COMPARATIVE ANALYSIS OF ICL AS AN ALTERNATIVE TO CRUDE OIL

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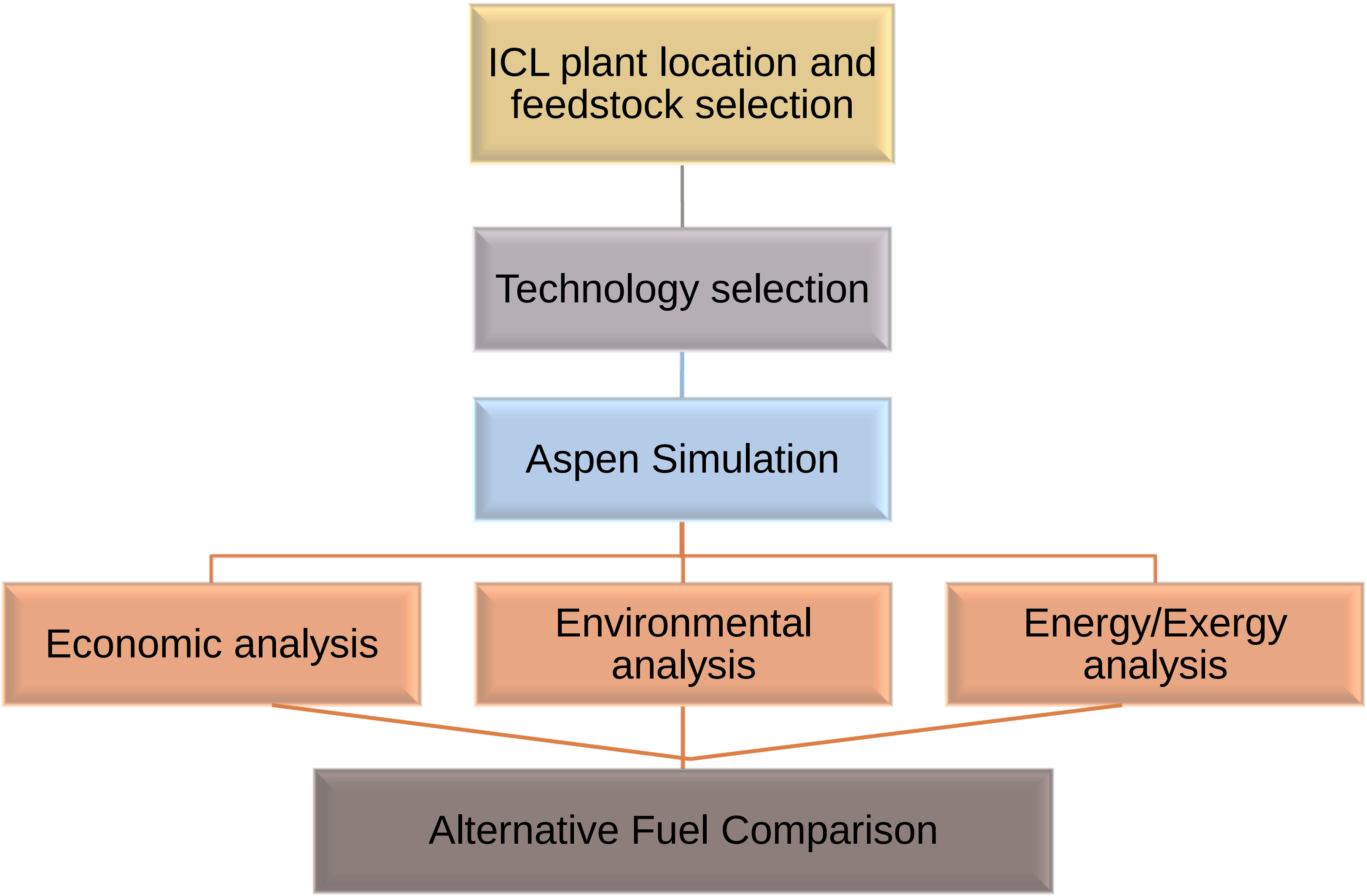
Problem Statement

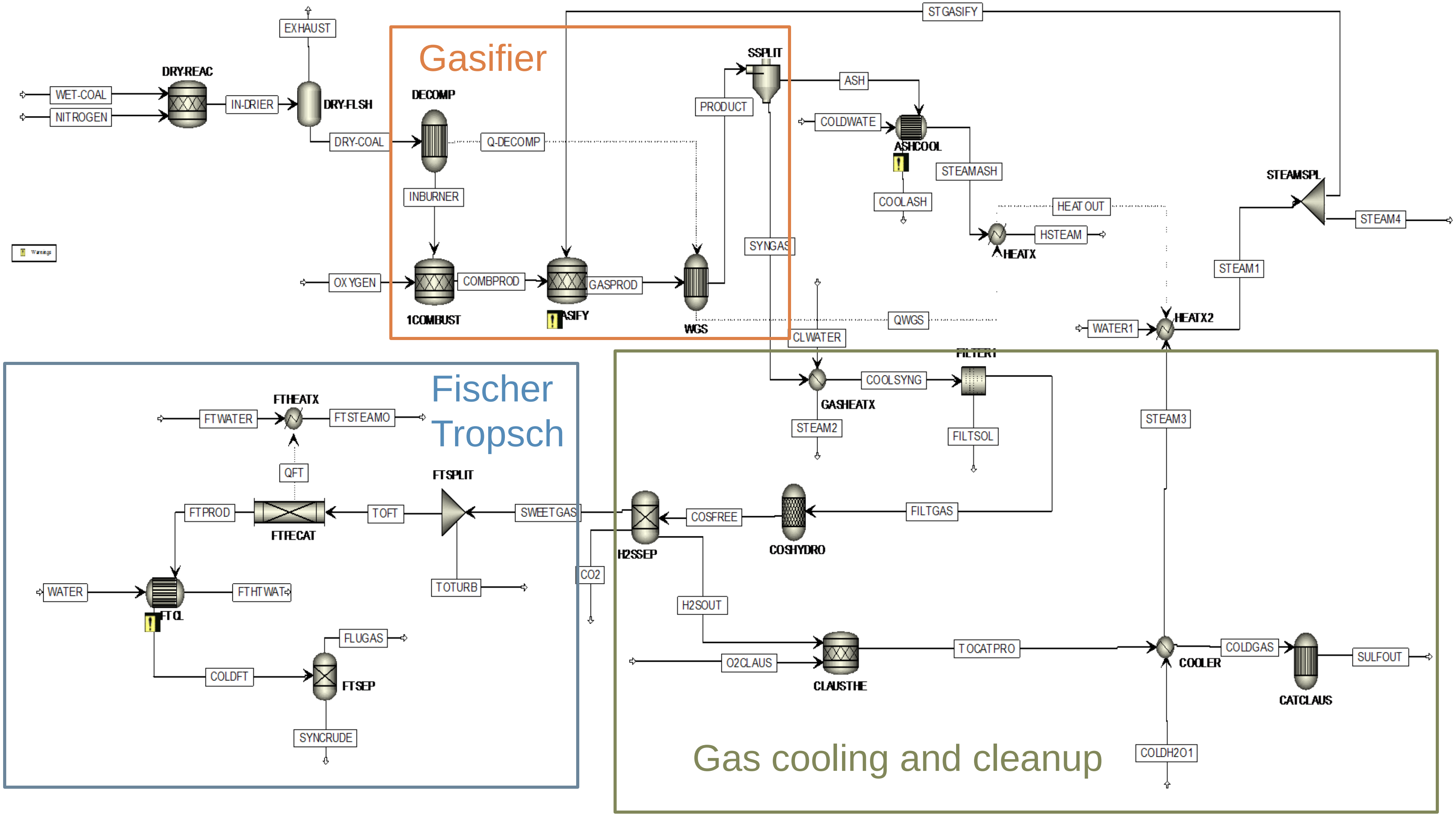
When the US can no longer rely on our current sources of crude oil, how will a domestic indirect coal to syncrude plant compare to other US crude oil alternatives for the transportation sector?

Project Scope

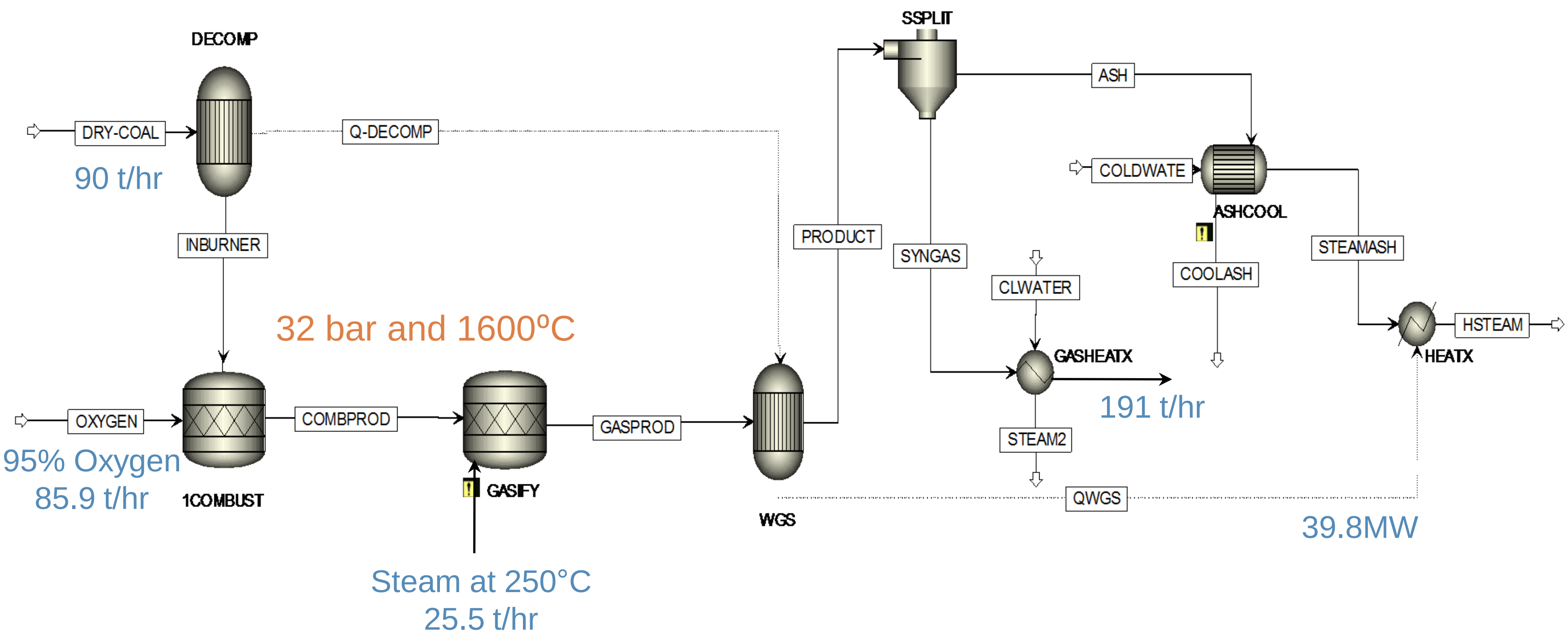


Aspen Plus simulation of designed CTL plant

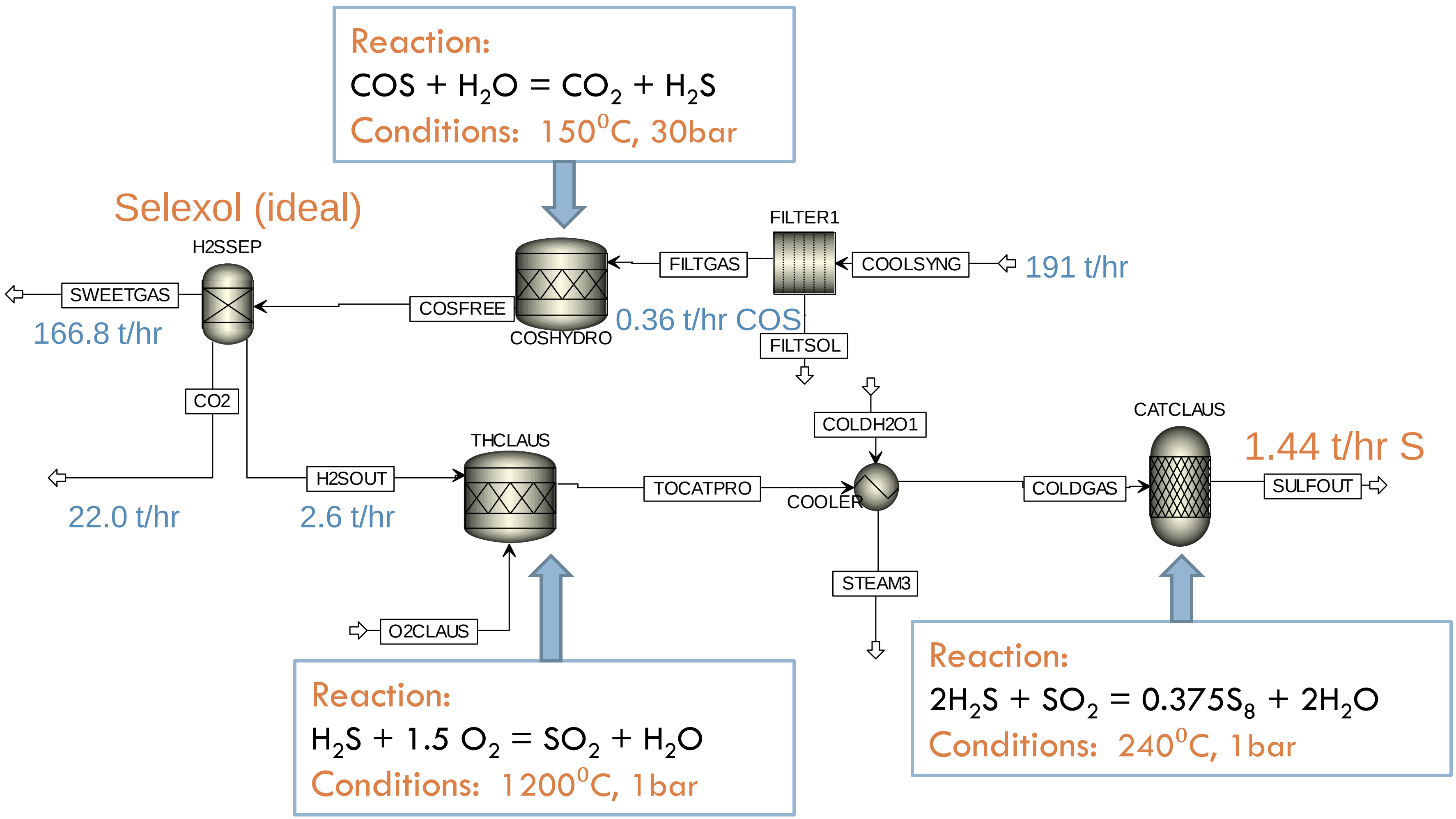
Final CTL plant simulation



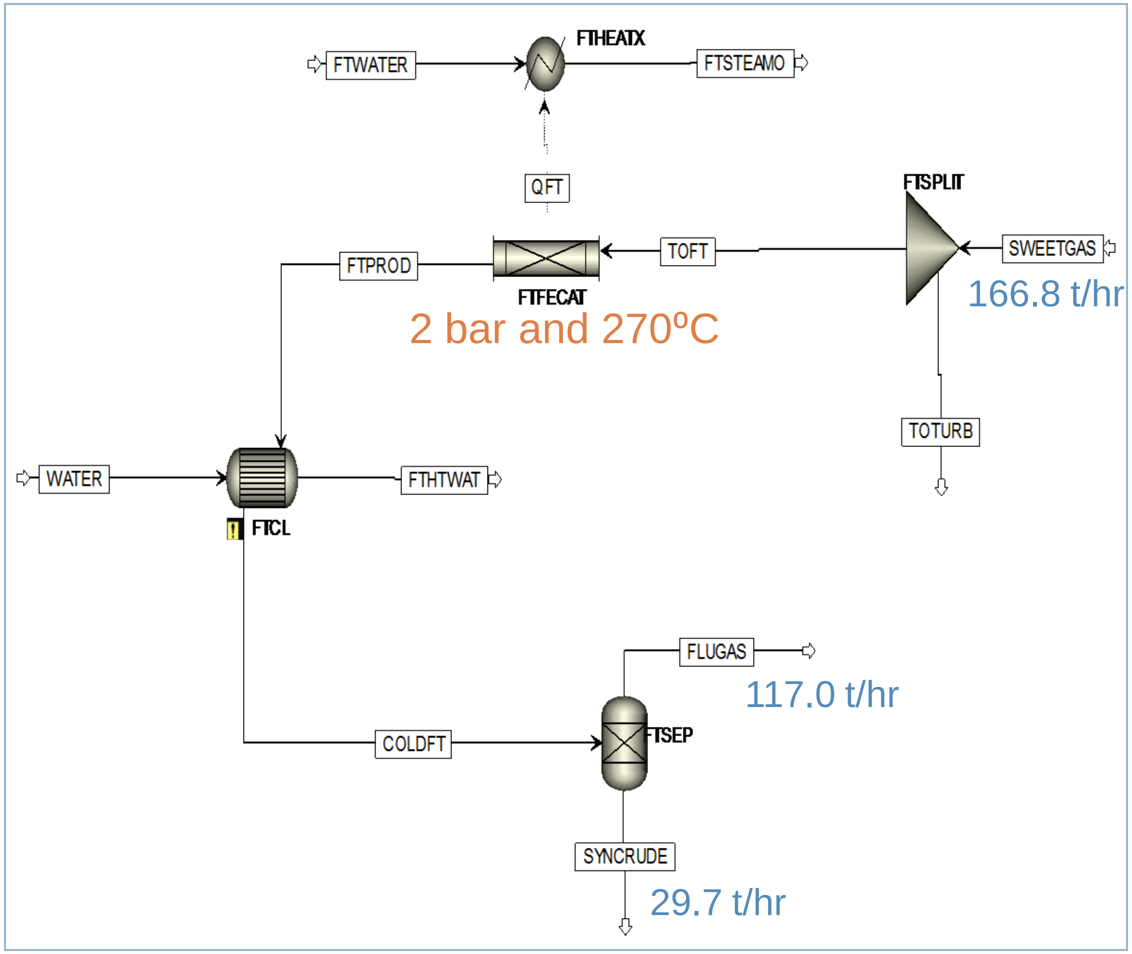
Aspen - Gasifier



Aspen – Gas cleanup



Aspen – F.T. Synthesis



- Kinetic model from Fernandes [1]

$$R_{FTS} = \frac{k_{FTS} P_{CO} P_{H_2}}{P_{CO} + a P_{H_2O}}$$

$$R_{WGS} = \frac{k_{WGS}\left(P_{CO} P_{H_2O} - \frac{P_{CO_2} P_{H_2}}{K_1}\right)}{\left(P_{CO} + K_2 P_{H_2O}\right)^2}$$

- Assuming steady-state operation and isothermal conditions *
- Valid for multi-tubular fixed bed [2]

[1] Fernandes, F. A. N. and E. M. M. Sousa (2006). "Fischer-Tropsch synthesis product grade optimization in a fluidized bed reactor." AIChE Journal 52(8): 2844-2850.
[2] Van der Laan, G. P. and A. A. C. M. Beenackers (1999). "Kinetics and selectivity of the Fischer-Tropsch synthesis: A literature review." Catalysis Reviews-Science and Engineering 41(3-4): 255-318

XTL simulations

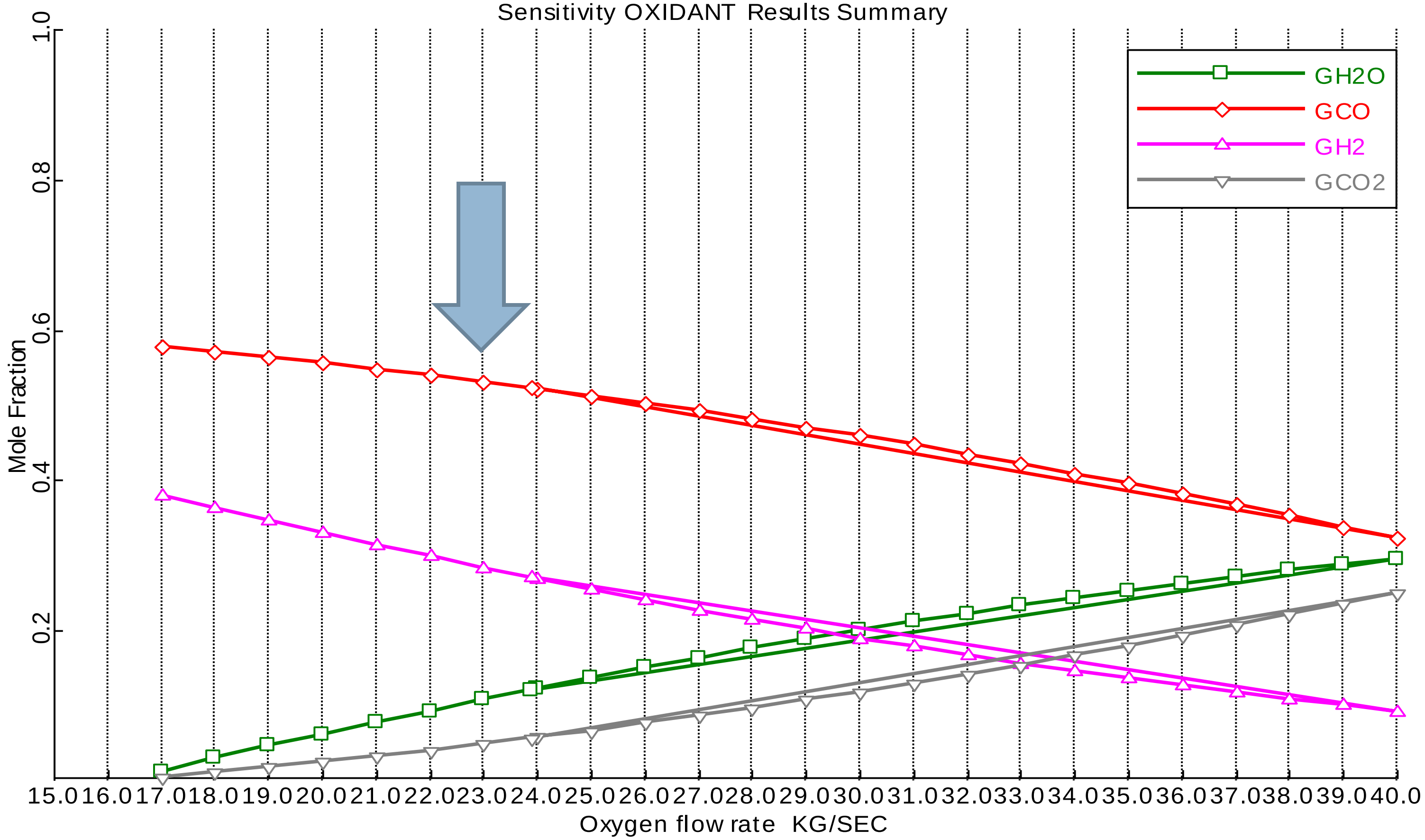
	CTL
Feed	100% Coal
Syngas composition	CO: 59.5% H_2: 30.7%
FT product	29.6 t/hr
Efficiency	51.2%

	CBTL
Feed	25% BM 75% Coal
Syngas composition	CO: 53.3% H_2: 33.1%
FT product	29.2 t/hr
Efficiency	51.3%

	BTL
Feed	100% Switchgrass
Syngas composition	CO: 41.6% H_2: 36.5%
FT product	17.8 t/hr
Efficiency	50.8%

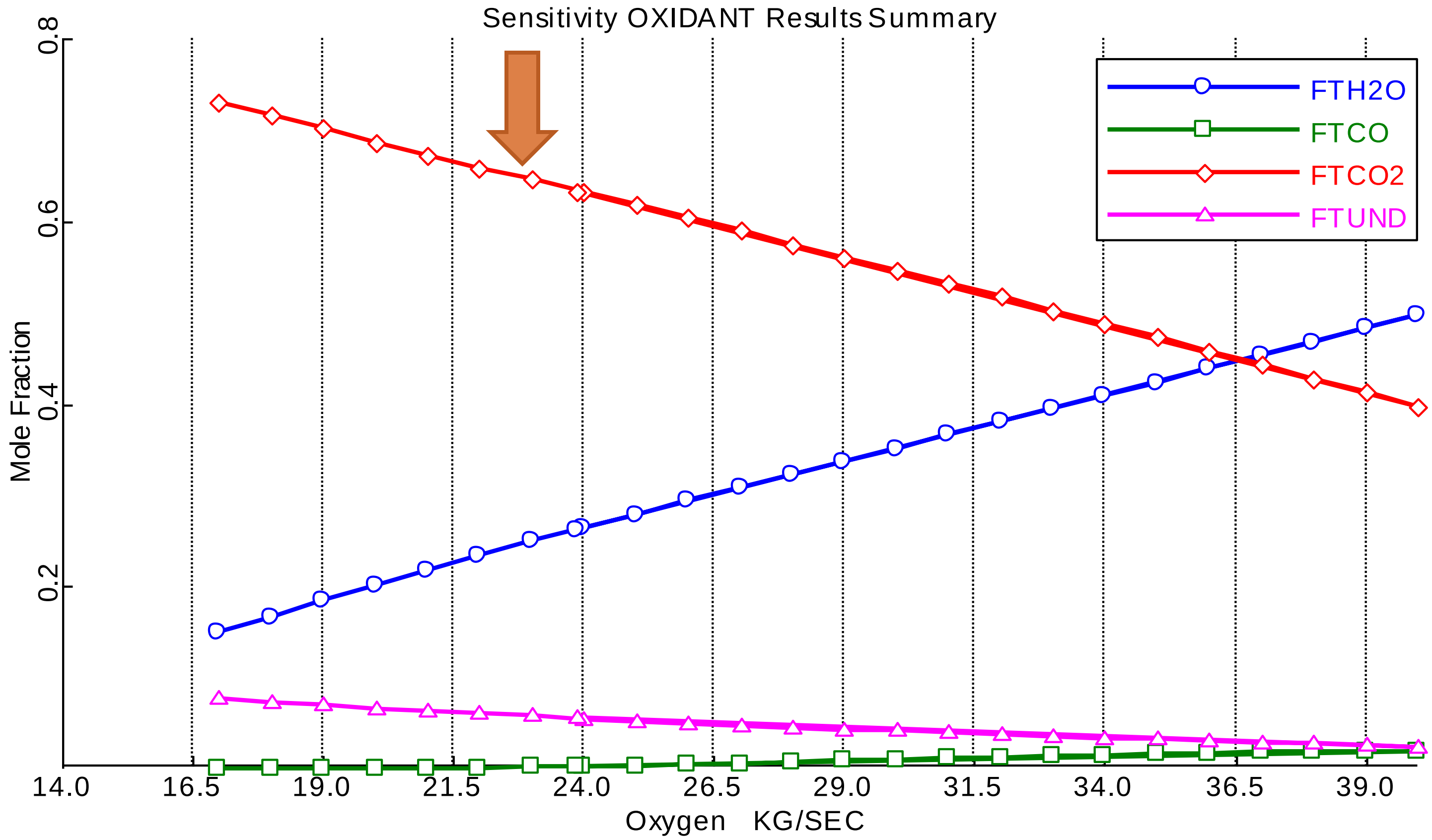
Sensitivity Analysis - Aspen

Gasifier



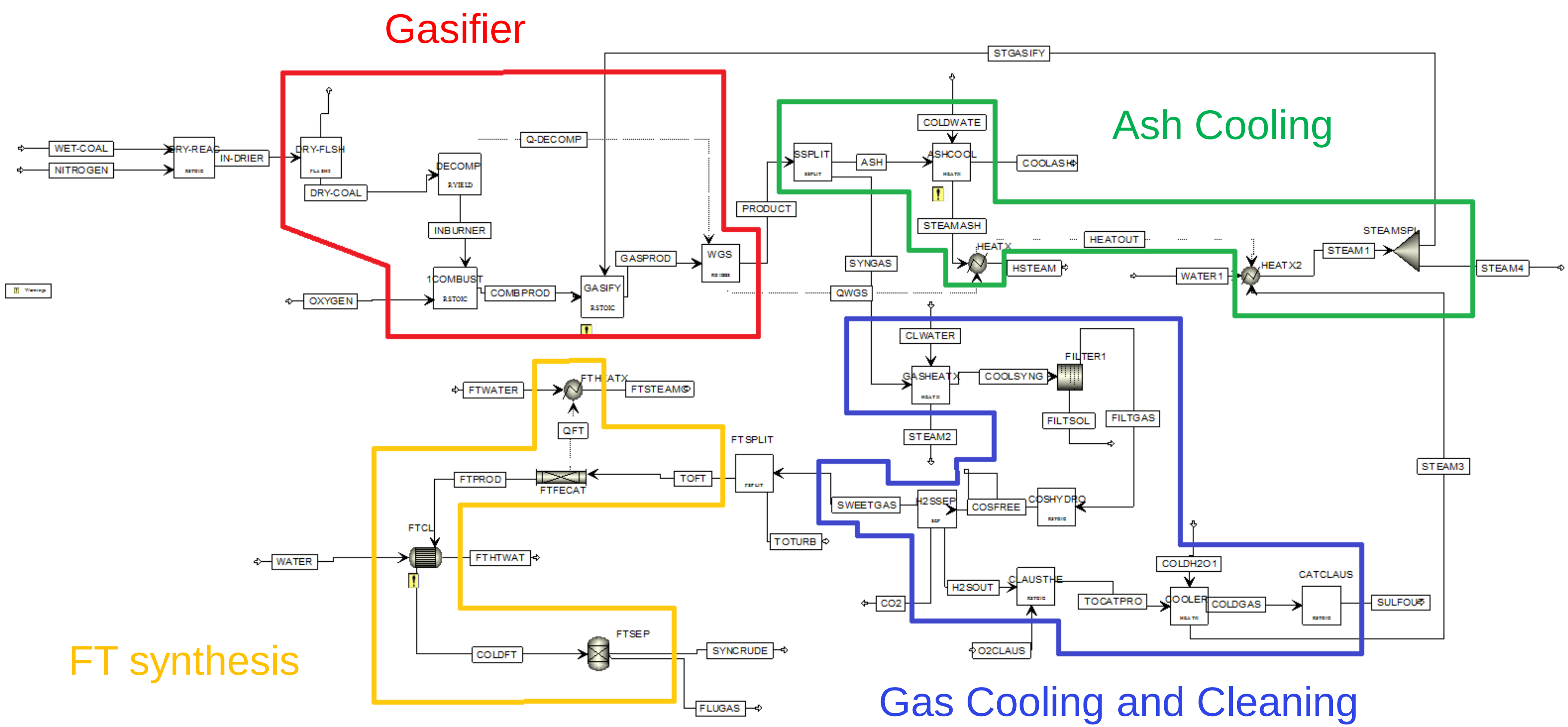
Sensitivity Analysis - Aspen

Fischer Tropsch

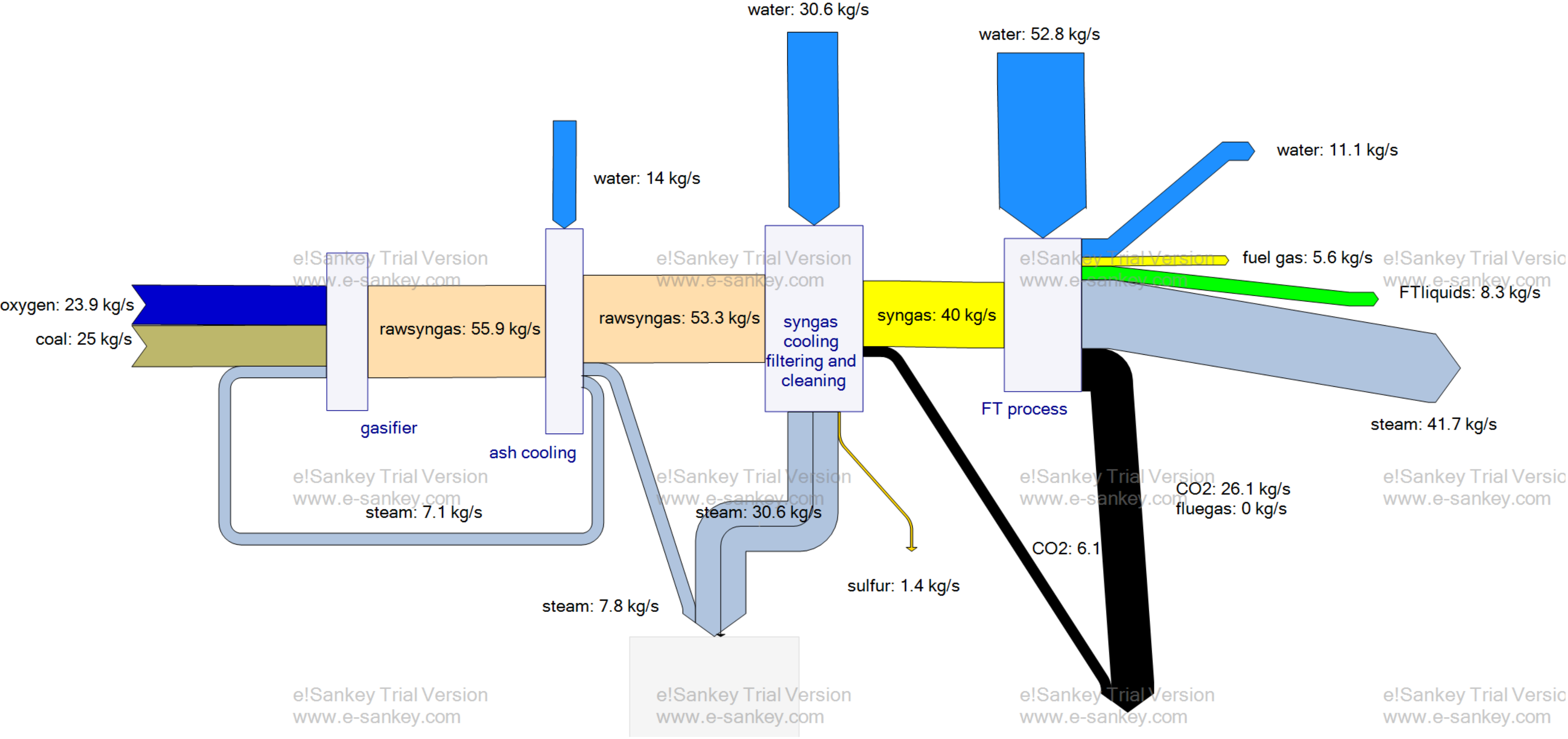


Energy and Exergy Analysis of designed CTL plant

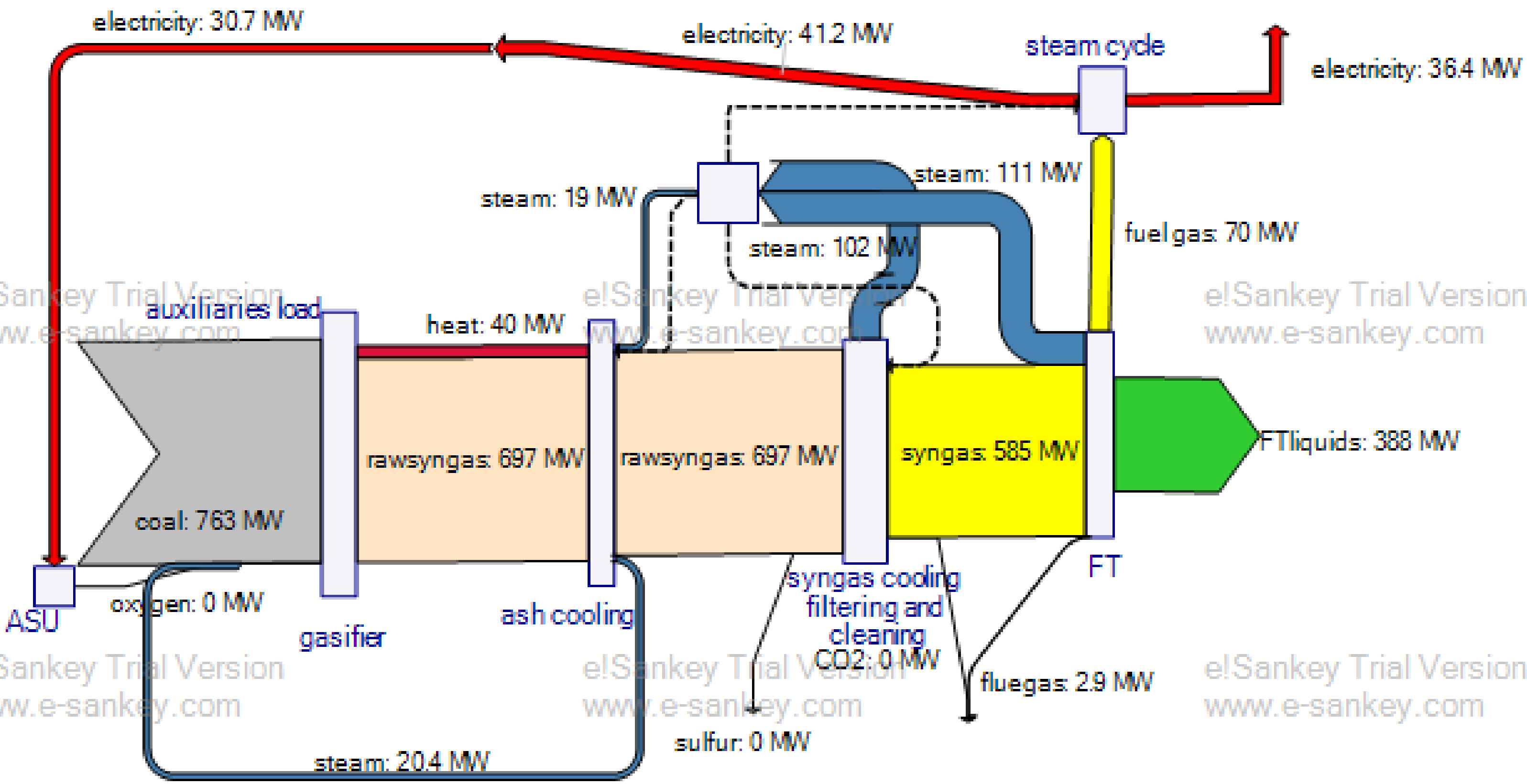
Main Sections of the Aspen Simulation



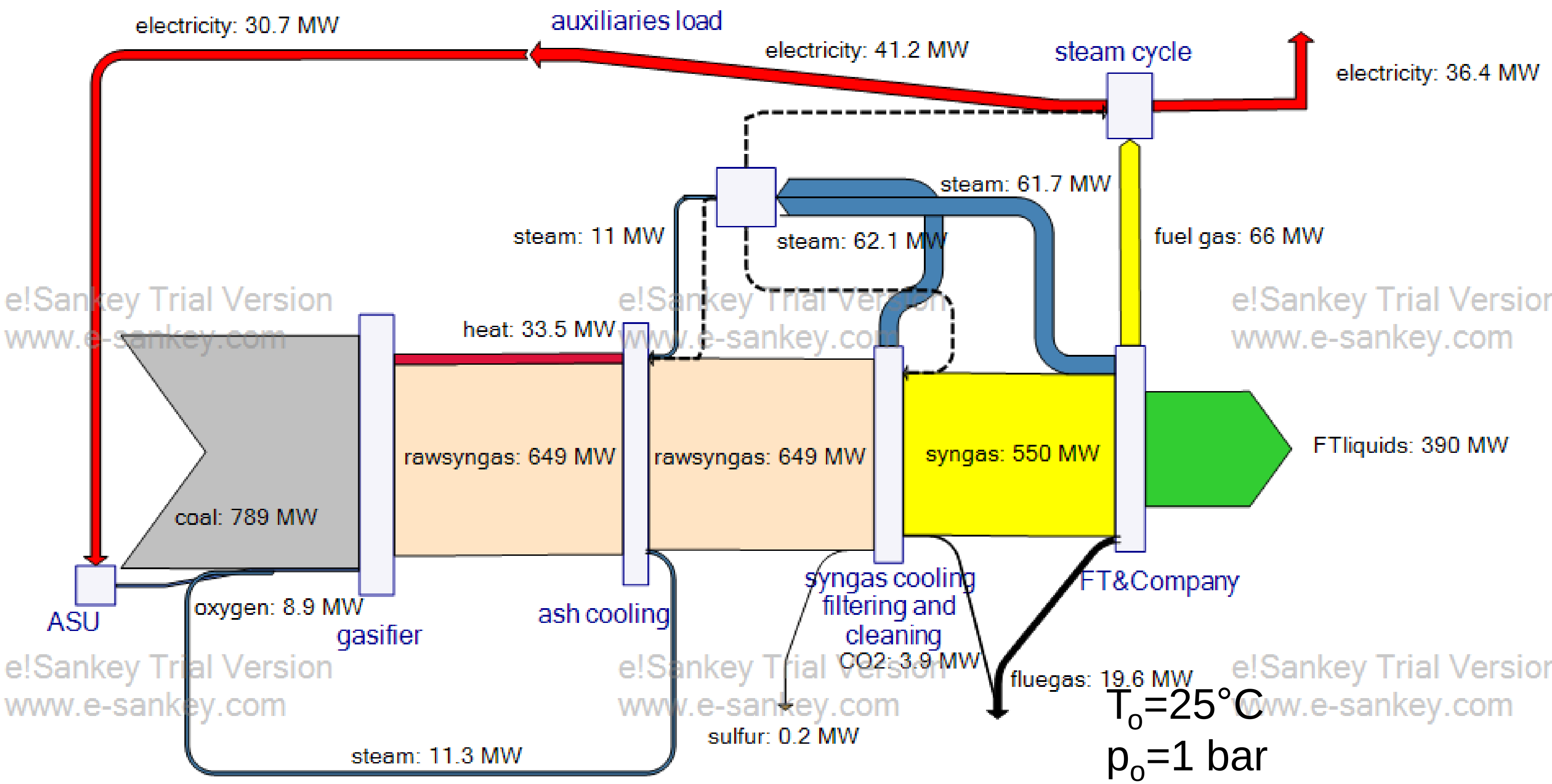
Mass flow diagram



Energy Flow Diagram

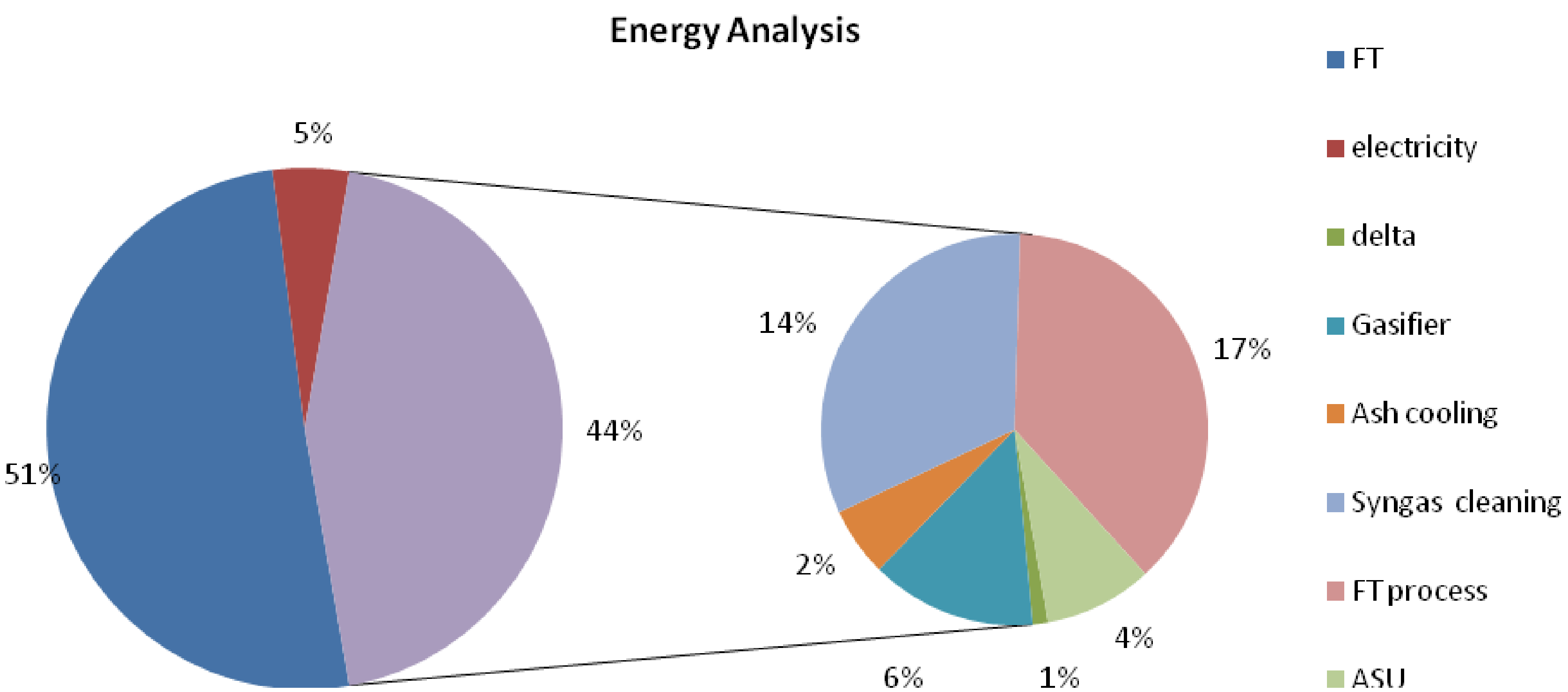


Exergy Flow Diagram



T_o=25°C
p_o=1 bar
Ideal gas
B=Bchem+Bphys+ΔGmix

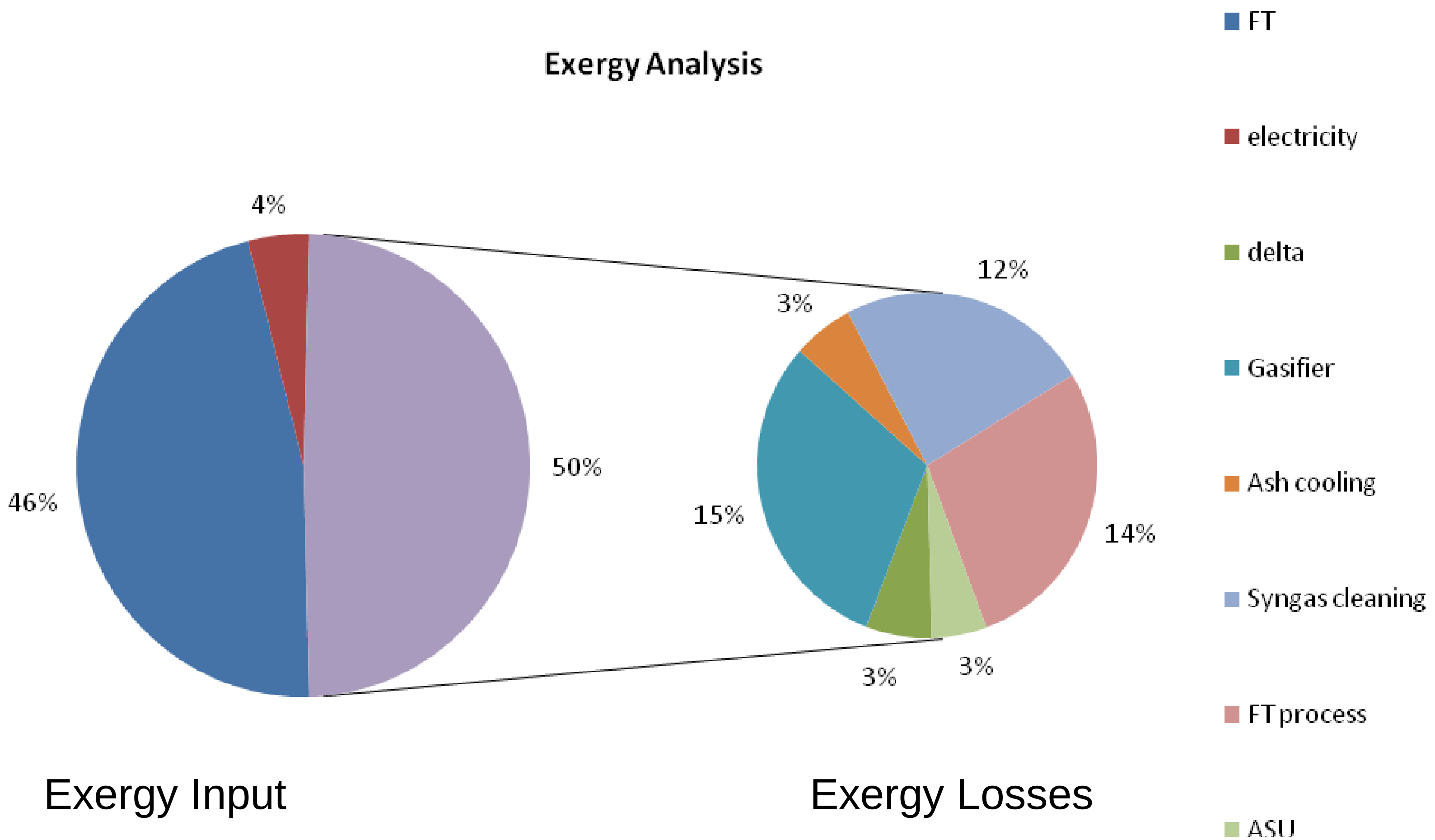
Energy Analysis



Energy Input

Energy Losses

Exergy Analysis



Exergy Input

Exergy Losses

Gasifier Sensitivity Analysis

An example, oxygen:

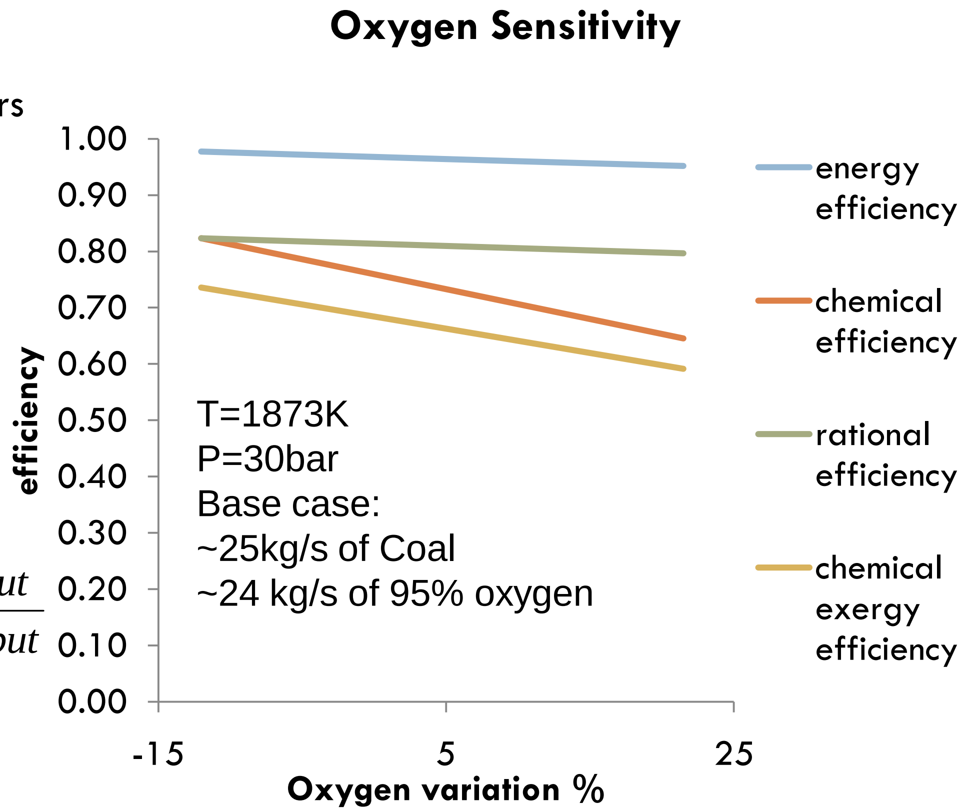
- Energy Efficiencies for well insulated gasifiers are very high ~1 [1]
- Rational Efficiencies lower than Energy ones ~ 0.8 [1]
- O_2 sensitivity shows a decreasing trend of the chemical and rational efficiencies.

$$energy\_efficiency = \frac{energy\_input}{energy\_output}$$

$$chemical\_efficiency = \frac{chemical\_energy\_input}{chemical\_energy\_output}$$

$$exergy\_efficiency = \frac{exergy\_input}{exergy\_output}$$

$$exergy\_efficiency = \frac{exergy\_input}{exergy\_output}$$

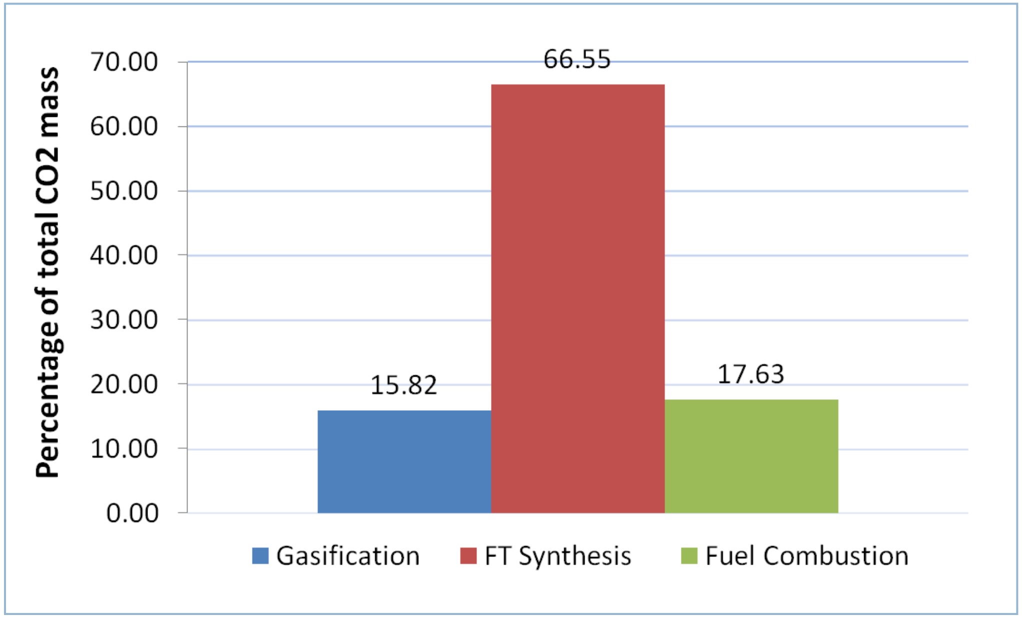


[1] Mark J. Prins “From coal to biomass gasification: Comparison of thermodynamic efficiency”, Energy, 2004

Environmental Analysis of designed CTL plant

CO_2 Emissions

Figure. Sources of CO2 emissions in CTL plant



- Considerations
  - Purity of captured CO_2 streams is quite good

Source	Purity (%)
Gasifier – post Selexol	99
FT Synthesis	95.28

  - 90% of the impurities in FT Synthesis 'Fluegas' is nitrogen

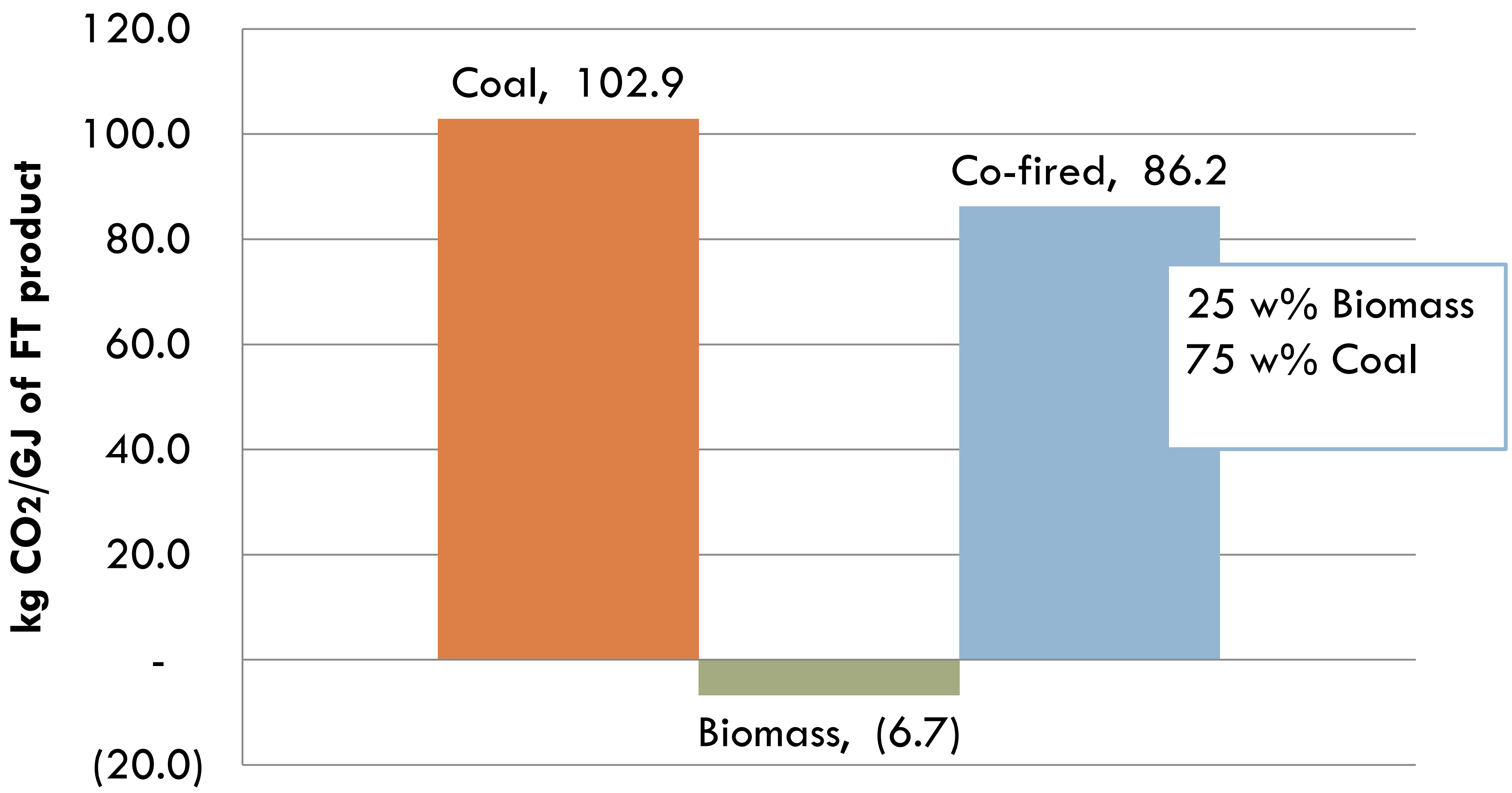
Table. Summary of CO2 emissions from CTL plant

CO2	TOTAL PRODUCED	TOTAL CAPTURE READY	TOTAL PRODUCED (Kreutz et al, 2008)
kg CO2 eq/GJ fuel (HHV)	102.9	85.0	99.0

~28,000 tonnes/day

Effect of Feedstock in Overall CO_2 Emissions: CTL, BTL, Co-firing

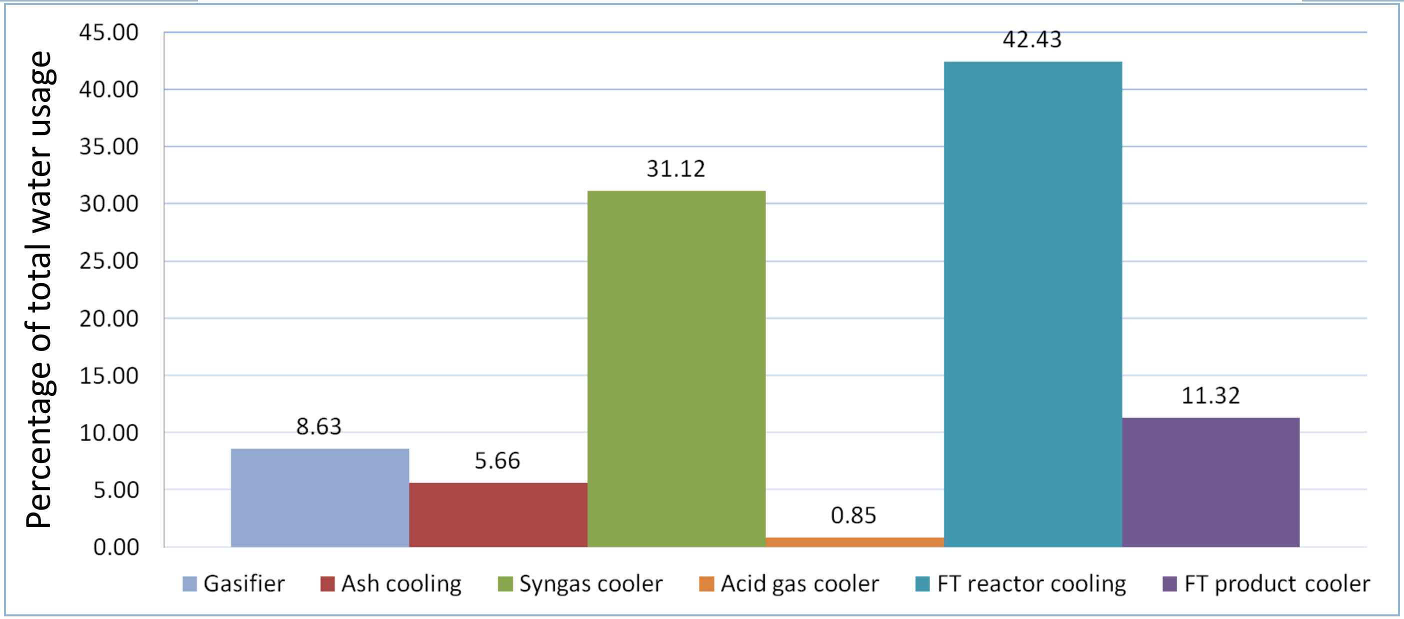
Figure. CO_2 emissions from various feedstock configurations



Assuming a biomass storage capacity = 17.2 kg Ceq/GJ HHV.

Water Usage

Figure. Allocation of water usage in CTL plant



Net consumption = Make-up water (3% total) + consumed process water

Table. Summary of water usage & distribution in CTL plant

	gal water/gal FT liq	Literature gal water/gal Ftliq	Reference
Water recycled in plant	7.70	-	
Water replaced/consumed	0.85	1.03	[1]
Water usage in the plant	**8.55**	**7.30, 8-10**	**[4], [5]**

Waste Management

- Bulk mass of waste comes as
  - Ash slag
  - Fly ash
- Concerns
  - Water leaching: hazardous to groundwater resources
  - Slag is less susceptible to leaching than bottom ash

Source: http://www.charah.com/

Table. Solid waste production from CTL plant

Solid waste lines	Content	From Equipment	Tonnes/day	kg ash-slag/bbl FT_{liq}
COOLASH	ash slag	Slagging Gasifier	1808.0	36.71
FILTSOL	fly ash	Particulate filter	9.4	0.19

- Management
  - Landfill disposal, ash-ponds (trouble)
  - Recycling of ash (cement industry)

Policy Prospects for CTL

Future government policies & environmental regulations → May promote or *discourage* early investment from the private sector for CTL projects

Possible barriers for CTL

- Remaining Uncertainties
  - Production costs
  - Management of GHG Emissions (CCS development)
  - Crude oil prices (competitiveness with conventional fuels) ☆

- Lack of effective policies to reduce GHG emissions will likely hold back government support ☆

Policy Prospects for CTL (cont.)

- **Policy Incentives for CTL**
  - Subsidies
    - Investment-tax credits (financial help from the beginning of the project at government's expense)
    - Production subsidies (favoring alternative vs conventional fuels)
    - Petroleum taxes
  - Price Floors
    - Encourages private investment for CTL by removing the financial constrains at times of low crude oil prices
  - Income Sharing
    - Beneficial for the government at times of high crude-oil prices to recover public funds from promoting CTL

Economic Analysis of designed CTL plant

Economic Model Considerations

Input categories

- Financing
- Escalation factors
- Technical design criteria
- General facility parameters
- Contingency factors
- 12% discount rate

Major Outputs

- Net Present Value (NPV)
- Return on Investment (ROI)
- Payback Period
- Year to year “At Hand” and “Discounted” Cash Flows

Model Input Parameters

Design Parameters of a 50,000 Barrel / Day Coal to Liquids Grassroots Facility / 15 yr depreciation

General Facility Parameters	
Expected Plant Lifetime (yrs)	30
Local Industrial Electrical Costs ($/kWhr)	$0.060
Capacity Utilization Factor	85%
Overall Contingency Factor	25%
Additional FT Contingency Factor	25%
Total O&M Costs	5%
Facility Electrical Capacity (MW_e)	620
Facility Electrical Needs (MW_e)	330
Typical Output to Grid (MW_e)	**290**

F-T Parameters	
Petro-Oil Market Value ($/bbl)	$97
Diesel / Naphtha ratio (% diesel)	65%
ULSD Premium vs. petro crude (multiplier)	1.25
Naphtha value of diesel	77%
F-T HHV (BTU/gallon)	126,500
Capital Investment per bbl capacity (thousand $)	$105

Economics, Interest, and Projections	
Tax Rate	40%
Financing Fee	3.0%
Debt to Equity Ratio (% Debt)	55%
General Inflation	2.0%

Base Year Values (MM$ / YR)	
Expected Plant Cost (+ contingency)	$5,232
Annual Fixed and Variable O&M (not including electricity & feed)	$262
Annual Feedstock Costs	$319
Annual Electrical Sale to Grid	$130
Annual F-T Revenue (pre-tax)	$1,628
Total Expenses	**$581**
Total Revenue	**$1,758**
Gross Income (pre-tax)	**$1,177**
Net Income (post-tax)	**$706**

NPV (MM$) :	**$1,036**
ROI :	**19.8%**
Payback Period :	**10**

Denotes User Input

Calculated Value

Sources

- Aspen simulation and exergy analysis
  - Thermal efficiency
  - Coal and oxygen requirements
  - Fisher Tropsch product quality and distribution
- DOE and NETL reports
  - Coal, electricity, and crude oil escalation,
  - Generally accepted debt to equity ratios
- DOE reports
  - Facility lifetimes
  - Scaling and contingency factors
  - Capacity utilization factors
  - Fixed maintenance and start up costs
- IRS 15 year Modified Accelerated Cost Recovery System (MACRS) depreciation schedule for gasification facilities

Year – to – Year Cash Flows

Year	5	6	7	8	9	10	11	12	13	14	15	16
PW Factor (from discount rate)	0.567	0.507	0.452	0.404	0.361	0.322	0.287	0.257	0.229	0.205	0.183	0.163
Cumulative Inflation Factor	1.082	1.104	1.126	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.294	1.319	1.346
Depreciation Schedule	0.0693	0.0623	0.059	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.059	0.0591	0.0295
Crude Oil Projection	109	112	116	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	142	147	151
Coal Projection	45	46	47	48	49	50	51	52	53	54	55	57
Electricity Projection	0.065	0.066	0.068	0.069	0.070	0.072	0.073	0.075	0.076	0.078	0.079	0.081
Capital Costs	0	0	0	0	[illegible]	[illegible]	[illegible]	0	0	0	0	0
Feedstock Costs	346	352	360	367	[illegible]	[illegible]	[illegible]	397	405	413	421	430
O&M Costs	283	289	295	301	[illegible]	[illegible]	[illegible]	325	332	338	345	352
Operational Expenses	**629**	**641**	**654**	**667**	**681**	**694**	**708**	**722**	**737**	**751**	**766**	**782**
F-T Sales Revenue	1,832	1,887	1,944	2,002	[illegible]	[illegible]	[illegible]	2,254	2,321	2,391	2,463	2,537
Electricity Sales Revenue	140	143	146	149	[illegible]	[illegible]	[illegible]	161	164	168	171	174
Total Sales Revenue	**1,973**	**2,030**	**2,090**	**2,151**	**2,214**	**2,279**	**2,346**	**2,415**	**2,486**	**2,559**	**2,634**	**2,711**
Gross Income (pre-tax)	1,344	1,389	1,436	1,484	1,534	1,585	1,638	1,693	1,749	1,807	1,867	1,929
Depreciation	363	326	309	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	309	309	309	154
Gross Income - Depreciation (pre-tax)	981	1,063	1,127	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1,440	1,498	1,558	1,775
Income Tax	393	425	451	470	490	510	531	554	576	599	623	710
Interest Payment	112	105	97	[illegible]	[illegible]	[illegible]	[illegible]	49	38	26	13	0
Principal Payment	125	132	140	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	199	211	224	0
Debt Services	237	237	237	237	237	237	237	237	237	237	237	0
At Hand Cash (post-tax)	714	727	748	777	807	837	869	902	936	971	1,007	1,219
Cumulative Cash Flow	-3,812	-3,085	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	**3,762**	**4,769**	**5,988**
Present Worth	405	368	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	215	199	184	199
Cumulative (Net) Present Worth	**-3,341**	**-2,973**	**-2,634**	**-2,321**	**-2,030**	**-1,760**	**-1,510**	**-1,279**	**-1,064**	**-866**	**-682**	**-483**

Escalation & Depreciation

Expenses

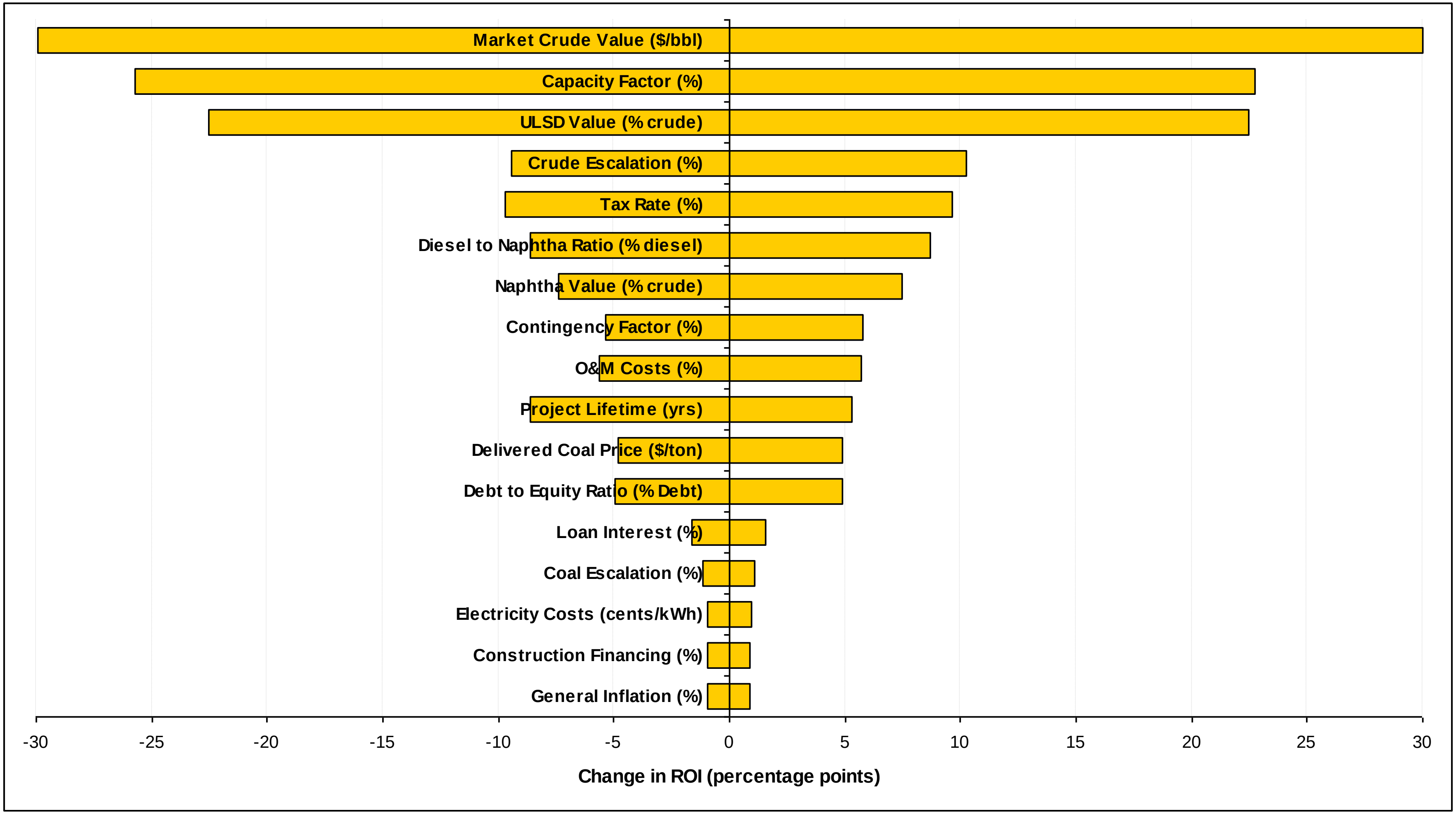
Sales

Income & Taxes

Loan Interest

Year-to-year Cash Flow

Sensitivity Analysis



Economic Scenarios

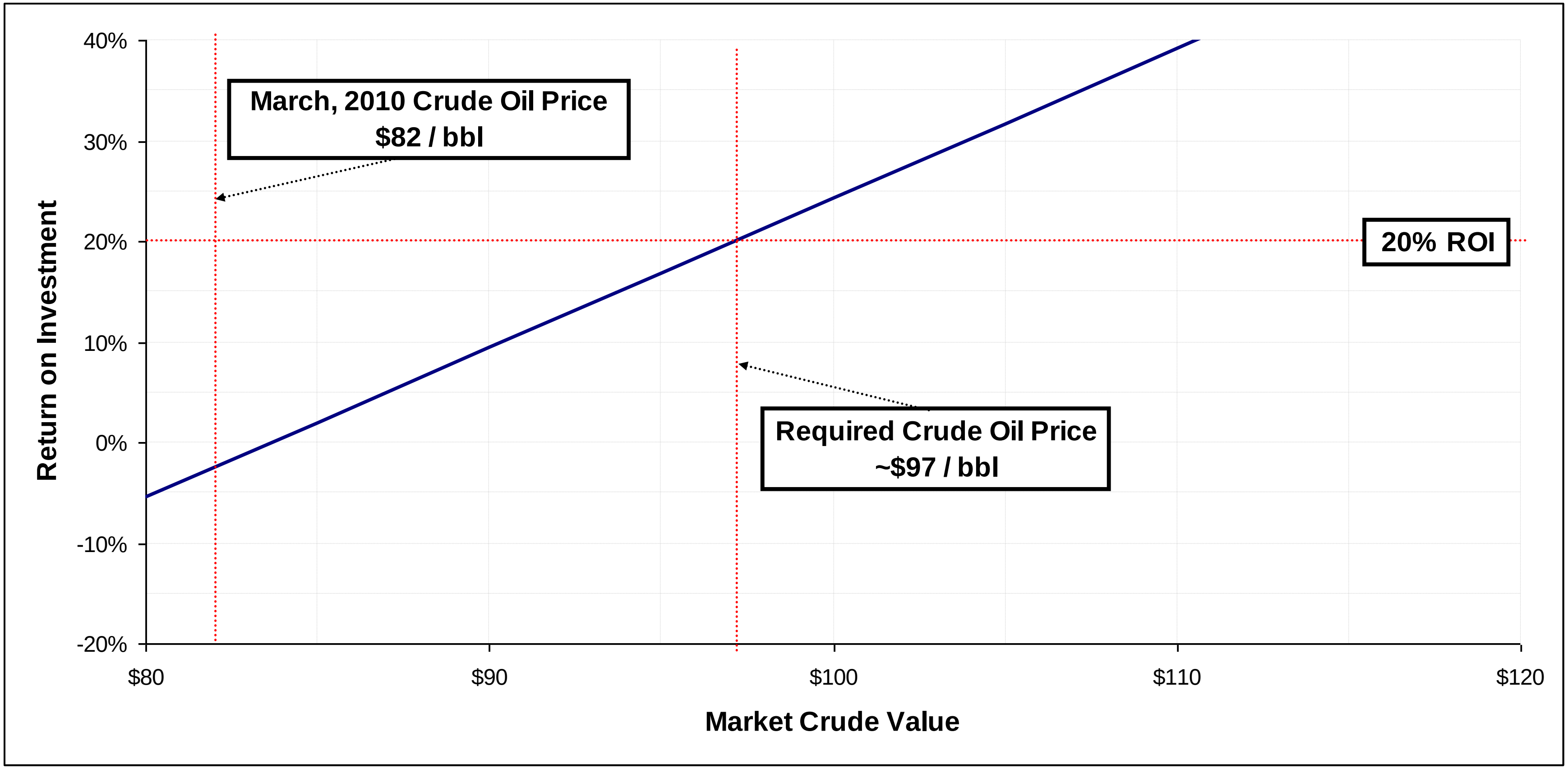
Scenarios not run

- Less than a three percentage effect on ROI
  - Loan interest
  - coal and electricity escalation
  - base year electricity costs
  - general inflation
- Lesser degree of uncertainty
  - Capacity factor
  - ULSD premiums
  - tax rates
  - ratio of diesel to naphtha product
  - O&M costs
  - Delivered price of coal.

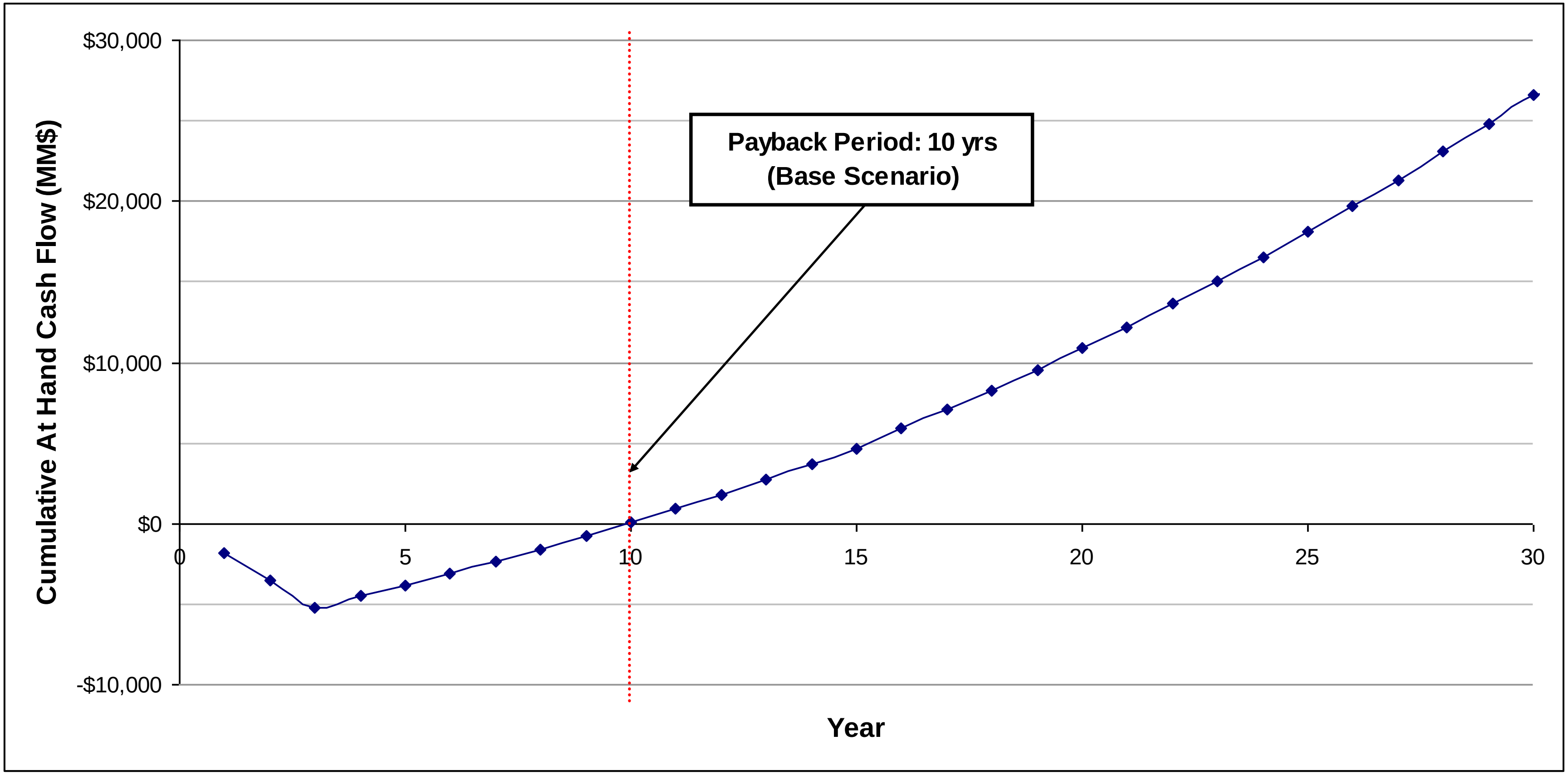
Economic Scenarios (cont.)

- **Scenario 1**: Base Case Scenario representing the required market value of crude oil to achieve 20% ROI. The payback period was calculated from this scenario.
- **Scenario 2**: The effect of plant lifetime on required market value and ROI
- **Scenario 3**: The effect of contingency factor
- **Scenario 4**: CCS

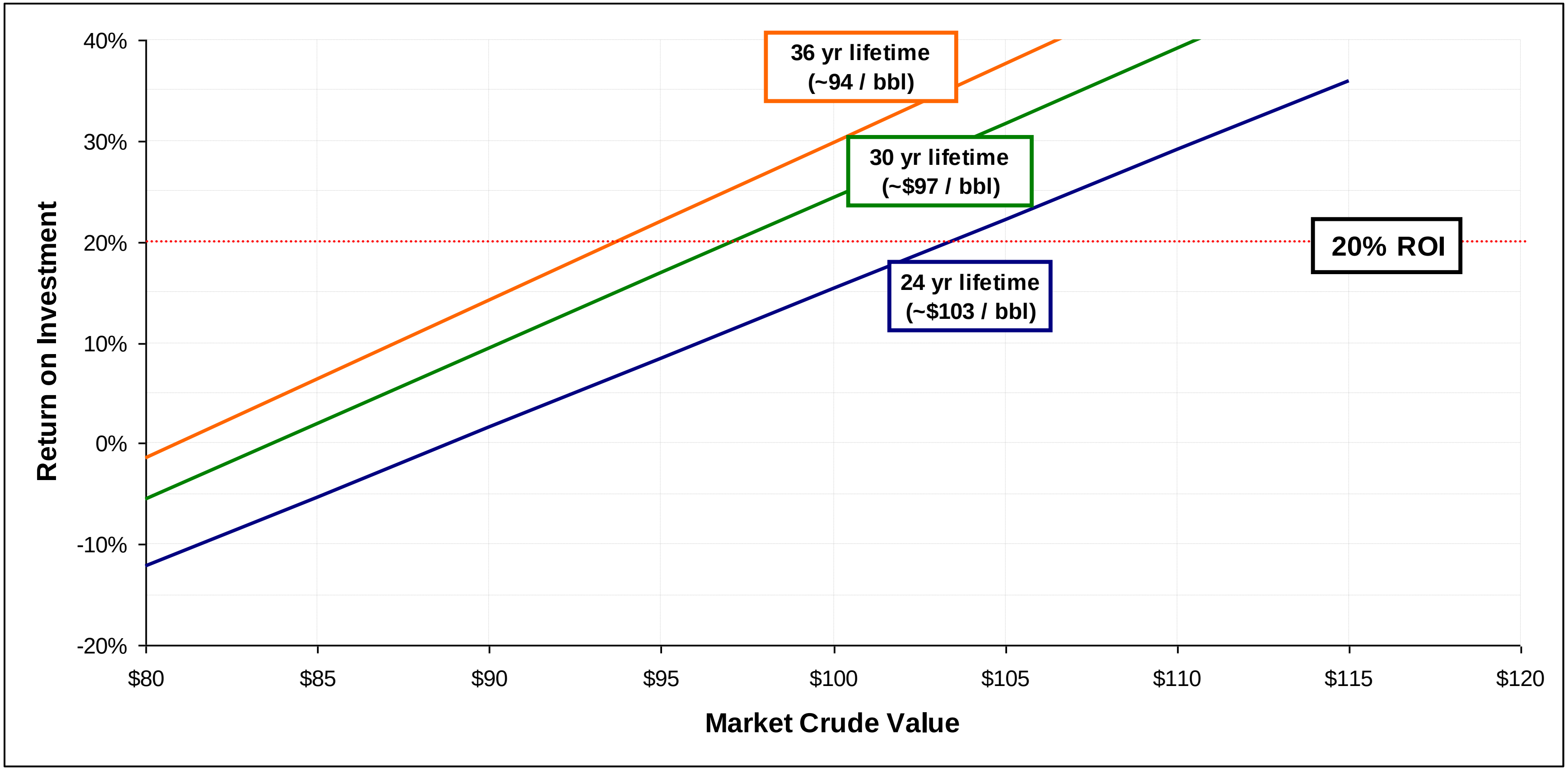
Base Case (Scenario 1)



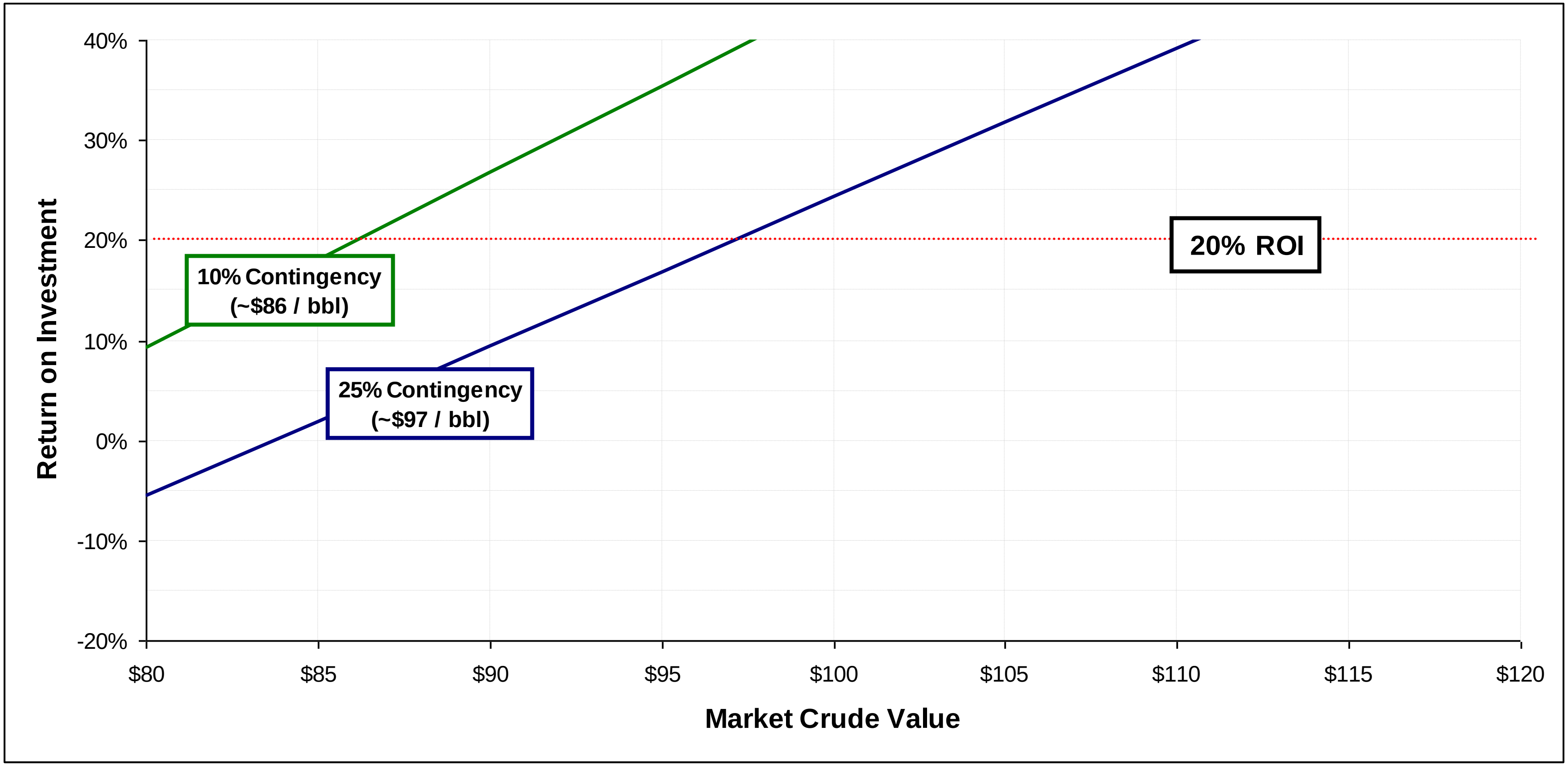
Payback Period



Plant Lifetime (Scenario 2)

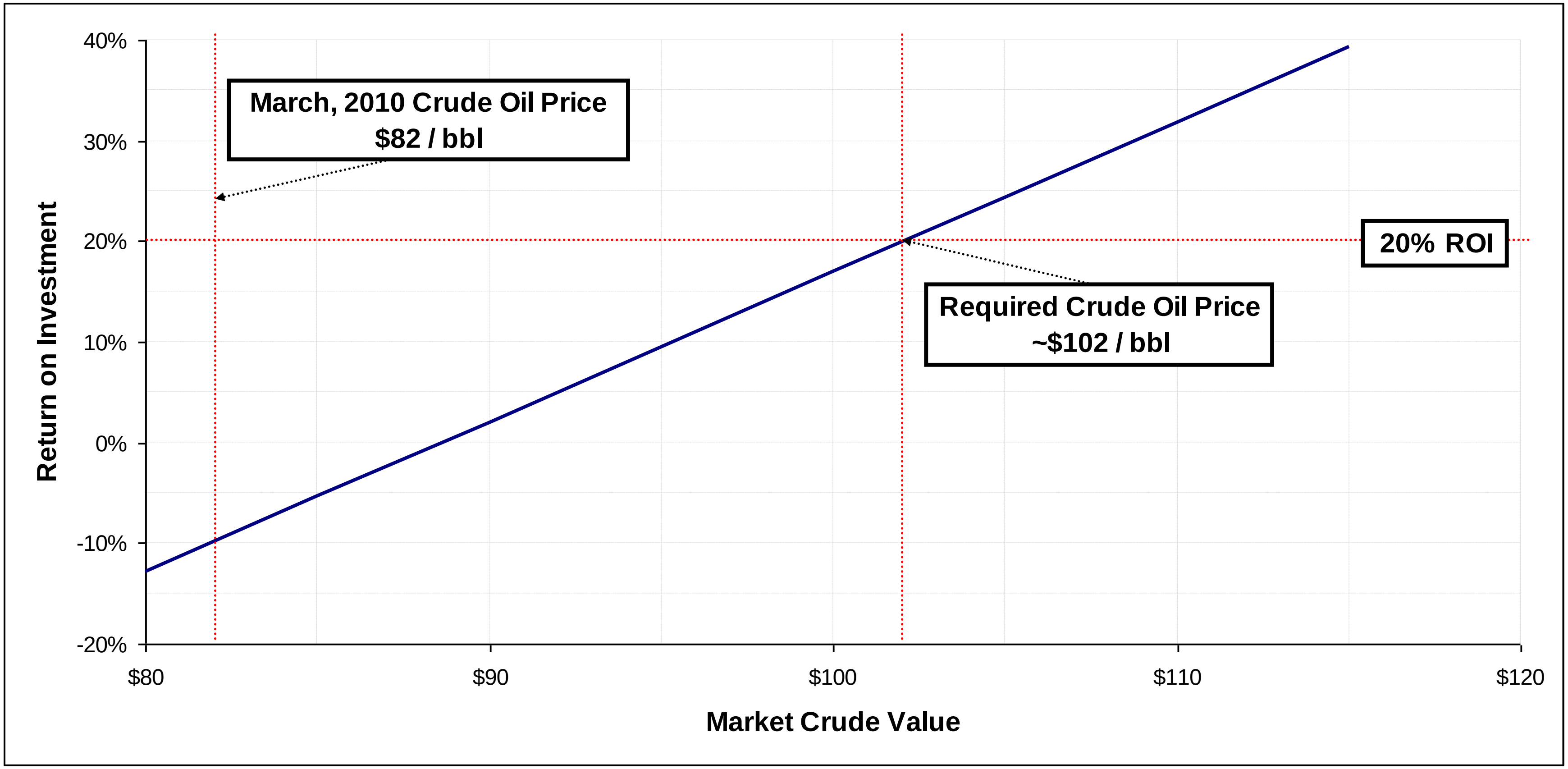


Contingency Factors (Scenario 3)



Considers uncertainties of pioneer plants vs. a plant of n^{th} design (3rd or 4th of its kind).

CCS (Scenario 4)



Assumes \$7 / ton to compress and transport CO_2
(2200psi & 200 miles)

Alternative Fuel Comparisons

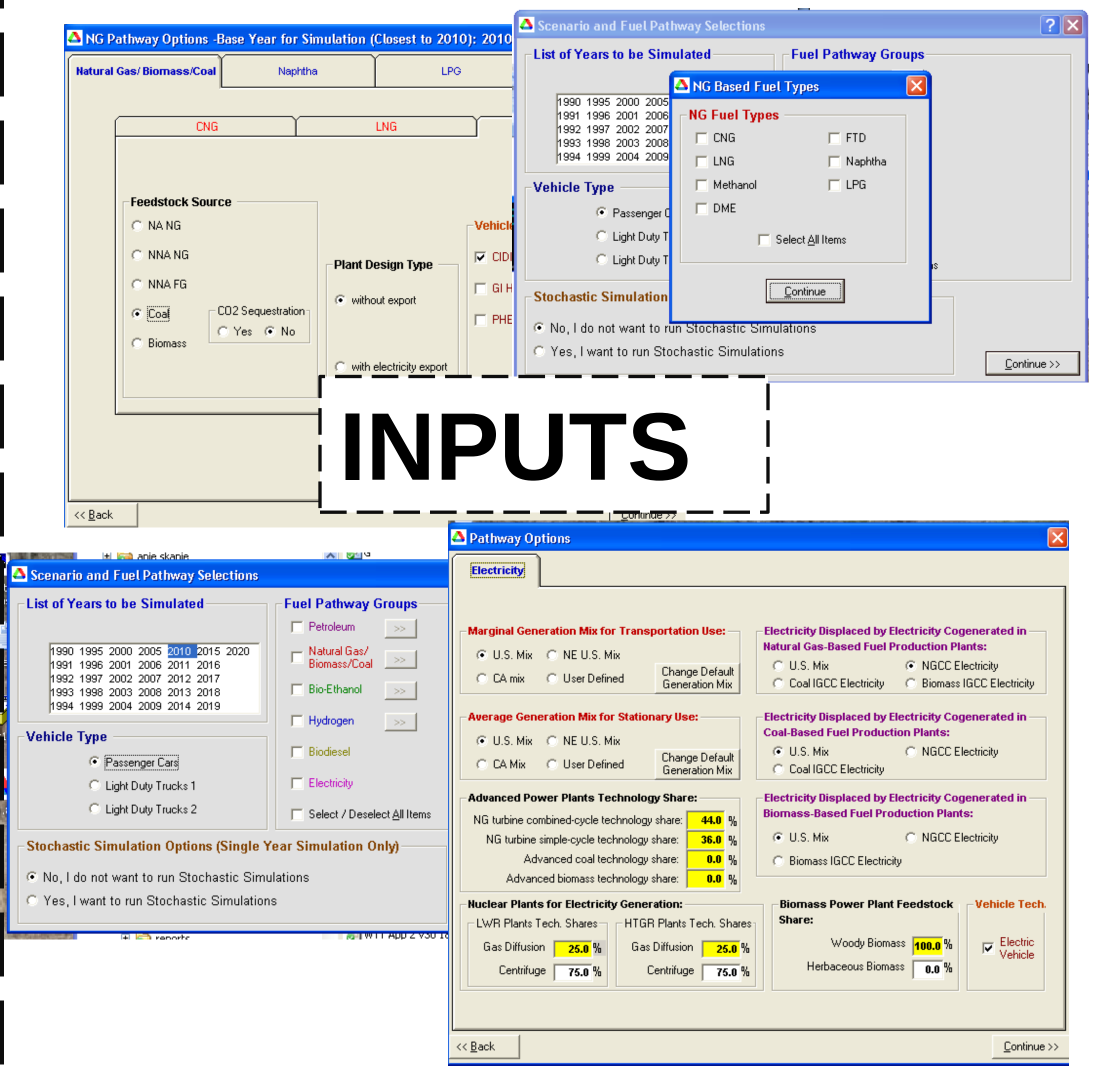
ICL Plant Comparisons

- Compared on an energy, economic and environmental basis
- Two methods
  1. Literature sources
  2. GREET - Greenhouse gases, Regulated Emissions, and Energy use in Transportation – Free software from Argonne National Laboratories

Comparison nomenclatures

- Our plant:
  - Indirect coal liquefaction diesel (ICL diesel)
  - Indirect biomass liquefaction diesel (IBL diesel)
- To other transportation fuels
  - Petroleum diesel @ $100/barrel of crude oil (Petro diesel)
  - Petroleum gasoline @ $100/barrel of crude oil (Petro gas)
  - Biodiesel soy and woody biomass (B100)
  - Ethanol from corn (E85)
  - Compresses natural gas, 200bar (CNG)
  - Synthetic natural gas from IGCC, 200bar (SNG)
  - Hydrogen from NG internal combustion at 200bar (H2 NG ICE)
  - Hydrogen from NG in a 80kW fuel cell vehicle, 200bar (H2 NG FCV)
  - Hydrogen from wind energy in 80kW fuel cell vehicle, 200bar (H2 WE FCV)
  - Electricity from fossil fuels in a 80kW electric vehicle (FF BEV)
  - Electricity from photovoltaic energy in a 80kW electric vehicle (PV BEV)

GREET modeling



OUTPUTS

Vehicle Technologies, Passenger Cars: Well-to-Pump Energy Consumption and Emissions

(Btu or grams per mmBtu of Fuel Available at Fuel Station Pumps)

Year: 2010	Baseline CG and RFG	Compressed Natural Gas	LNGV: Dedicated, NG	EtOH FFV: E85, Corn	CIDI Vehicle: FT100	CIDI Vehicle: BD100	Electricity (transportation)	FCV: L.H2
Total Energy	220,945	149,651	189,072	1,224,066	993,316	1,809,360	1,564,518	1,789,512
WTP Efficiency	81.9%	87.0%	84.1%	45.0%	50.2%	35.6%	39.0%	35.8%
Fossil Fuels	217,085	139,333	187,892	586,750	1,011,958	303,996	1,352,836	1,617,188
Coal	36,929	48,252	5,677	153,929	1,024,866	31,774	988,566	804,854
Natural Gas	84,637	85,122	169,384	352,510	-27,097	192,802	326,524	775,801
Petroleum	95,519	5,959	12,831	80,310	14,189	79,419	37,745	36,534
CO2 (w/ C in VOC & CO)	17,491	11,468	12,693	-10,314	150,163	-60,316	213,067	196,244
CH4	106.744	246.596	199.097	108.205	234.098	43.373	287.165	477.353
N2O	0.278	0.171	0.261	30.329	-0.118	10.737	2.808	1.633
GHGs	20,242	17,684	17,748	1,429	155,980	-56,032	221,083	208,664
VOC: Total	26.614	6.593	6.731	49.507	14.112	107.262	18.912	19.988
CO: Total	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	51.464
NOx: Total								163.064
PM10: Total								154.750
PM2.5: Total								50.062
SOx: Total								259.263
VOC: Urban								2.340
CO: Urban								14.622
NOx: Urban								32.541
PM10: Urban	1.871	0.093	0.080	0.719	-0.094	0.181	2.417	9.736
PM2.5: Urban	1.089	0.061	0.064	0.430	-0.055	0.116	1.430	9.245
SOx: Urban	7.248	2.547	0.536	5.845	-4.154	2.058	81.285	40.331

Vehicle Technologies, Passenger Cars: Well-to-Wheel Energy Consumption and Emissions (per Mile)

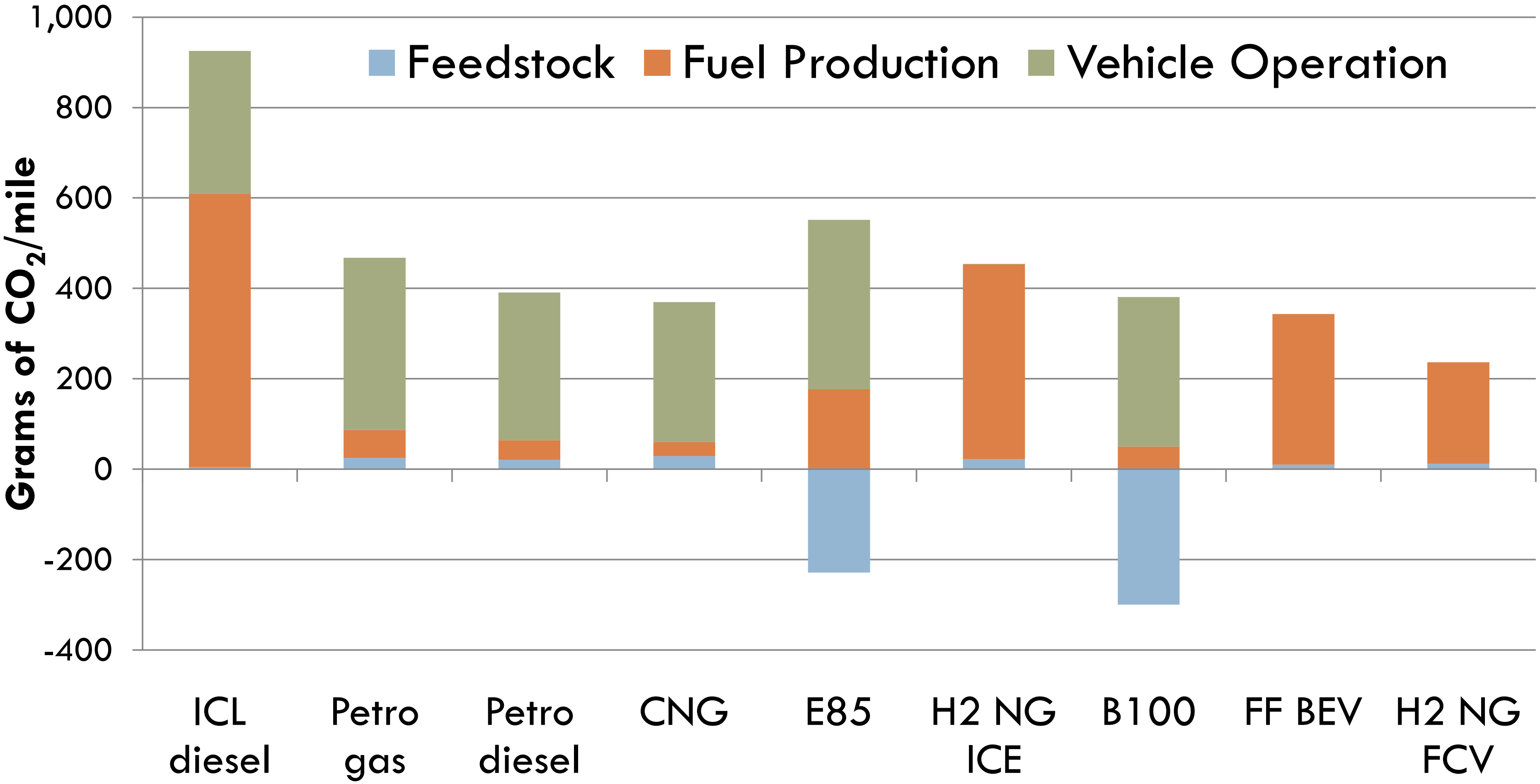
Gasoline Vehicle: CG and RFG

	Btu/mile or grams/mile		
Item	Feedstock	Fuel	Vehicle Operation
Total Energy	266	831	4,961
Fossil Fuels	257	820	4,961
Coal	39	144	0
Natural Gas	160	260	0
Petroleum	59	415	4,961
CO2 (w/ C in VO	25	62	381
CH4	0.461	0.068	0.015
N2O	0.000	0.001	0.012
GHGs	36	64	385
VOC: Total	0.018	0.115	0.180
CO: Total	0.033	0.034	3.745
NOx: Total	0.122	0.102	0.141
PM10: Total	0.010	0.039	0.029
PM2.5: Total	0.005	0.015	0.015
SOx: Total	0.041	0.069	0.006
VOC: Urban	0.003	0.074	0.112
CO: Urban	0.001	0.018	2.329
NOx: Urban	0.005	0.047	0.088
PM10: Urban	0.000	0.009	0.018
PM2.5: Urban	0.000	0.005	0.009
SOx: Urban	0.003	0.033	0.004

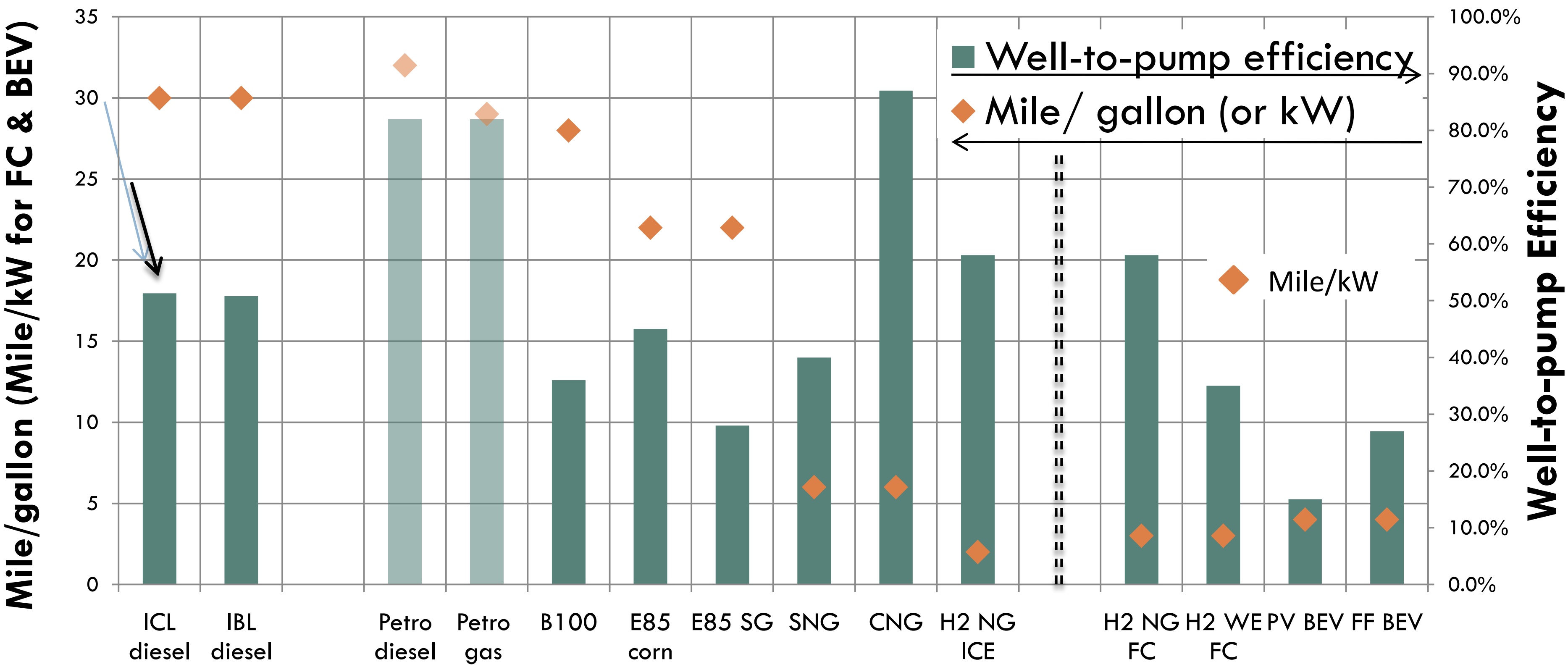
Dedicated CNGV

	Btu/mile or grams/mile		
Item	Feedstock	Fuel	Vehicle Operation
Total Energy	405	376	5,222
Fossil Fuels	402	325	5,222
Coal	14	238	0
Natural Gas	366	79	5,222
Petroleum	22	9	0
CO2 (w/ C in VO	29	31	310
CH4	1.246	0.042	0.146
N2O	0.000	0.000	0.012
GHGs	60	32	317
VOC: Total	0.032	0.003	0.139
CO: Total	0.045	0.008	3.745
NOx: Total	0.127	0.033	0.141
PM10: Total	0.005	0.042	0.029
PM2.5: Total	0.003	0.011	0.015
SOx: Total	0.061	0.072	0.001
VOC: Urban	0.001	0.000	0.086
CO: Urban	0.002	0.002	2.329
NOx: Urban	0.004	0.005	0.088
PM10: Urban	0.000	0.000	0.018
PM2.5: Urban	0.000	0.000	0.009
SOx: Urban	0.001	0.012	0.001

CO_2 emissions from GREET modeling



Fuel economies and production efficiencies



ASPENplus Software; GREET Software
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David Pimentel and Tad W. Patzek "Ethanol Production Using Corn, Switchgrass, and Wood; Biodiesel Production Using Soybean and Sunflower" *Natural Resources Research, Vol. 14, No. 1, March 2005 pages 65-76*
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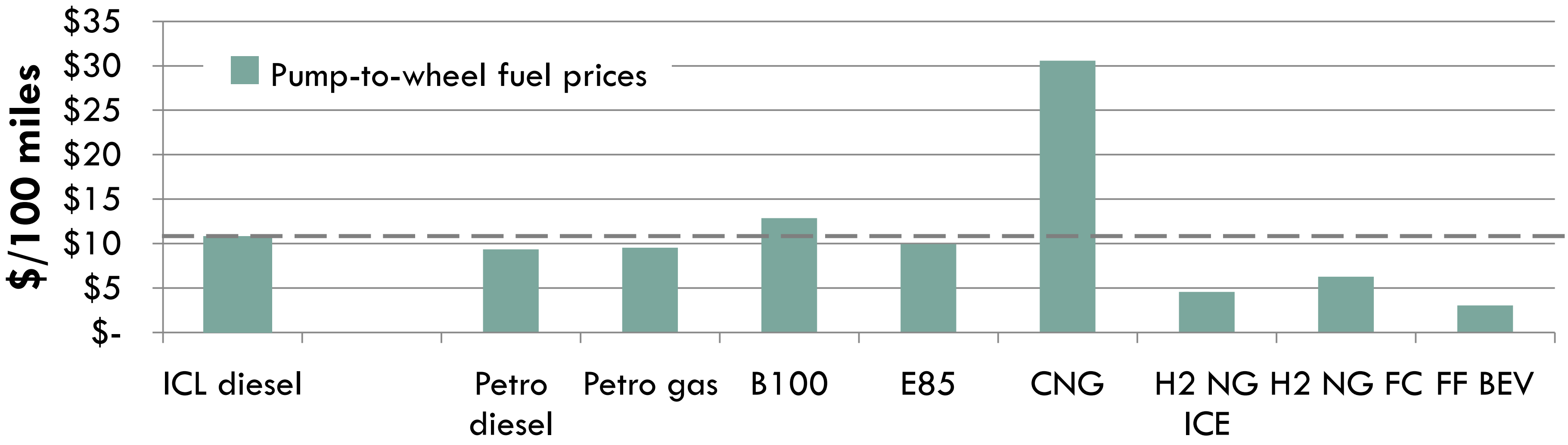
Yan, X. Y.; Inderwildi, O. R.; King, D. A., Biofuels and synthetic fuels in the US and China: A review of Well-to-Wheel energy use and greenhouse gas emissions with the impact

Economic and other comparisons



Other consideration examples:

- Environmental - 1 liter of ethanol -13 liters of wastewater; B100 - High NOx
- Energy - Farming considerations: Corn-9438 kWh/ha; Soy-4357 kWh/ha
- Economic – FC vehicles cost an average of $3,600 more with an average fuel cell costing 121$/m^2

"Liquid transportation fuels from coal and biomass" America's Energy Future Panel on Alternative Liquid Transportation Fuels, THE NATIONAL ACADEMIES PRESS Washington, DC www.nap.edu

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Conclusions

An indirect coal liquefaction plant in the US was simulated and results appeared comparable to the literature.

- Efficiency = 50%
- ROI ICL = 20% @ $97/bbl ($102/bbl w CCS)
- Emissions CO_2 = 102.9 kgCO_2/GJ fuel

ICL appears to be technically and economically sufficient to develop in the US and the main constraint at the moment is the environmental impact from CO_2 emissions compared to other transportation options.

THANK YOU

QUESTIONS?

F.T. model

- Assumptions:

  Steady-state operation; isothermal conditions; large-bubble flow in plug-flow regime due to its velocity; assumption of hydrocarbon products in the gas and liquid phases to be in equilibrium at the reactor outlet; negligible mass and heat transfer resistances between the catalyst and the liquid; location of the gas-liquid mass transfer limitation in the liquid phase; intrinsic kinetics for FT synthesis

- Kinetic parameters

Table 1. Kinetic Parameters for Fischer−Tropsch Synthesis in Iron Catalyst and for Water Gas Shift[2] [a]

k_{FTS}	0.1106 [mol/kg·s·MPa]
a	3.016
k_{WGS}	0.0292 [mol/kg·s]
K_1	85.81
K_2	3.07

[a] Obtained experimentally[2] at $T = 270$ °C, $P = 0.5-3.0$ MPa, and H_2:CO = 0.67−1.7.

[1] Fernandes, F. A. N. and E. M. M. Sousa (2006). "Fischer-Tropsch synthesis product grade optimization in a fluidized bed reactor." AIChE Journal 52(8): 2844-2850.