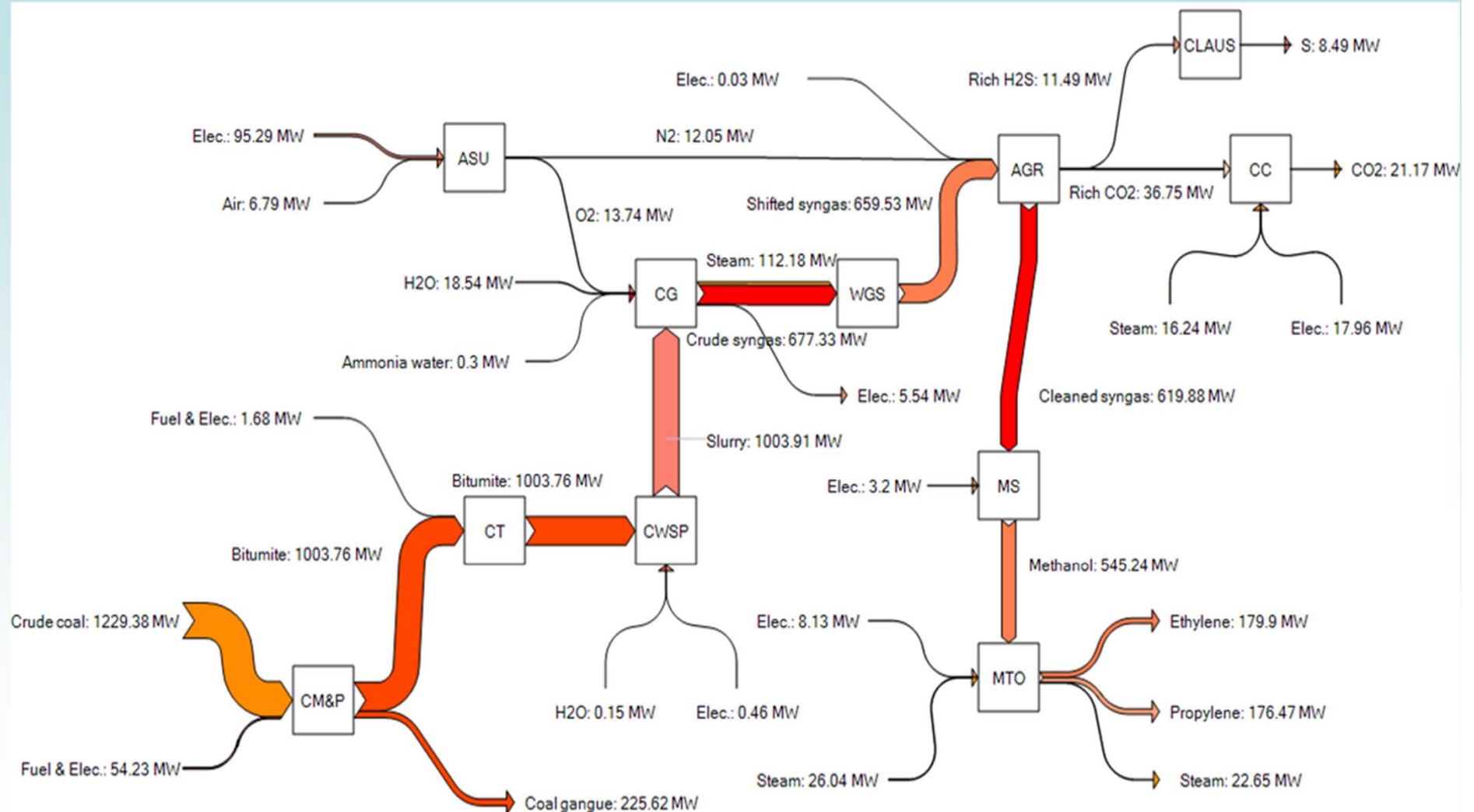
Life cycle boundary of the CTO process



LCA

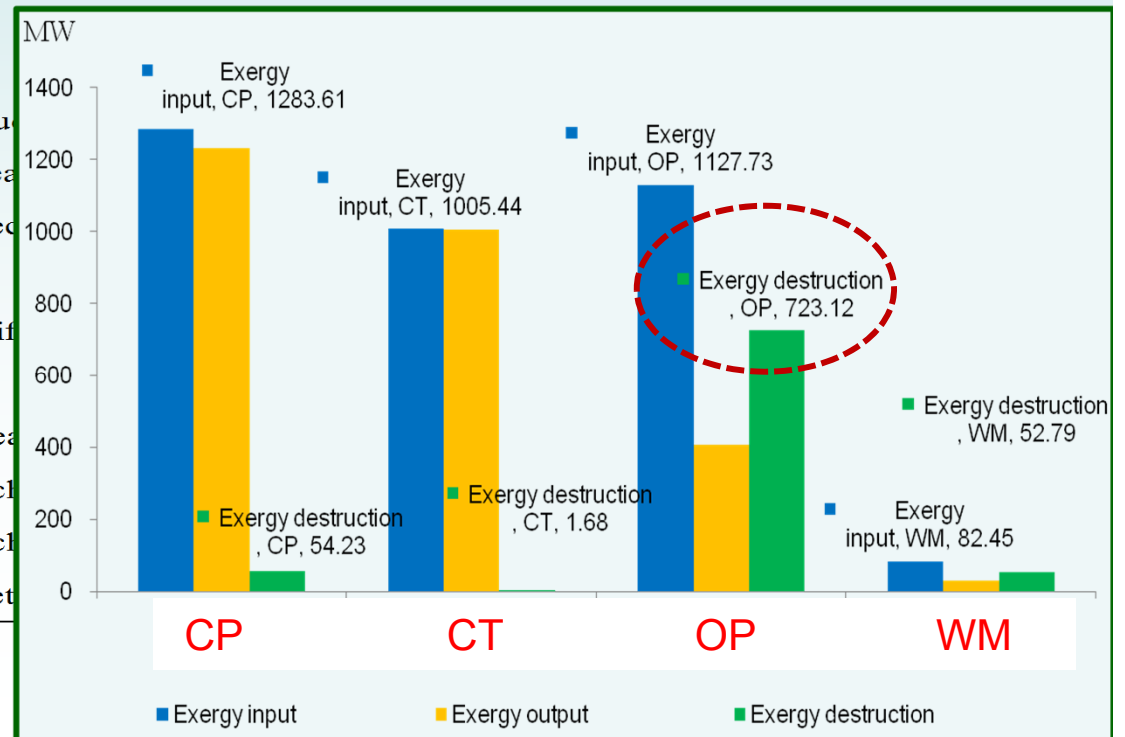


Life cycle exergy flow diagram of CTO

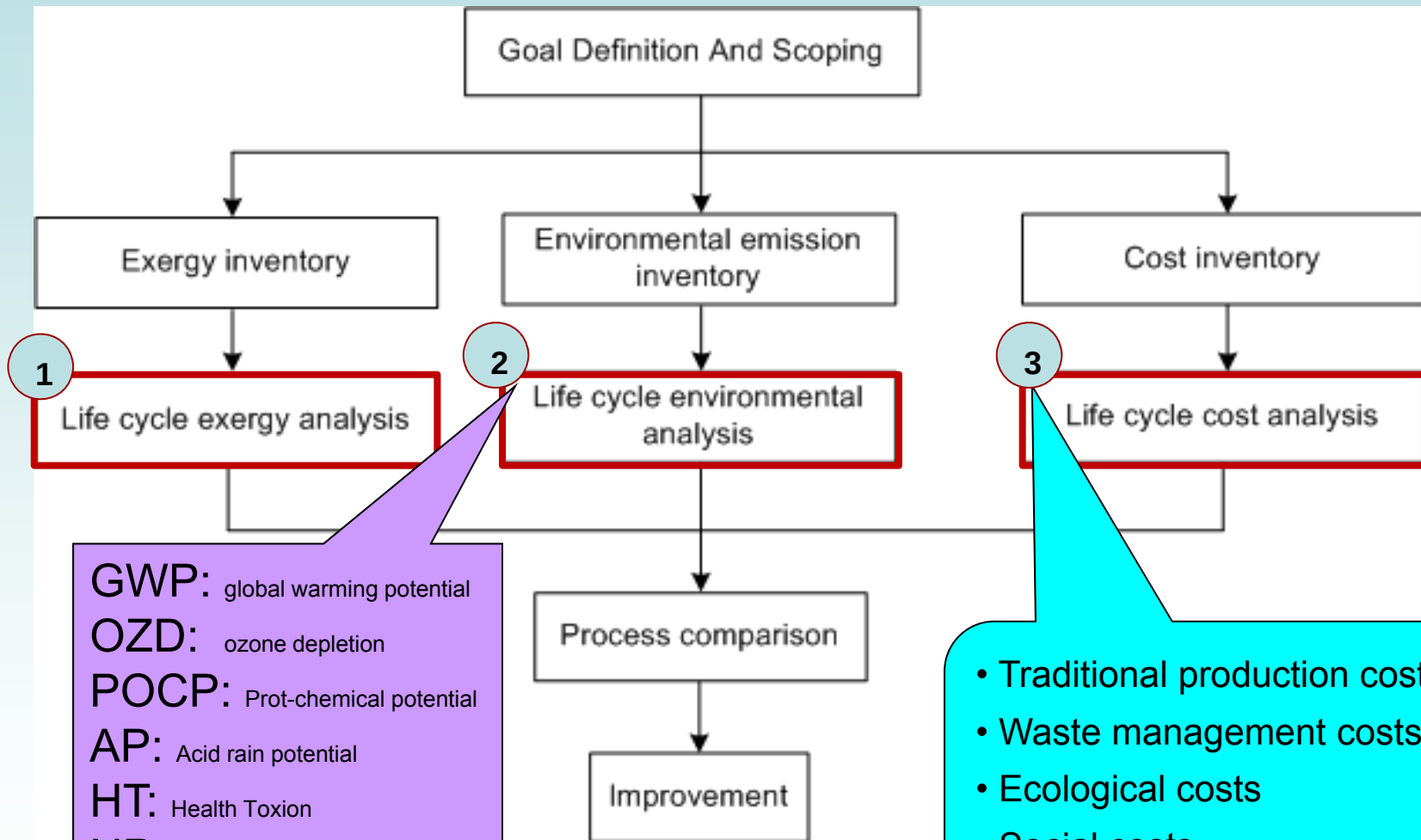


Life cycle exergy inventory of CTO

Stage	Unit	Input		Output		$Ex_{dest.}$ (MW)	η
		Item	Ex_{flow} (MW)	Item	Ex_{flow} (MW)		
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	CG	Slurry	1003.91	Crude syngas	677.33		
		O ₂	13.74	Steam	112.18		
		Cooling water	18.54	Shifted syngas	659.53		
		Ammonia water	0.30	N ₂	12.05		
				Elec.	0.03		
AGR	AGR	Cleaned syngas	619.88	Met			



LCA

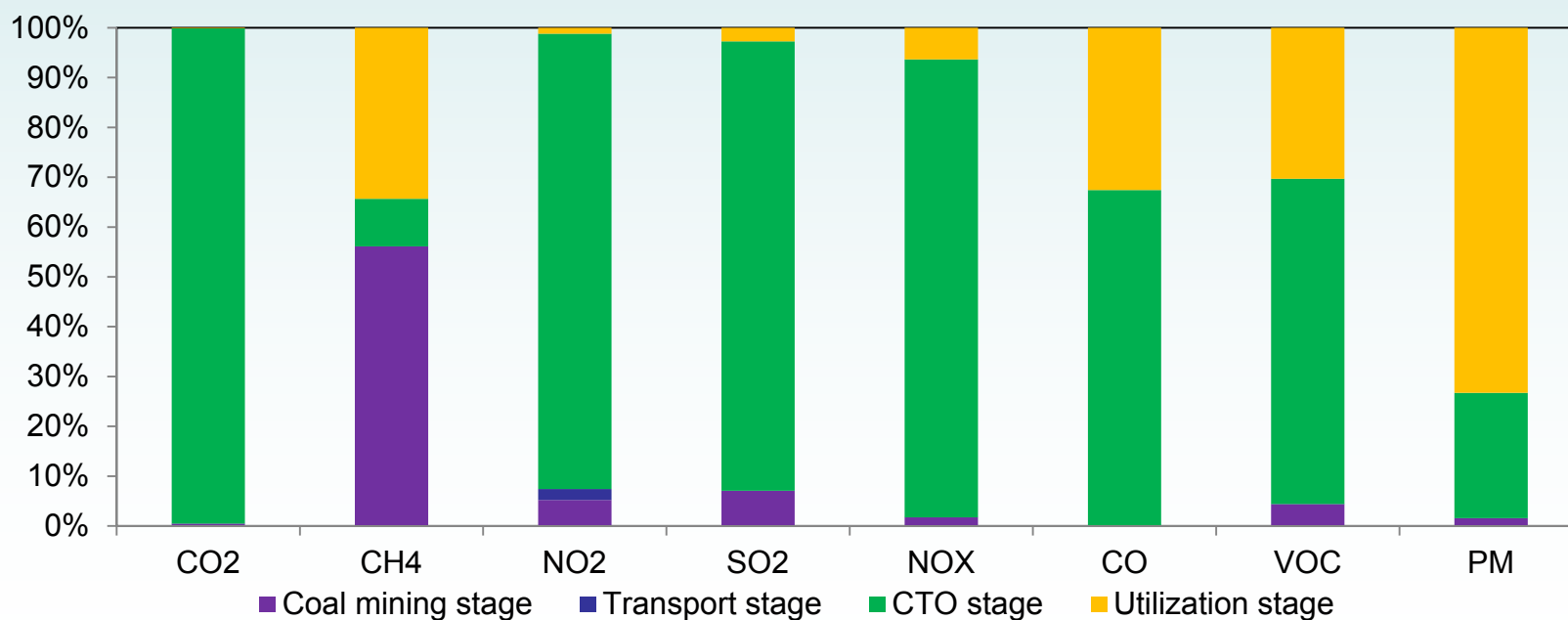


GWP: global warming potential
OZD: ozone depletion
POCP: Prot-chemical potential
AP: Acid rain potential
HT: Health Toxion
NP: Nutrition potential
ETP: Ecological Toxion potential
RDP: Resource depletion potenti

- Traditional production costs
- Waste management costs
- Ecological costs
- Social costs

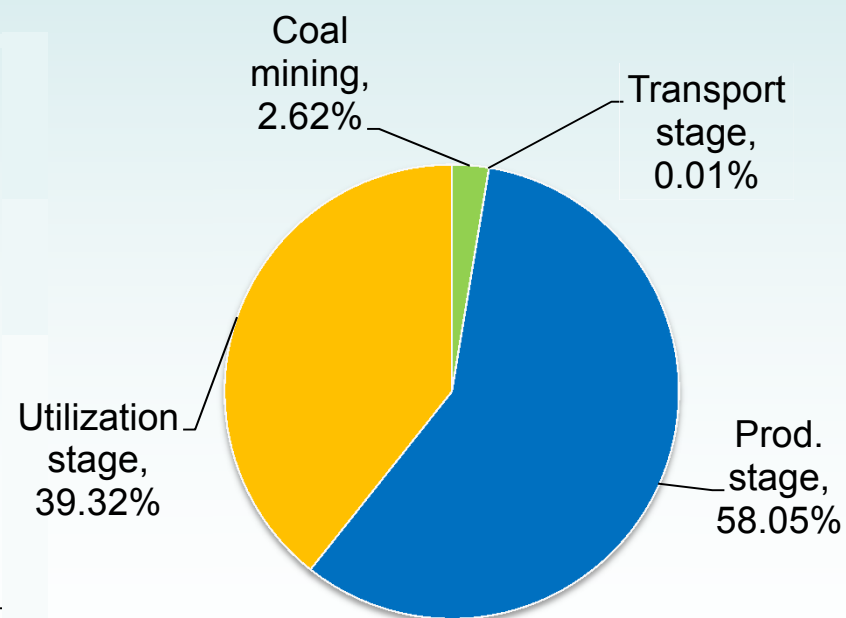
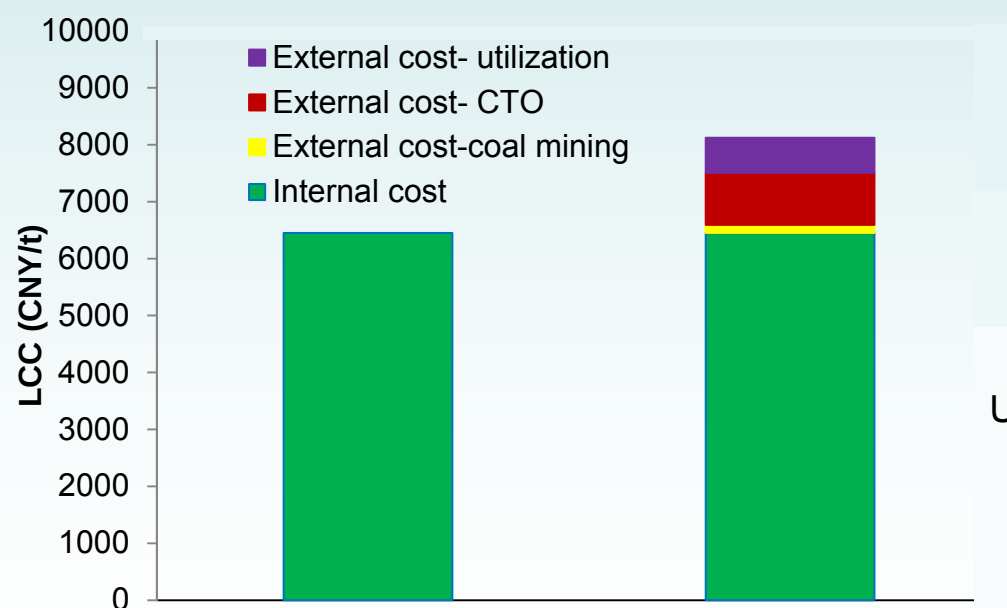
Life cycle environmental inventory of CTO

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

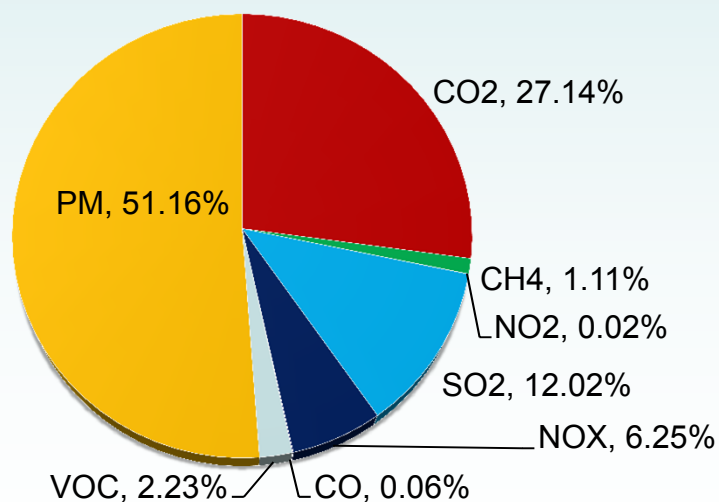
CNY/t olefins	CO ₂	CH ₄	NO ₂	SO ₂	NOX	CO	VOC	PM	Total
Coal mining stage	2.1	9.83	0.02	13.3	1.7	0.00	1.6	12.8	41
Transport stage	0.0	0.00	0.01	0.0	0.1	0.00	0.0	.01	0.1
Production stage	424.4	1.67	0.34	170.5	90.3	0.66	22.9	202.4	913
Utilization stage	0.5	6.01	0.00	5.2	6.2	0.32	10.6	589.7	618
Total	427.0	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

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

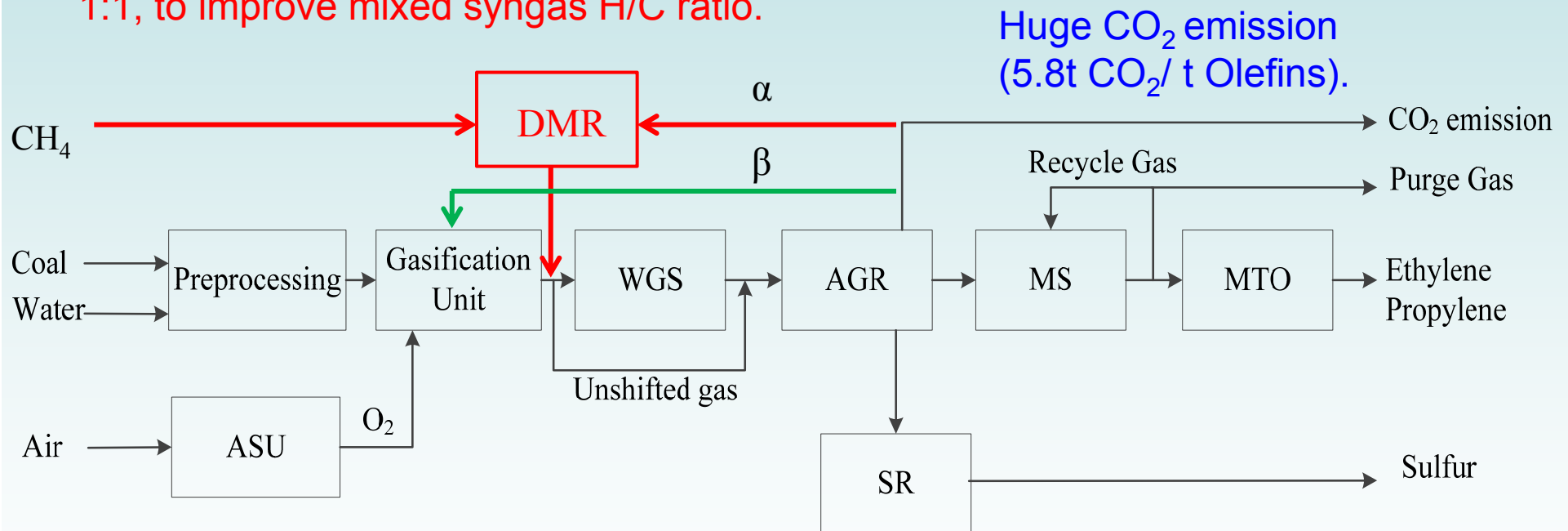


In LCC of CTO,
PM treatment is the largest
external cost.
CCS cost is the second.

How to improve the sustainability of CTO? **Process innovation.**

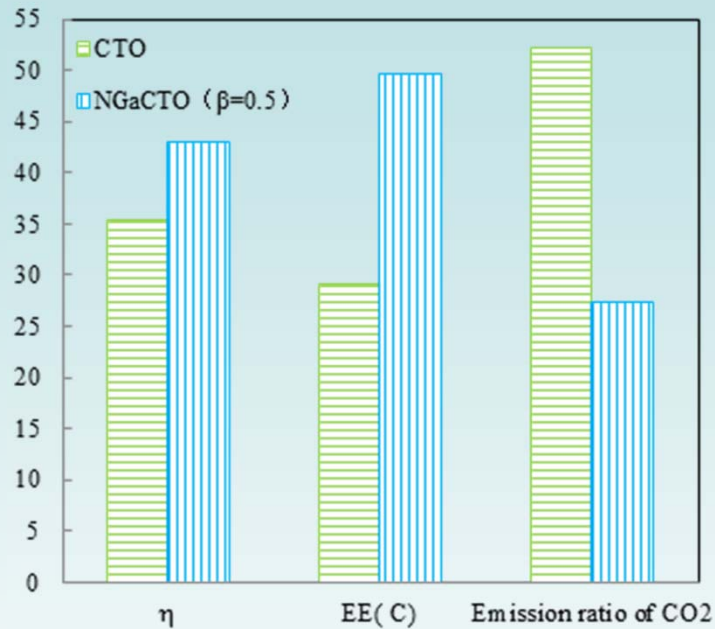
1. Natural Gas and Coal to Olefin (NG-CTO)

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

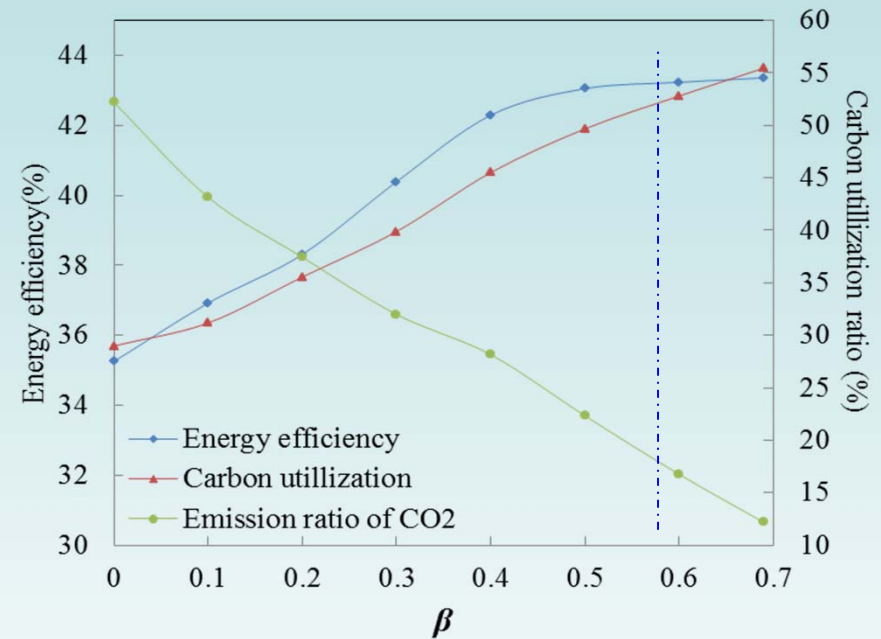


(2) A part of pressurized hot CO₂ is recycled to the gasifier, as a gasification agent, to increase syngas production.

Mass and Energy Efficiency Improvement



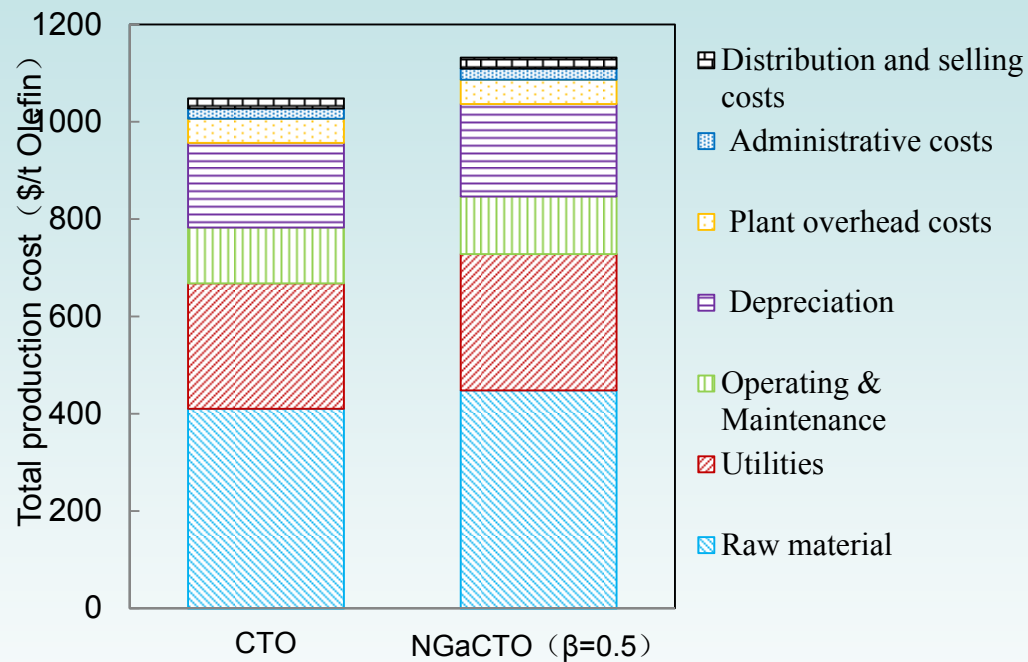
NG-CTO efficiency for material, energy, and CO₂ emission.



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

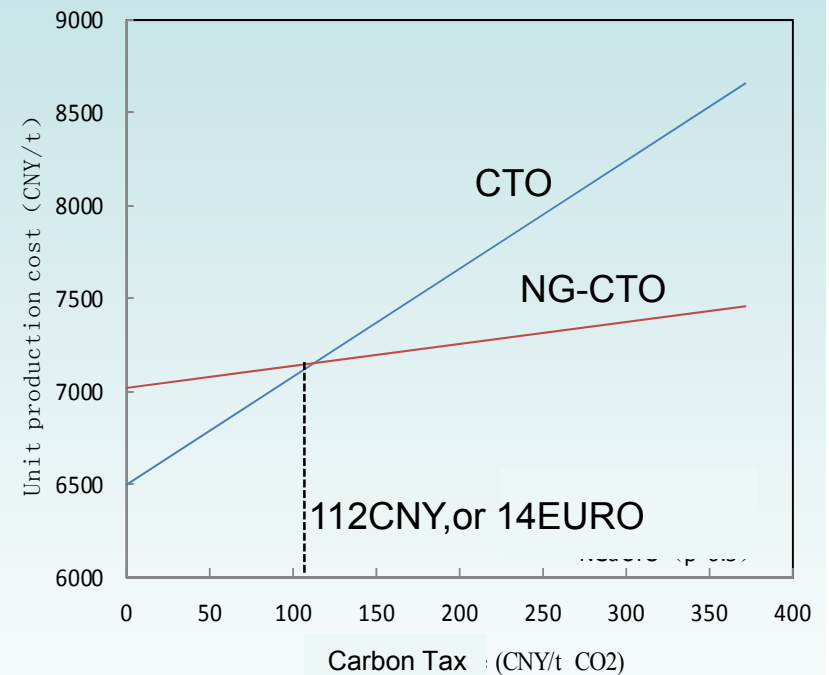
Methane dry reforming reaction is strongly endothermic. It is important to select CO₂ recycle rate for a rational energy integration.

Economic performance of CTO



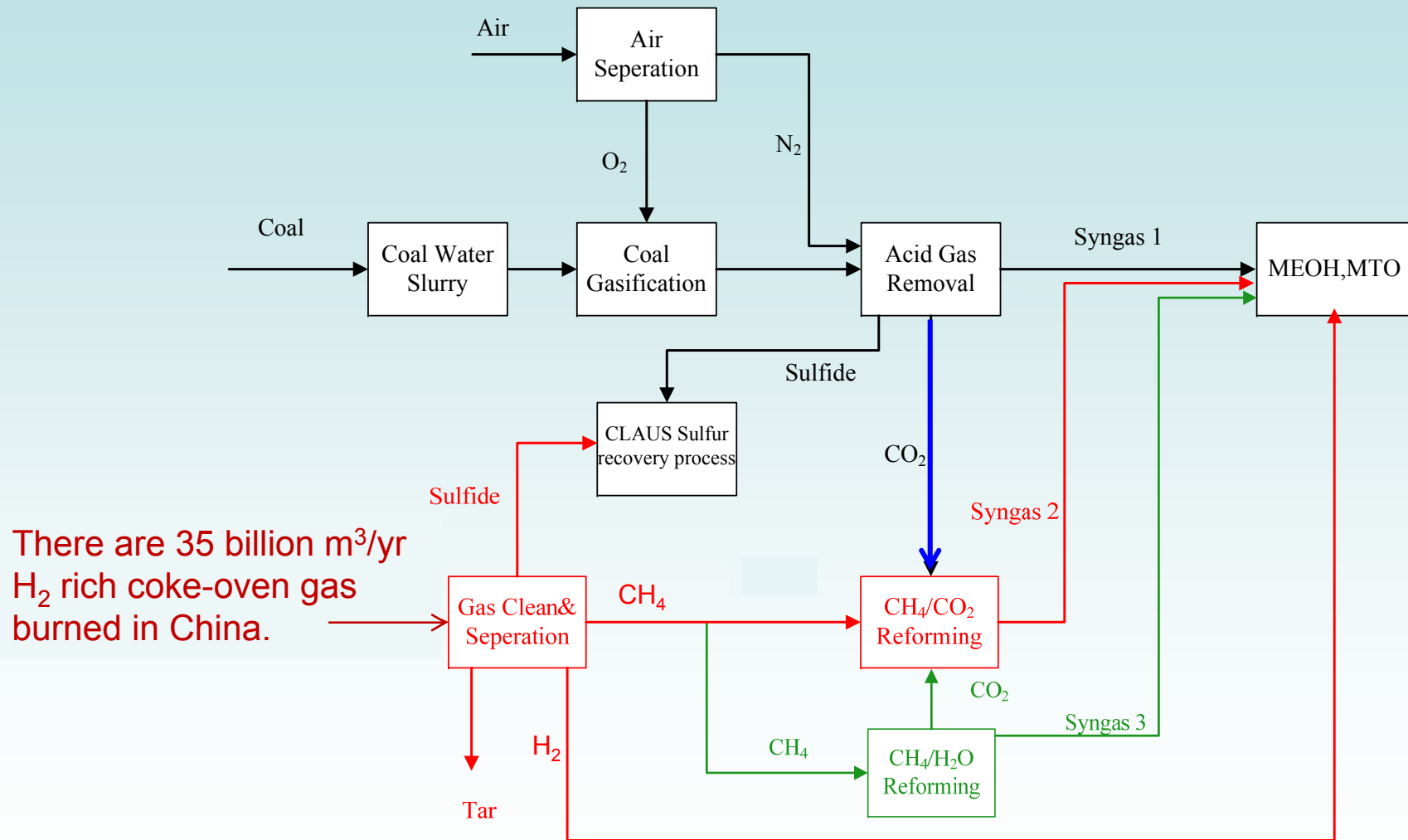
NG-CTO production cost 7020 CNY/t, slightly higher than CTO 6500 CNY/t.

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)

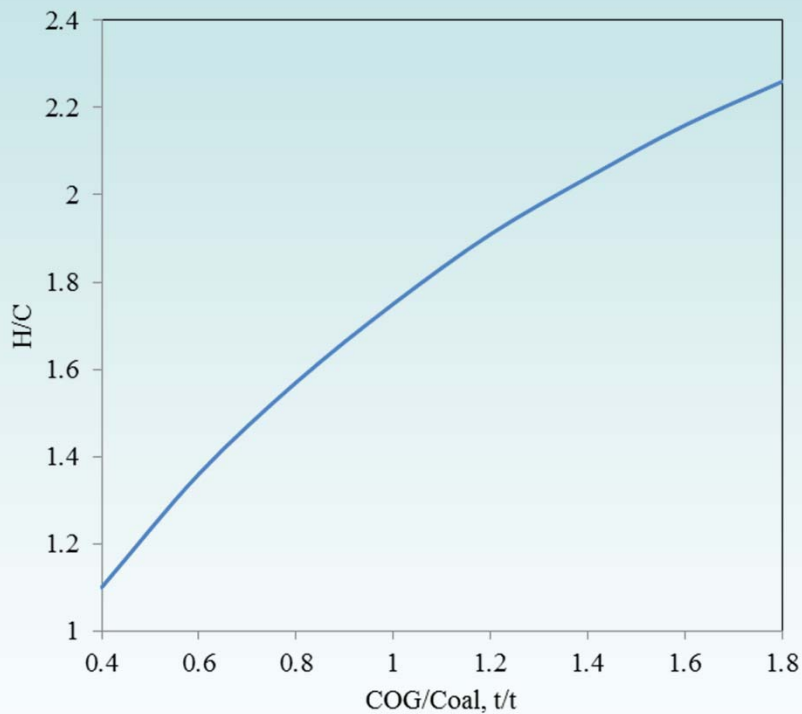


There are 35 billion m³/yr H₂ rich coke-oven gas burned in China.

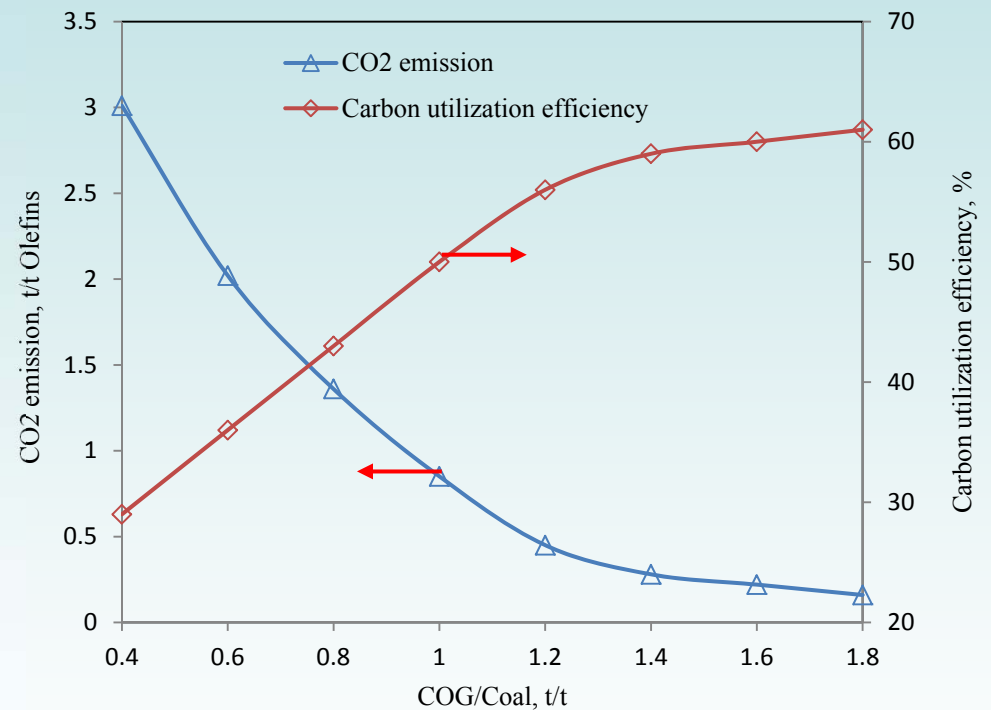
- H₂-rich coke-oven gas fed, CH₄/CO₂ reforming raise H/C ratio to 1.

CH₄/H₂O reforming raise H/C further to 2

Material and Environmental performance of GCTO



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

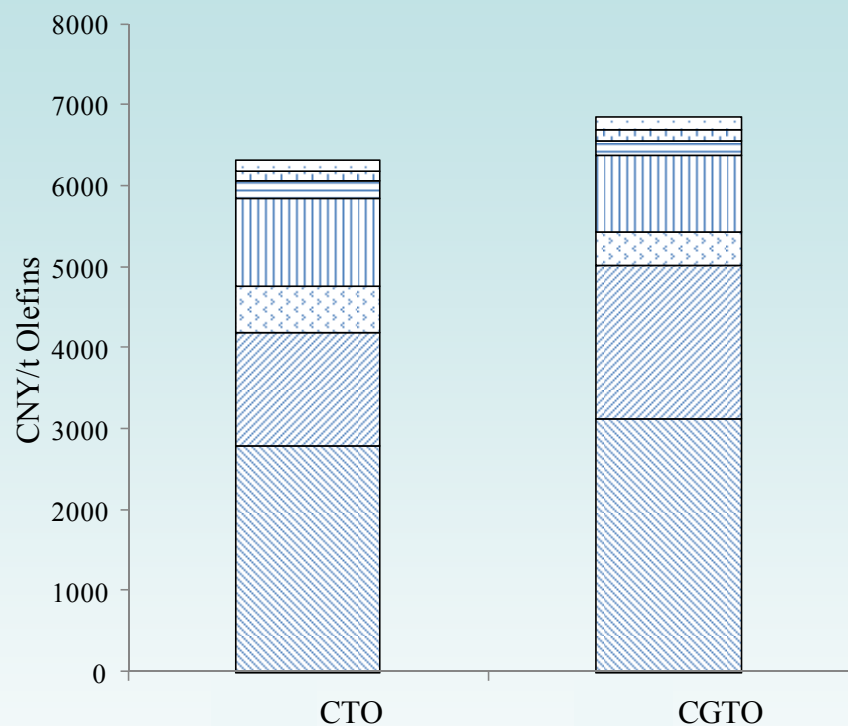


As introduce of coke oven gas, C utilization efficiency rises, while CO₂ emission decreases.

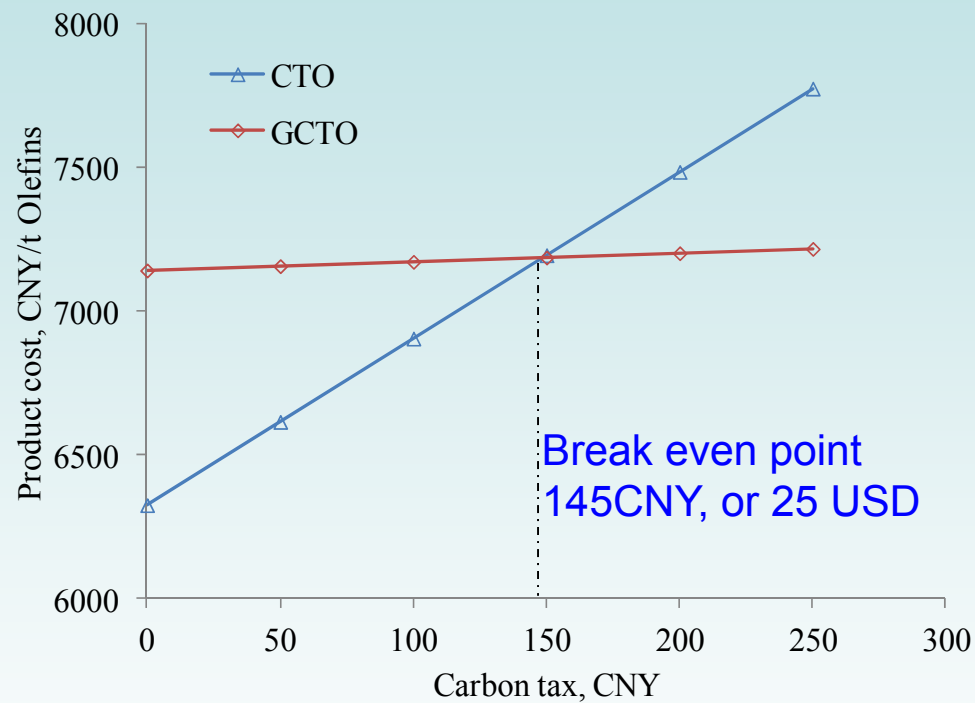
Energy efficiency and CO₂ release of GCTO

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

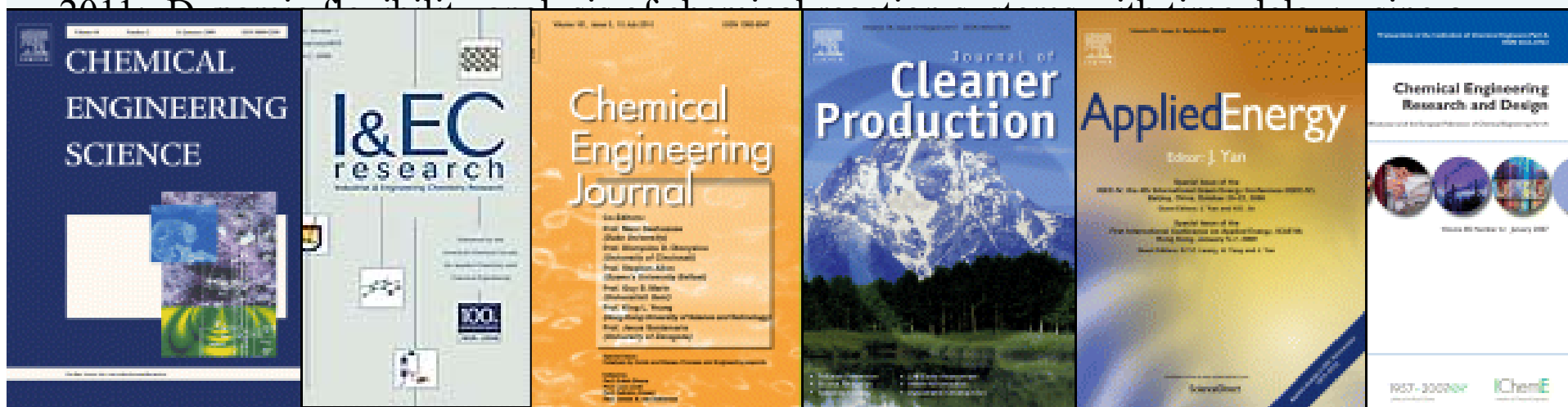
* Feedstock: 620 CNY/t coal, 0.8 CNY/m³ coke-oven gas.

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

- 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.



Acknowledgements

- National Science Foundation of China (21136003);
- China Major Fundamental Research Project (973).
- My colleagues and PhD students at South China University of Tech.



Questions and comments please.

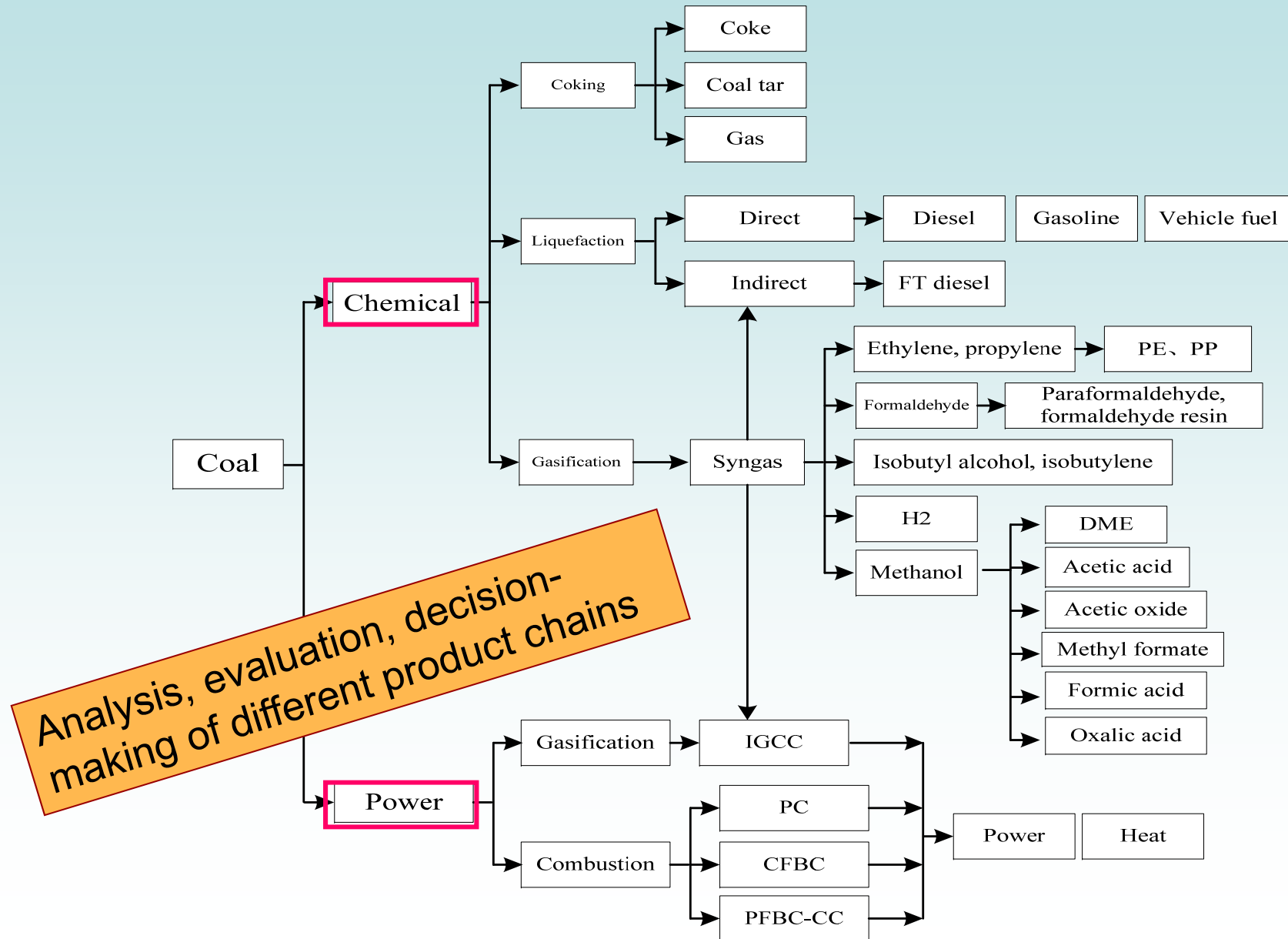
ceyuqian@scut.edu.cn



Outline

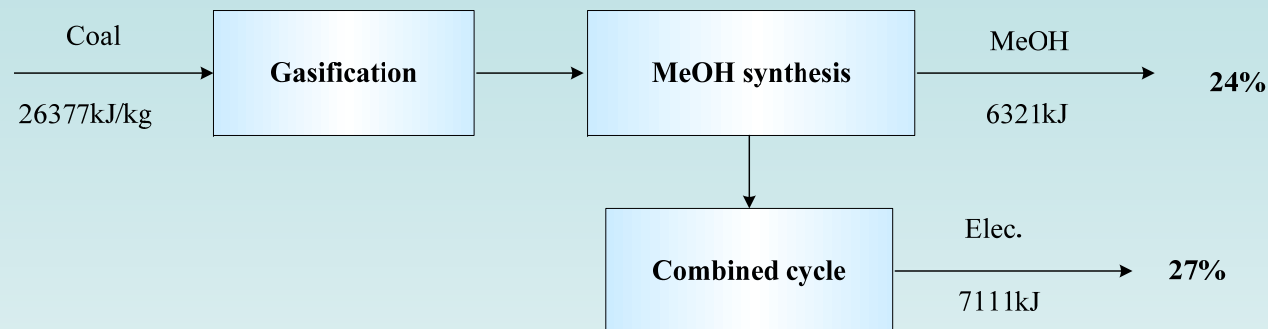
- Background
- Objectives and approaches of sustainability analysis
- Energy efficiency analysis and process integration
- Sustainability analysis
 - Industrial Case: coal to olefins
- Concluding remarks

Coal-based Energy and Chemical Product Chains



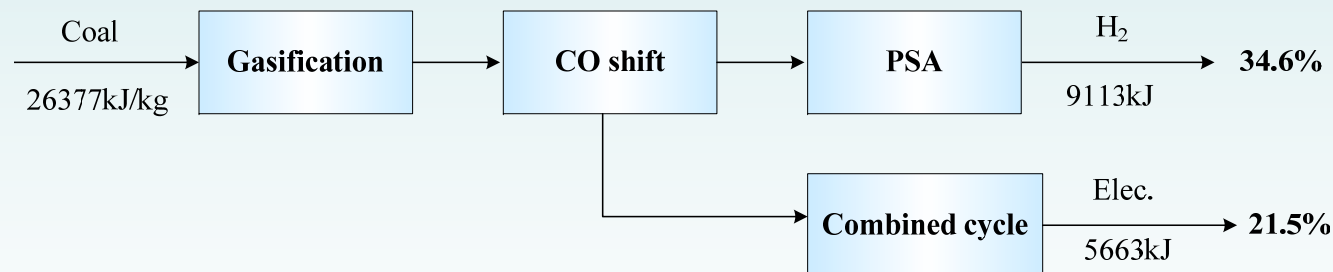
Alternative Co-production processes

Methanol-Power Co-production



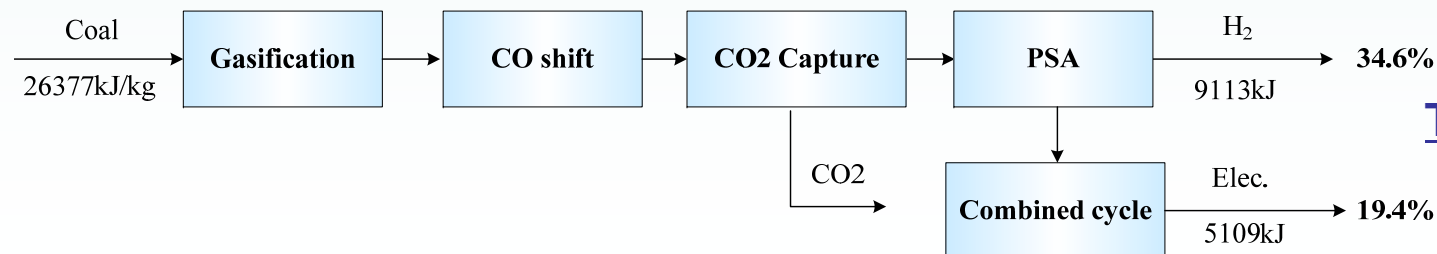
Total: 51%

Hydrogen-Power Co-generation



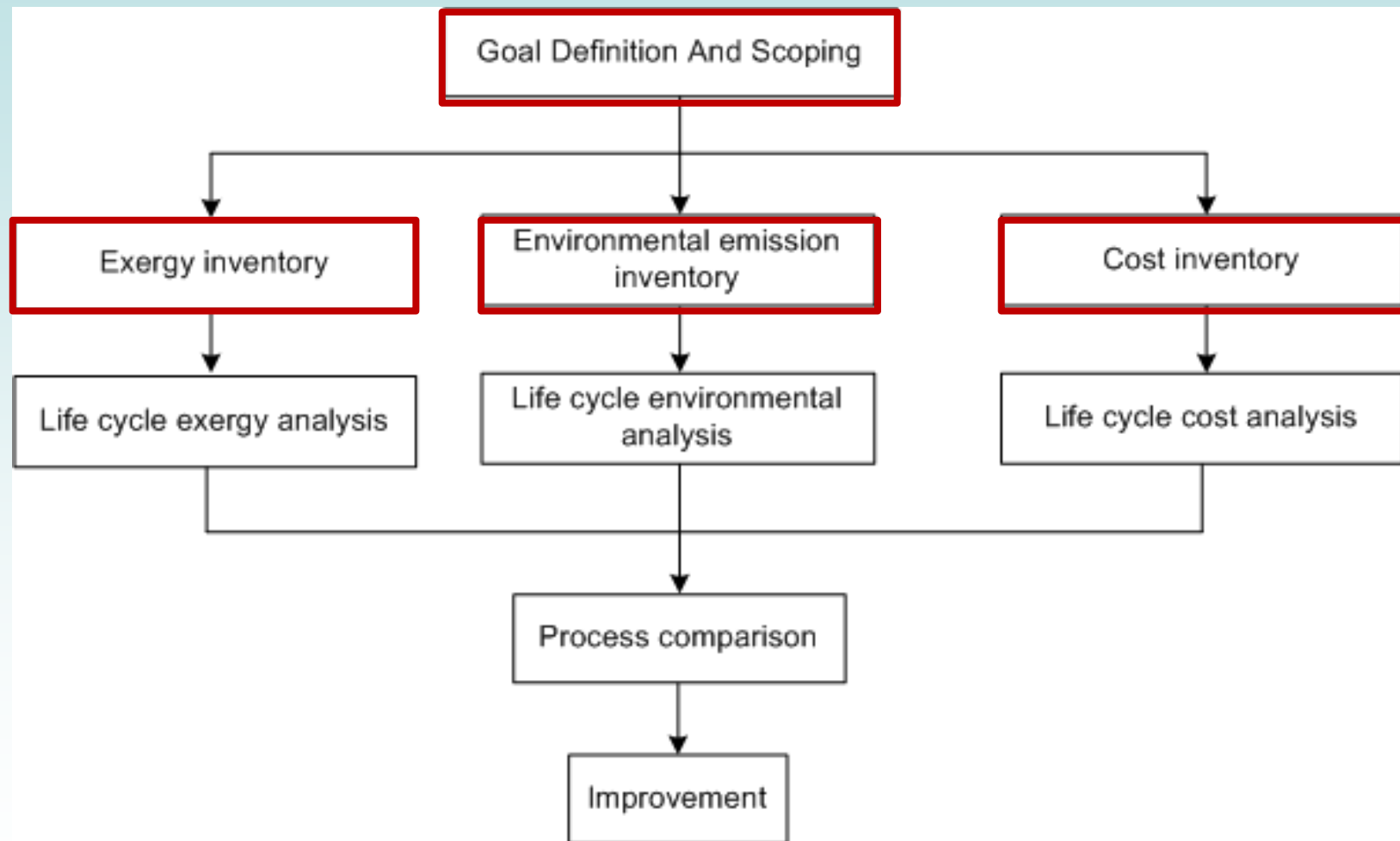
Total: 56%

With CO₂ Capture

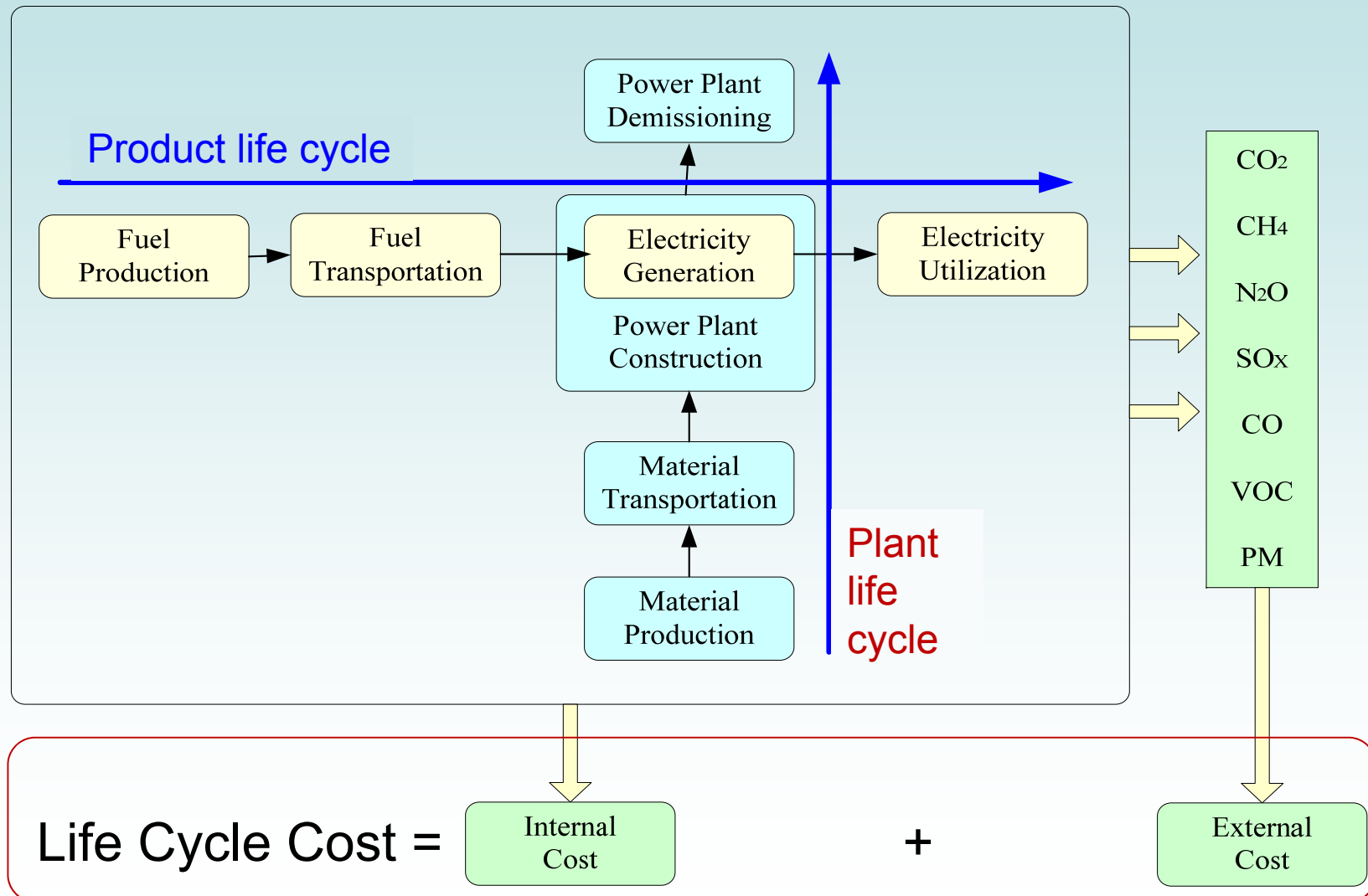


Total: 54%

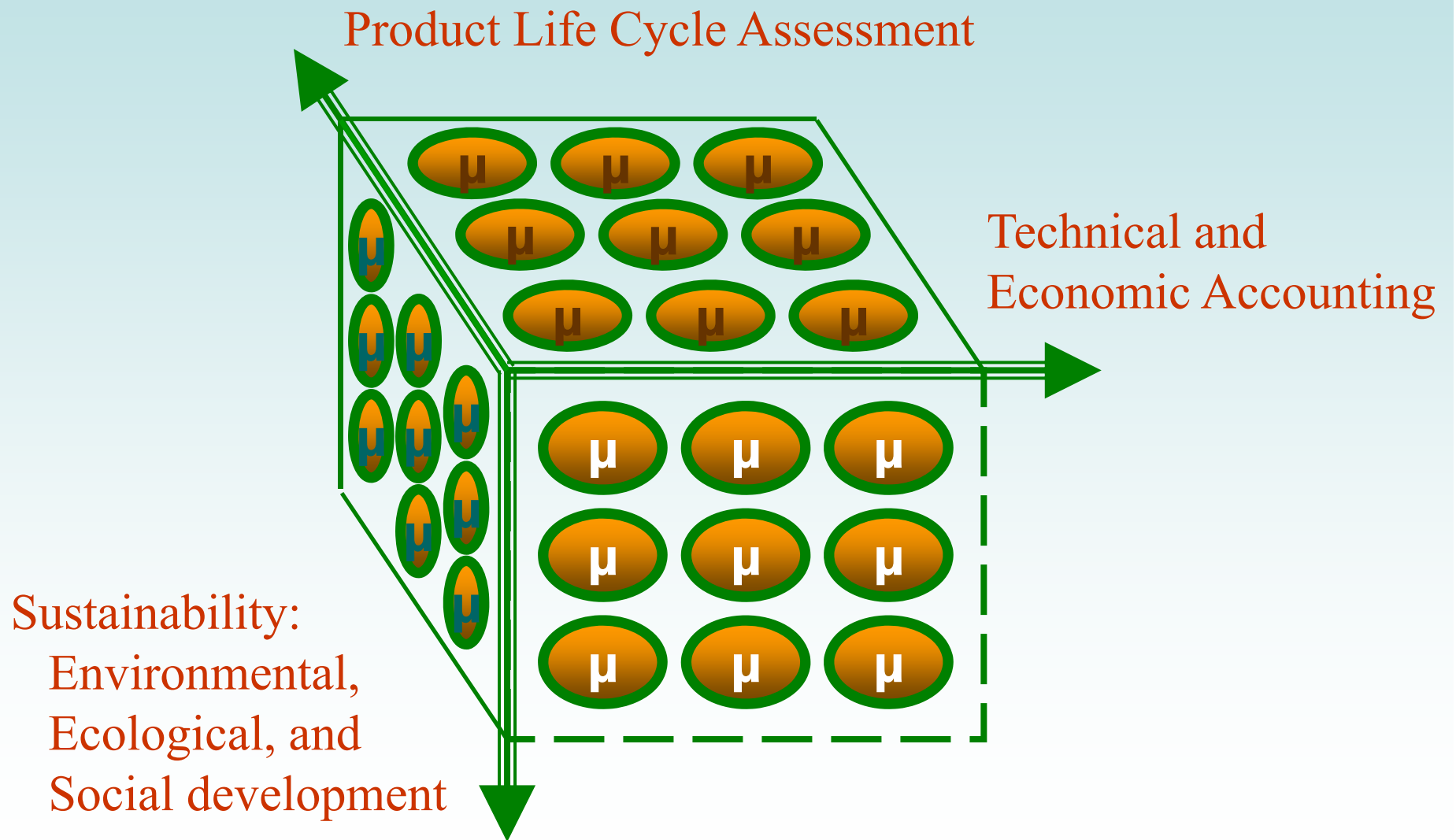
LCA Approach



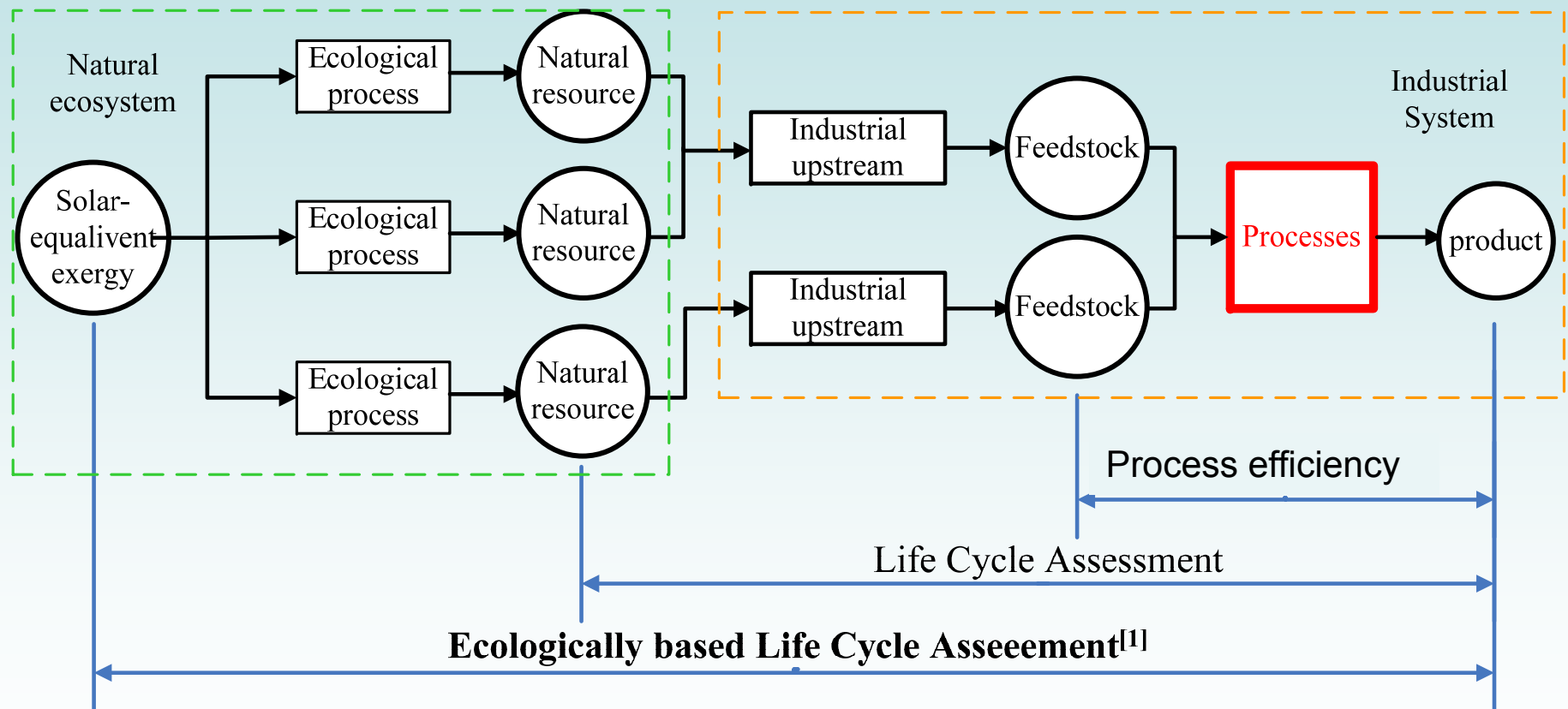
Life Cycle Boundary and Scope



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. Sustainable exploitation

$$\alpha = a^{aver} \cdot a^{min}$$

2. Economic effectiveness

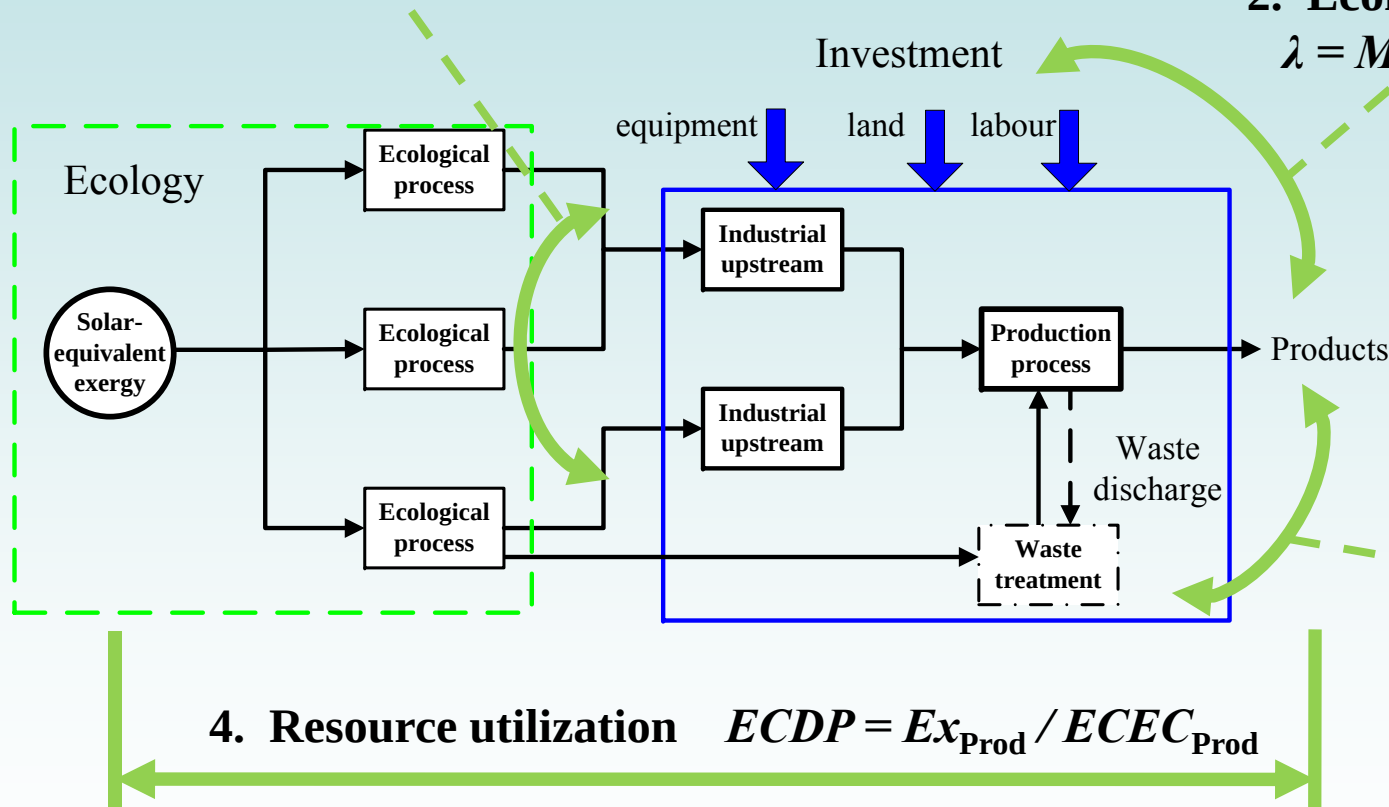
$$\lambda = \text{Money}_{\text{Prod}} / \text{Money}_{\text{Inv}}$$

3. Environmental compatibility

$$\psi = \text{EMR} / \text{IVP}$$

4. Resource utilization

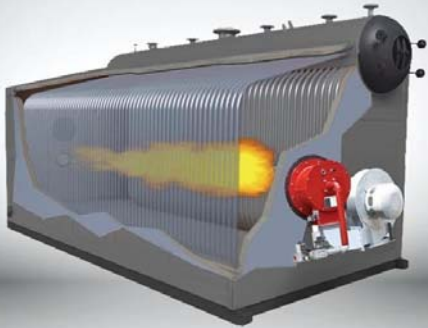
$$\text{ECDP} = \text{Ex}_{\text{Prod}} / \text{ECEC}_{\text{Prod}}$$



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. $\psi = \text{EMR} / (\text{ECEC}_{\text{Prod}} / \text{Money}_{\text{Prod}})$

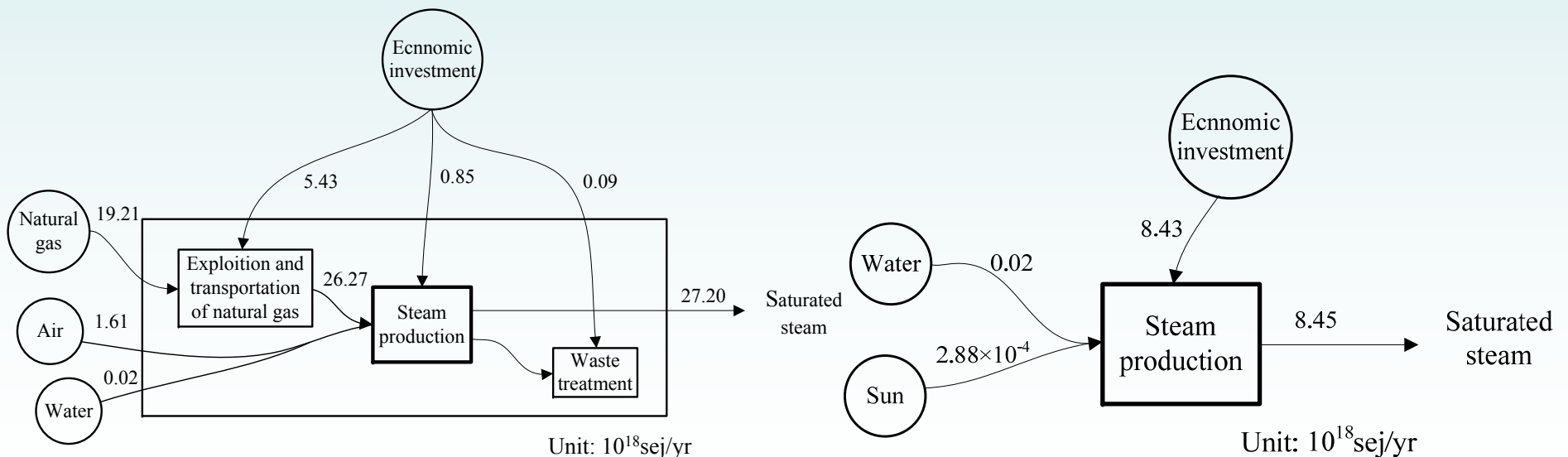
Eco-LCA of Steam Production



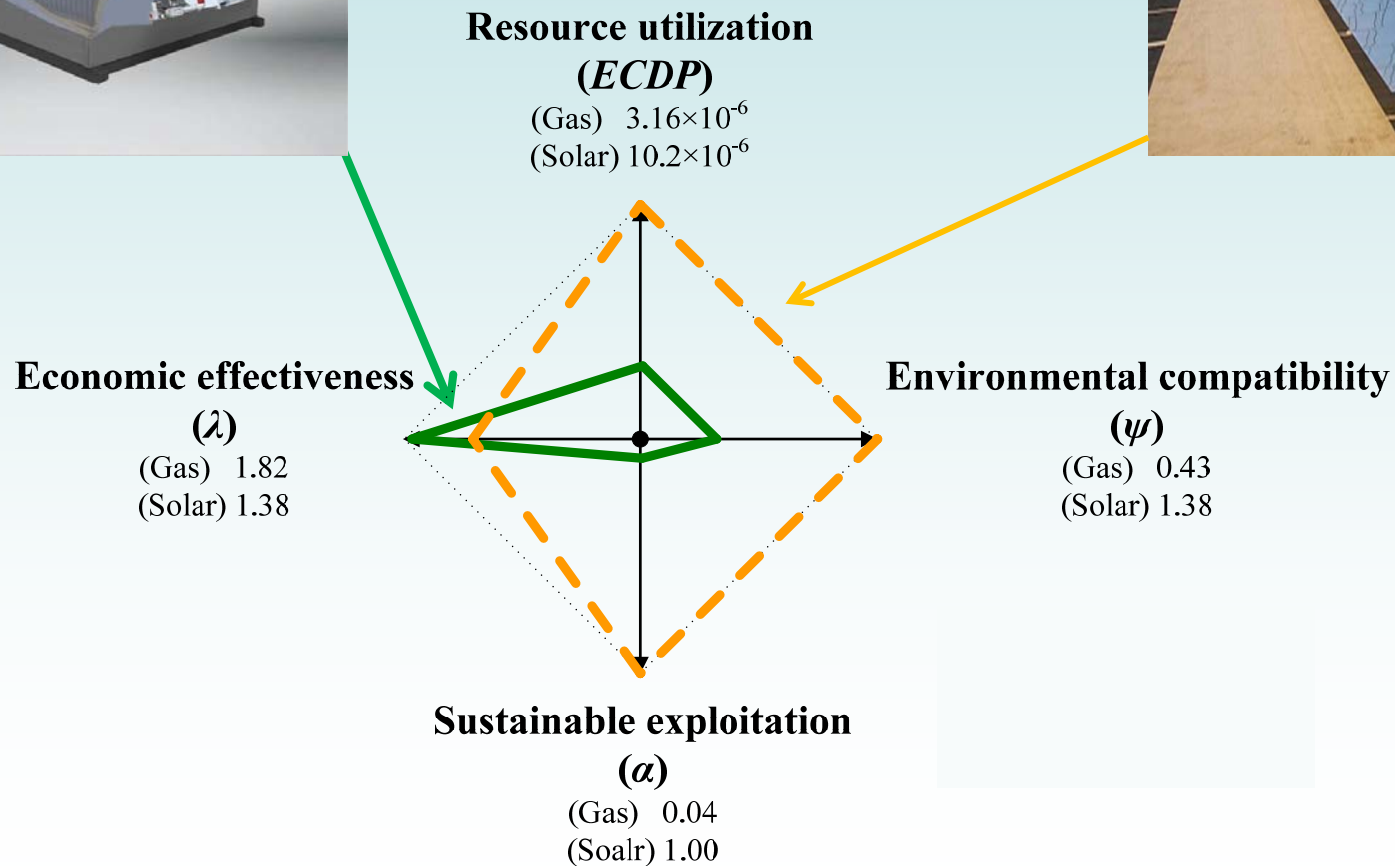
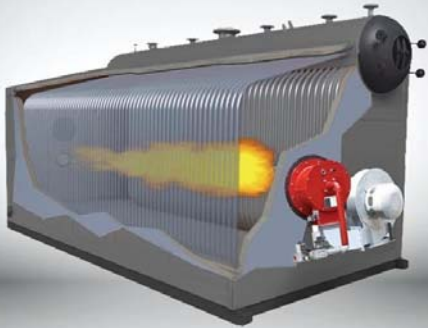
the **functional unit** produces
80 kt/yr of 3.5MPa saturated
steam.



Gas boiler v.s. Solar boiler



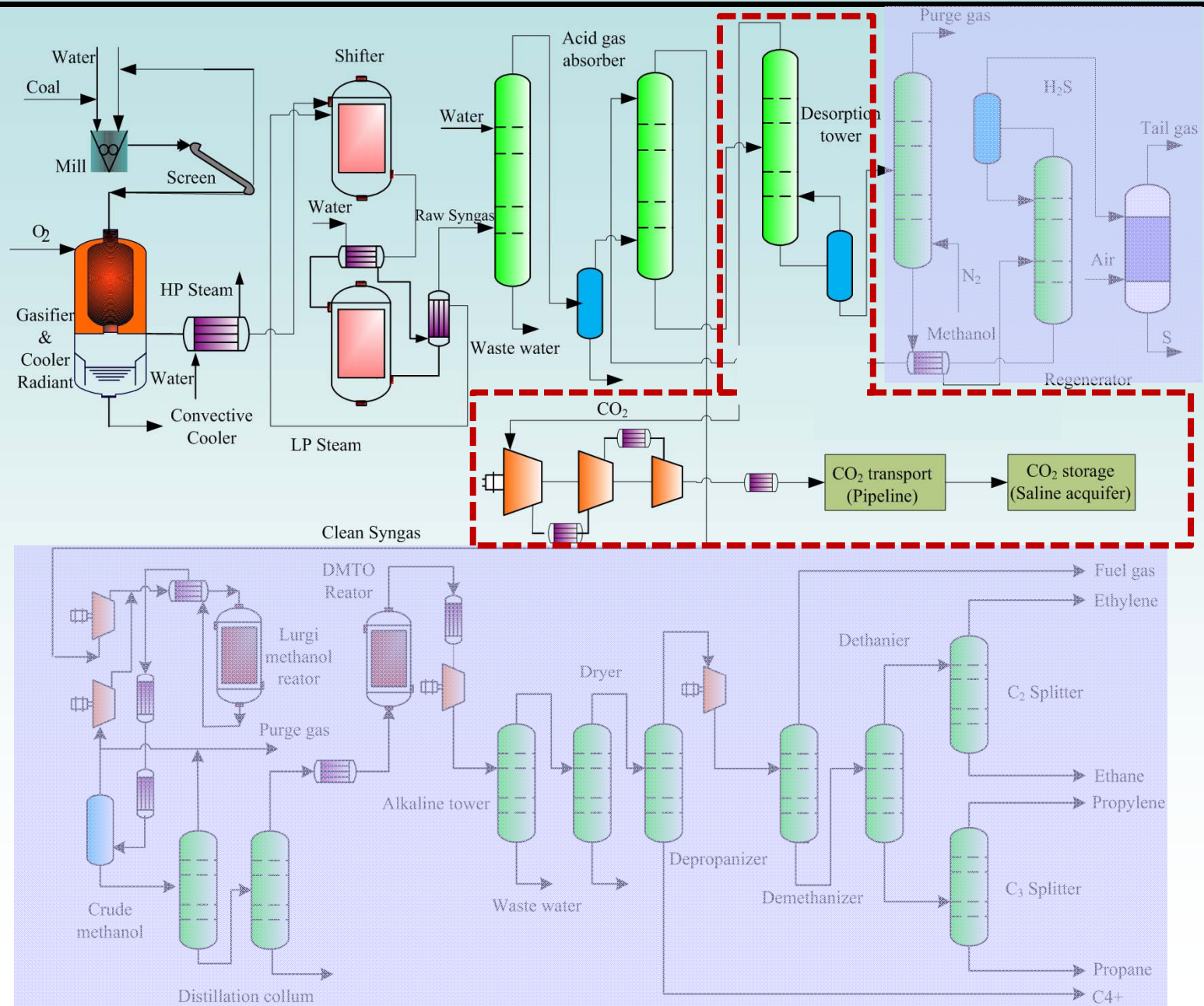
Eco-LCA of Steam Production



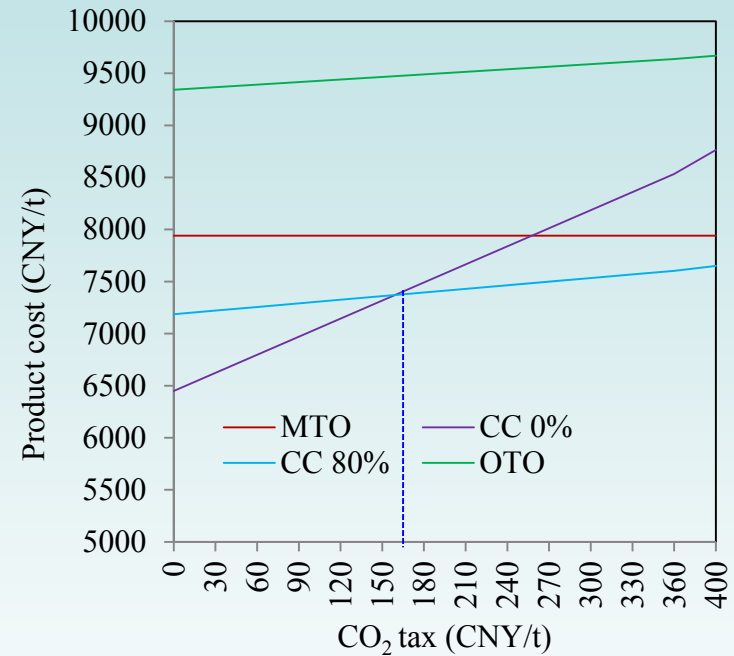
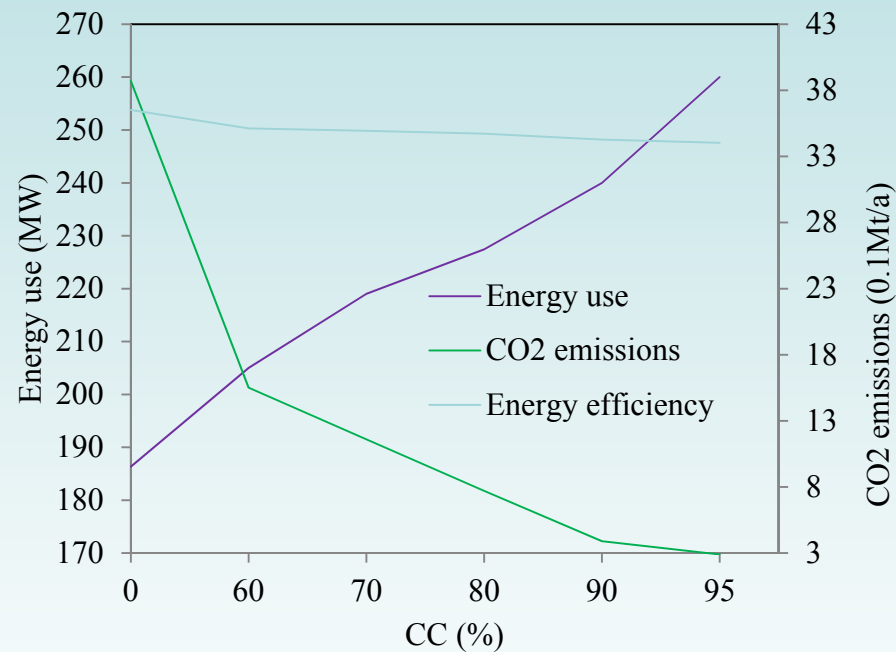
Sustainability analysis on resource, energy, environment, and economy

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

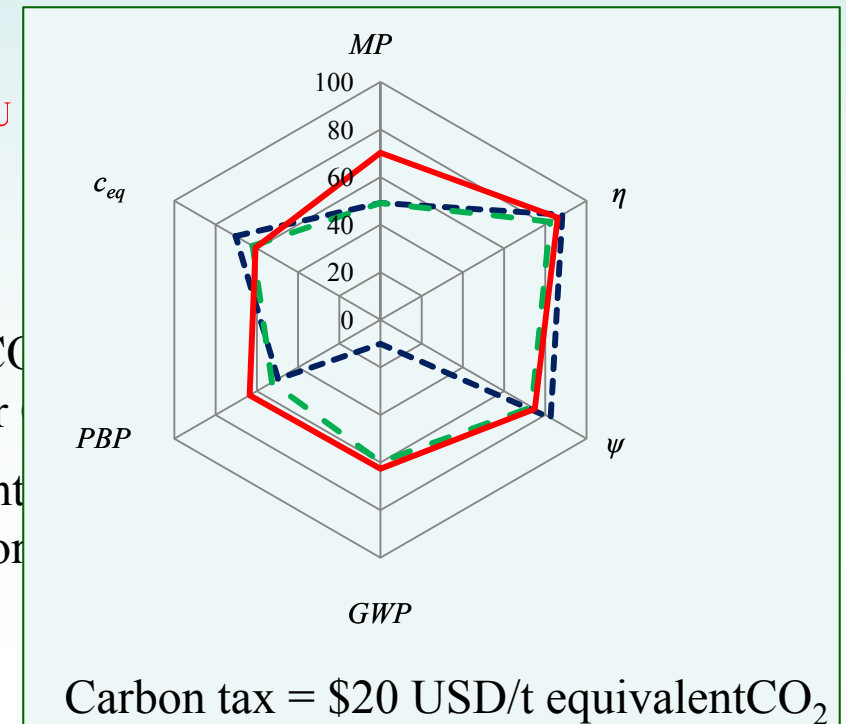
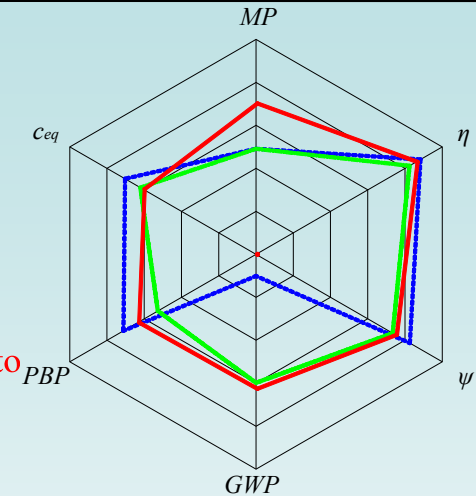
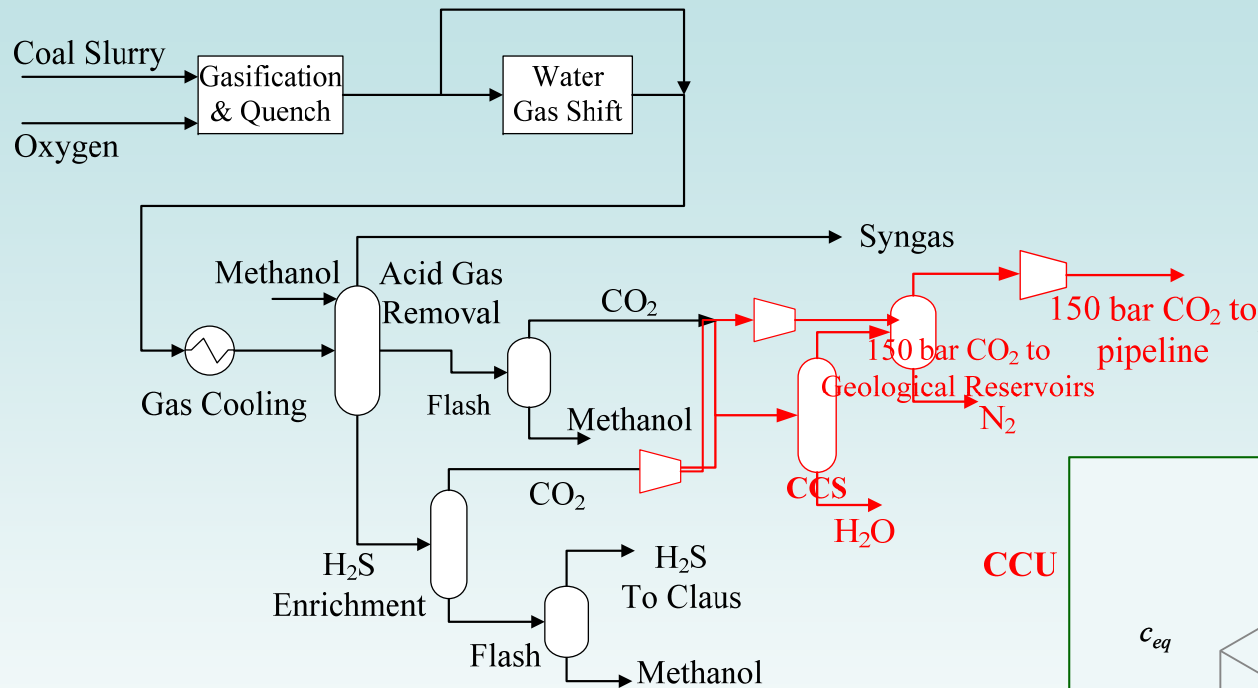


Energy consumption, economic and environmental performance with CC rate



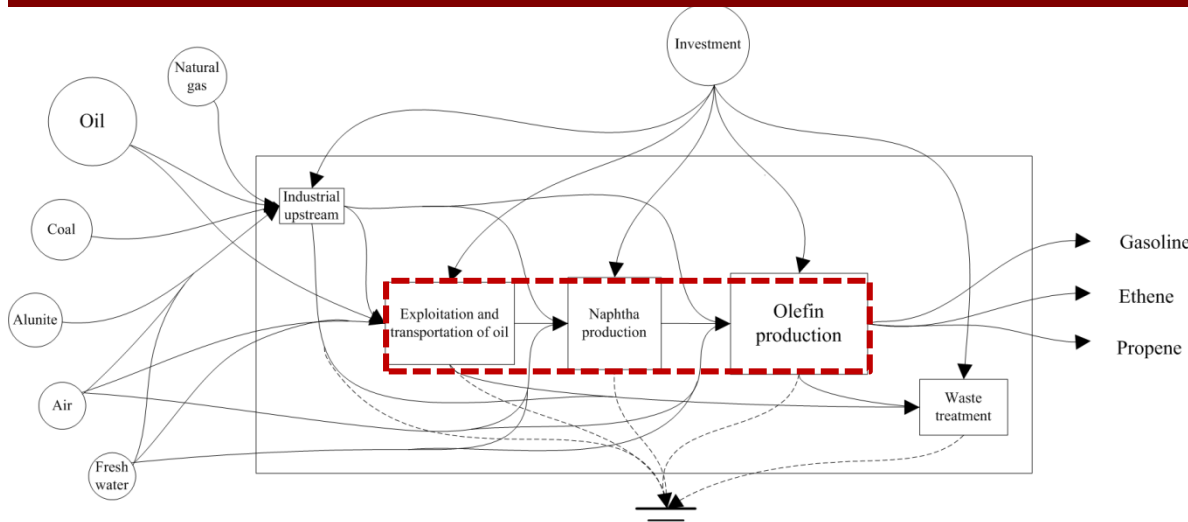
In considering carbon tax (at 20Euro), CTO with 80% CCR is economically attractive than OTO, MTO, or CTO without CC.

Coal gasification with CCS or CCU?

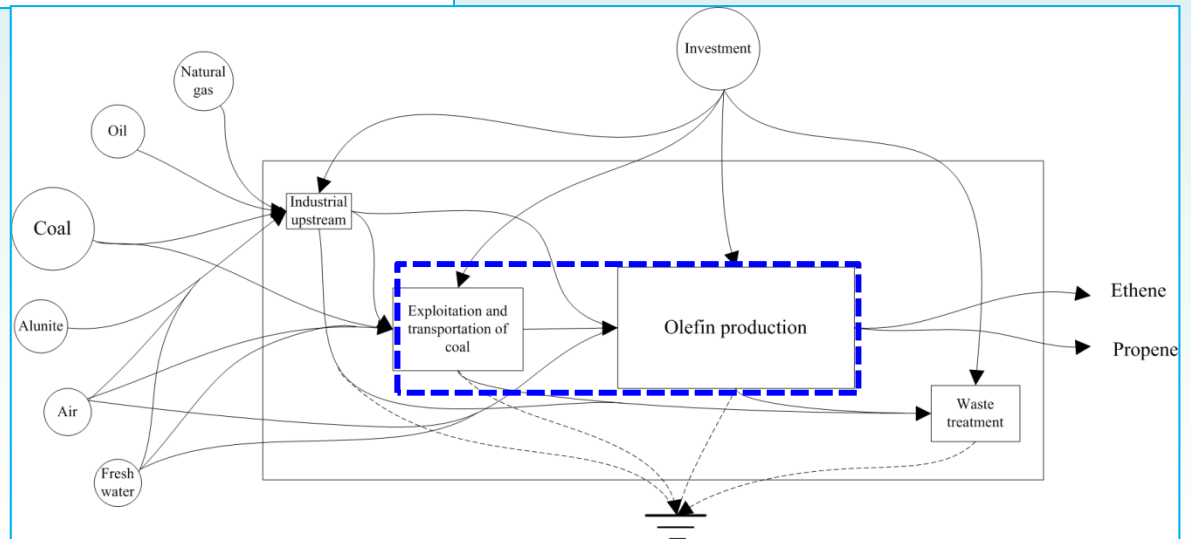


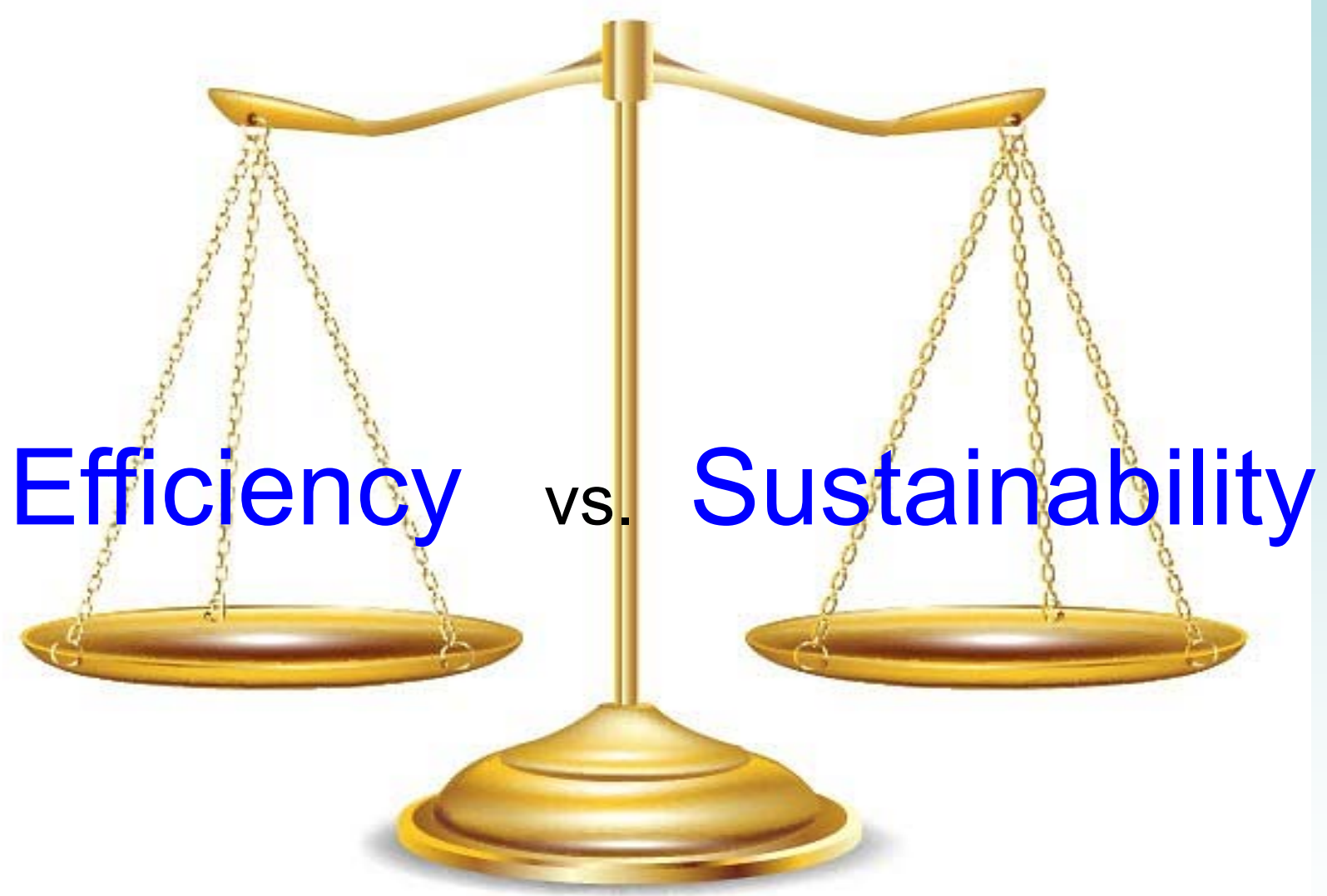
- As shown in the chart, although GWP reduced, CO₂ (90%) for oil extraction/geo-storage are of higher
- On the other side, CO₂ enriched to higher concentration is better for resource utilization and economic performance
- Quantitative sustainability analysis helps rational decision making on CCUS approaches.

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.

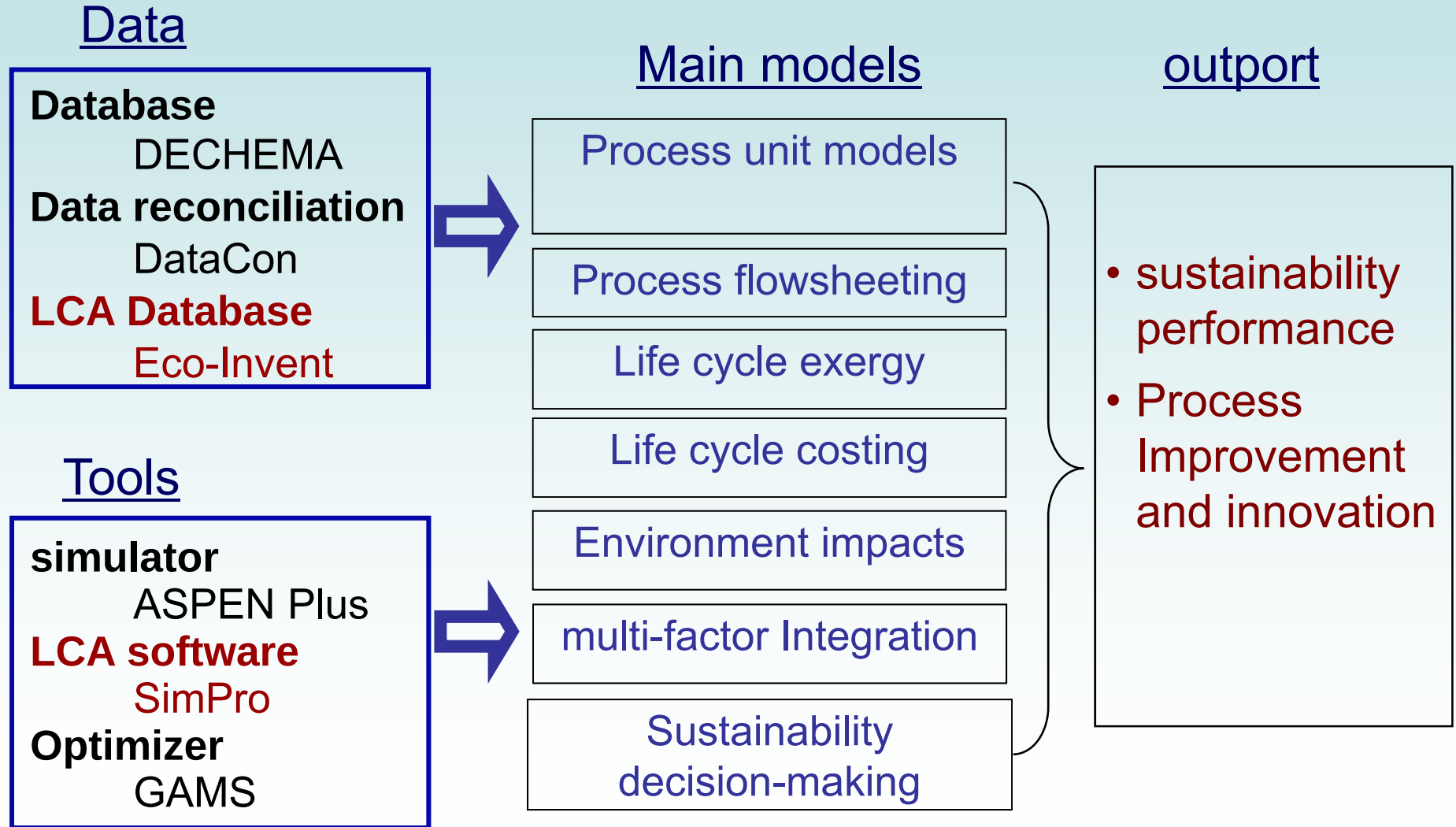




Efficiency vs. Sustainability

Coordinate, Balance, Trade off

A platform for sustainability assessment and decision-making



Process integration, and Innovation

