

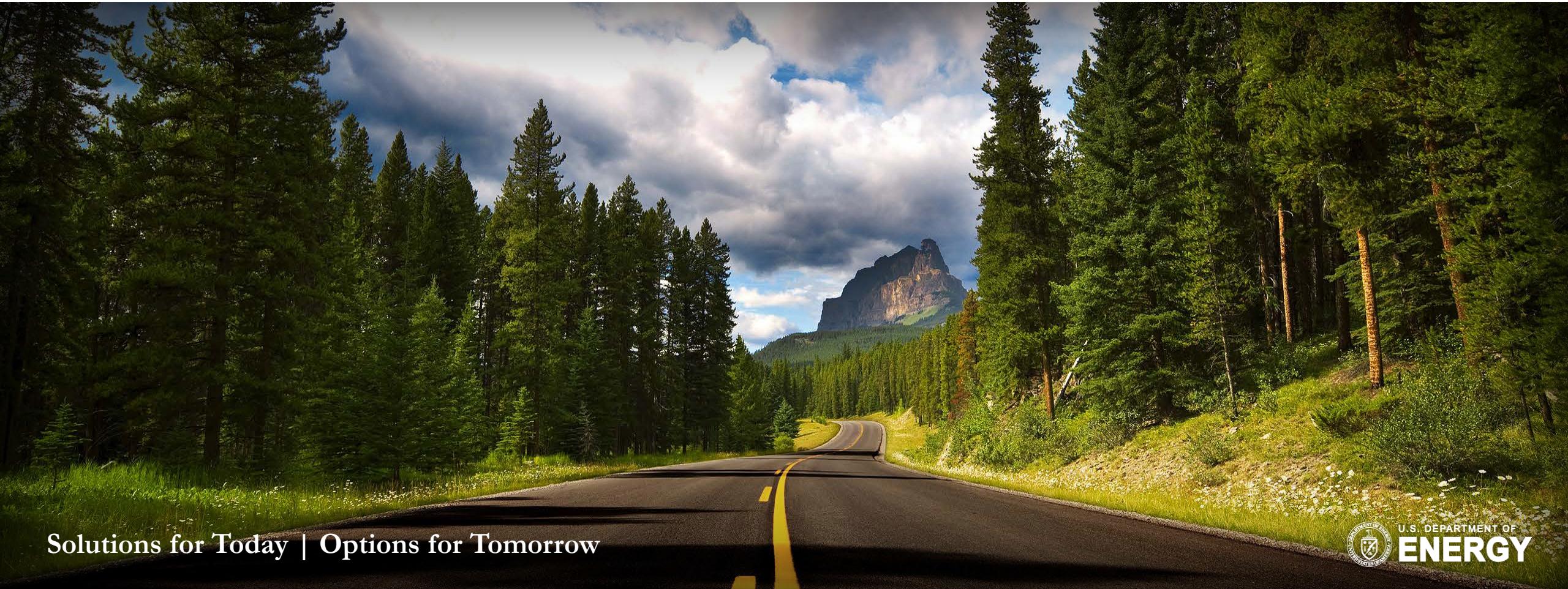
# Catalytic Gasifier-Based Direct Supercritical Carbon Dioxide (sCO<sub>2</sub>) System Study (NETL-PUB-21640)



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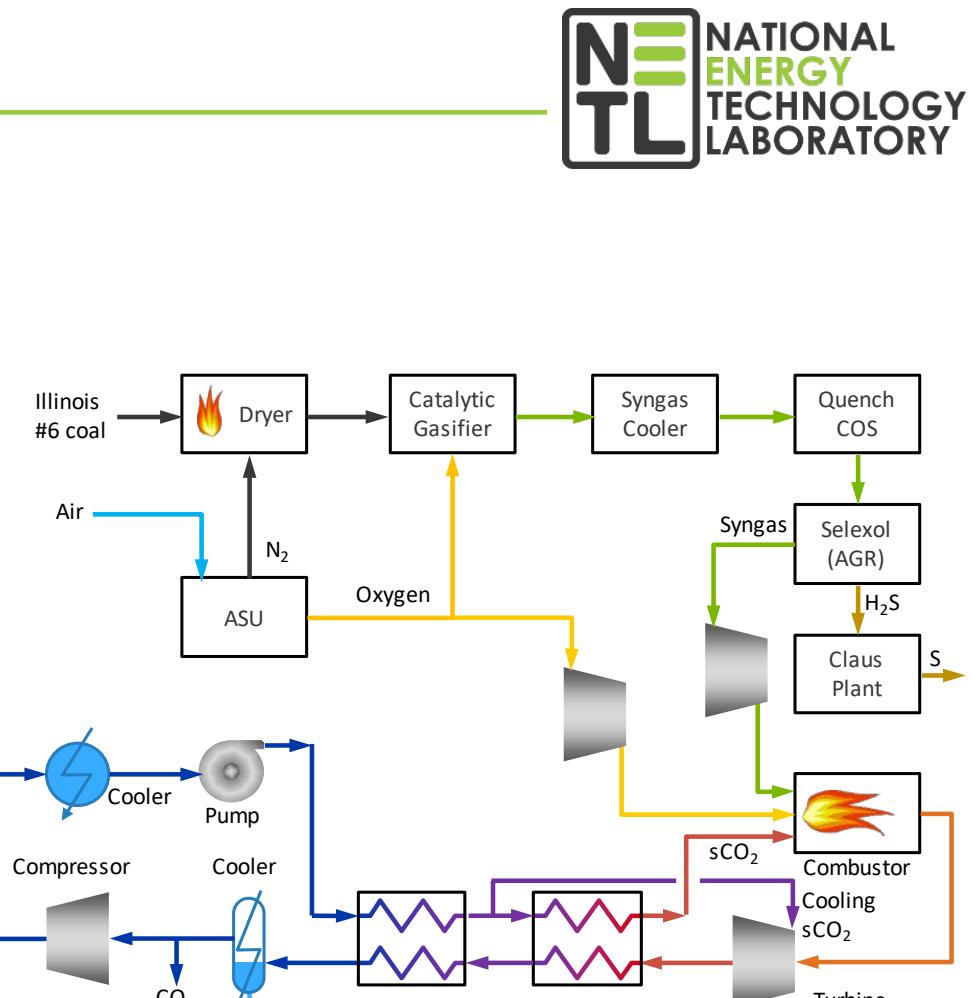
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# Outline

- Overview
- Catalytic Gasification
- Screening Study
- Options for thermal integration
- Process Tradeoffs
- Cases/Configurations
- Techno-economic Analysis Methodology
- Preliminary Performance Results
- Preliminary Conclusions

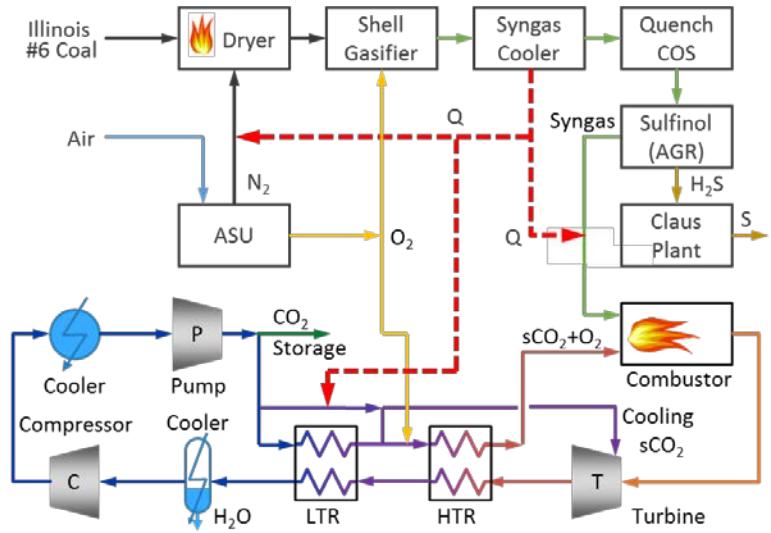


Source: NETL

# Overview

## NETL's Integrated Gasification Direct sCO<sub>2</sub> Cycle Study<sup>1,2</sup>

- Modeled two thermally-integrated Shell gasifier/direct sCO<sub>2</sub> plants with carbon capture<sup>1,2</sup>
  - Net plant thermal efficiency of 40.6% (HHV) with 99% carbon capture
  - 20% Cost of Electricity (COE) improvement over Shell IGCC system with carbon capture, mostly due to higher thermal efficiency
- Future gasification/direct sCO<sub>2</sub> analyses will consider different gasifier types and/or syngas cleanup strategies to improve plant efficiency
  - Catalytic gasification, GE quench and radiant gasifiers
  - In-situ syngas cleanup (i.e. 8 Rivers' approach) may improve efficiency to ~44%



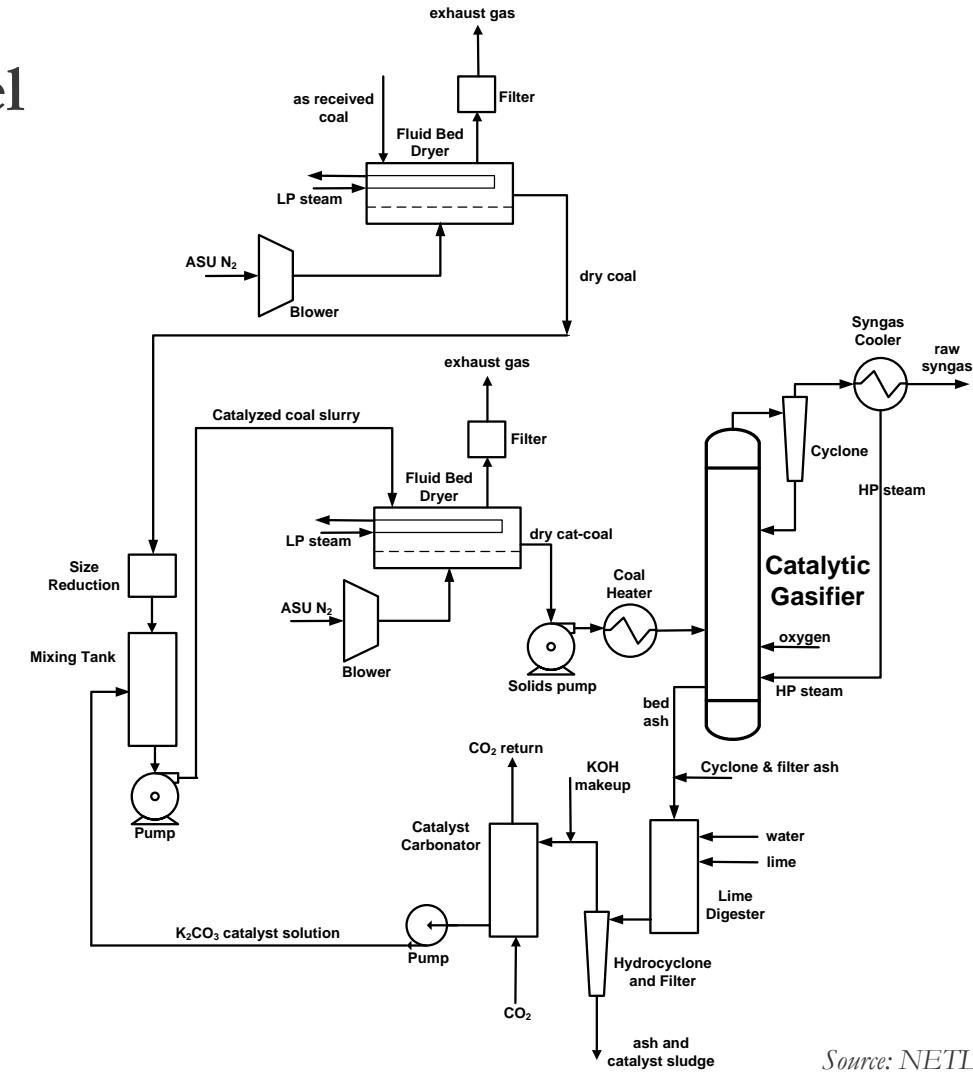


# Catalytic Gasification

## Why Catalytic Gasification?



- Potentially attractive process that reacts a fossil fuel (e.g. coal or petcoke) with steam using heat, pressure, and a suitable catalyst to produce a high heating value syngas (> 30% methane)
- Advantages include:
  - Single reactor for multiple processes (gasification, water gas shift, methanation)
  - Minimal oxygen, operation at 600 – 700 °C
  - Higher gasifier cold gas efficiency compared to conventional gasifiers
- Most recently in 2014 NREL conceptual study<sup>1</sup> which showed significant performance improvement for plants based on SOFC (Solid Oxide Fuel Cell) technology



Source: NETL

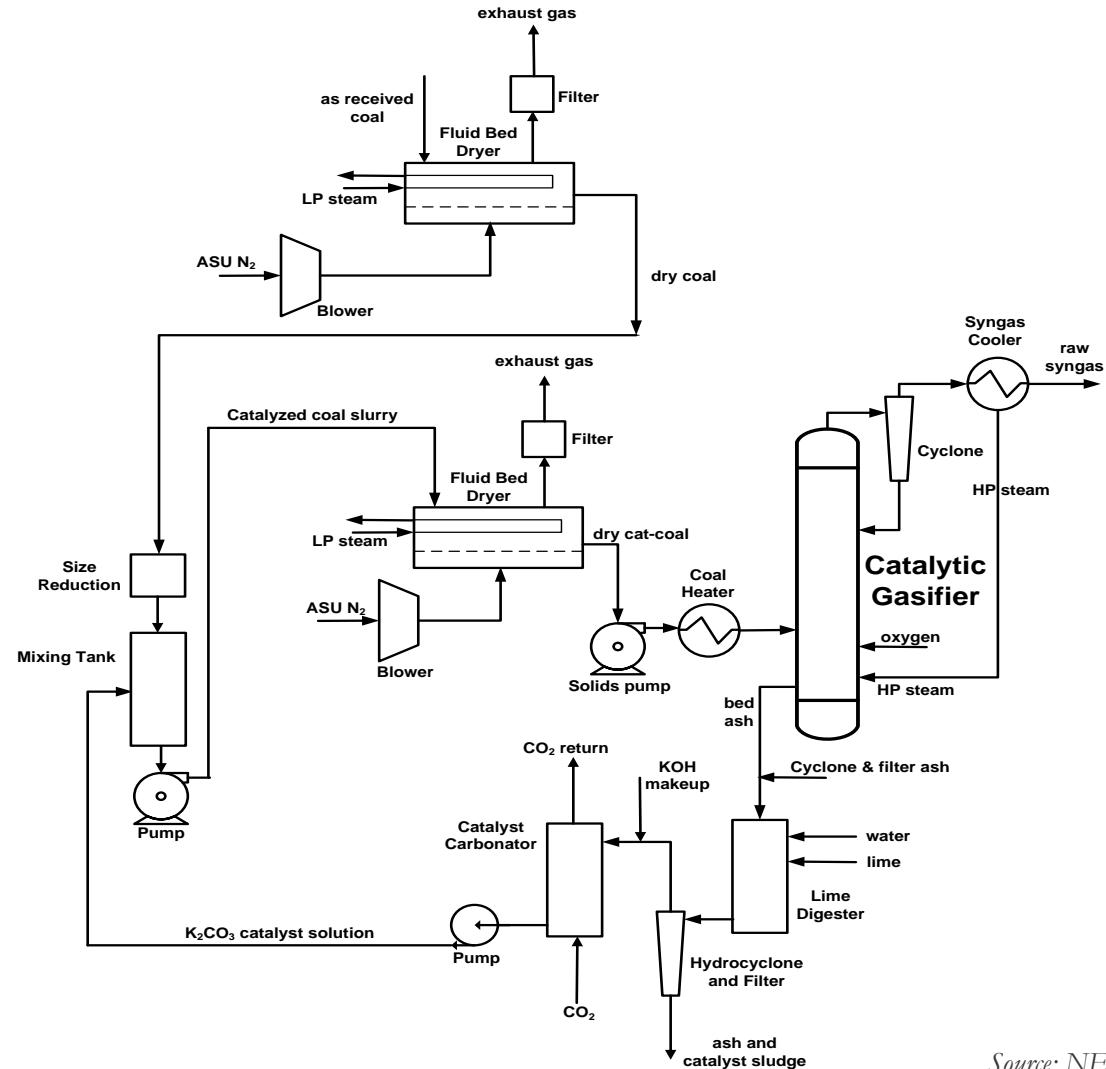


<sup>1</sup> Iyengar, A.K.S., Newby, R.A., Keairns, D.L., "Techno-Economic Analysis of Integrated Gasification Fuel Cell Systems", DOE/NETL- 341/112613, Pittsburgh, PA, November, 2014.

# Catalytic Gasification

# Pathway to High-methane Syngas

- High methane concentration in syngas favored by:
  - Low gasifier temperature
  - High gasifier pressure
  - High hydrogen content in feed streams
- Lower gasifier temperature necessitates catalyst to attain reasonable carbon conversions in reasonably sized vessels
- Only potential hydrogen sources are recycle hydrogen from syngas and steam

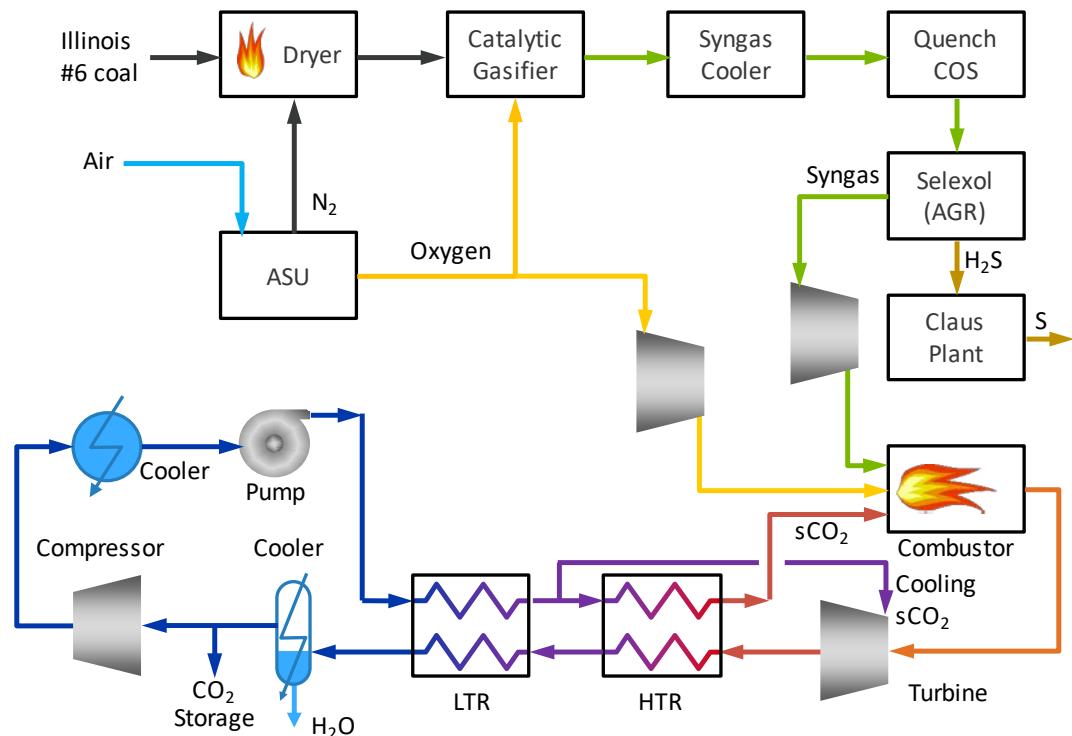


Source: NETL

# Screening Study

Objective: Determine if a catalytic gasifier offers advantages over the previously studied Shell-like gasifier as a fuel source for direct-fired sCO<sub>2</sub> power cycles with carbon capture and storage (CCS)

- Approach: Develop a performance and cost baseline for a syngas-fired direct sCO<sub>2</sub> cycle based on catalytic gasifier (CG)
- CG-direct sCO<sub>2</sub> plant design:
  - Oxy-fired catalytic gasifier designed to produce a high methane syngas
  - Low pressure cryogenic Air Separation Unit (ASU) with 99.5% oxygen purity
  - Oxy-syngas Combustor
  - Cooled sCO<sub>2</sub> turbine
  - Condensing sCO<sub>2</sub> cycle operation (CIT = 27 °C)
  - CO<sub>2</sub> purification unit (CPU) required to meet CO<sub>2</sub> pipeline purity specs



<sup>1</sup> Weiland, N.T., Shelton, W., Shultz, T., White, C.W., and Gray, D. "Performance and Cost Assessment of a Coal Gasification Power Plant Integrated with a Direct-Fired sCO<sub>2</sub> Brayton Cycle." Report: NETL-PUB-21435, 2017.

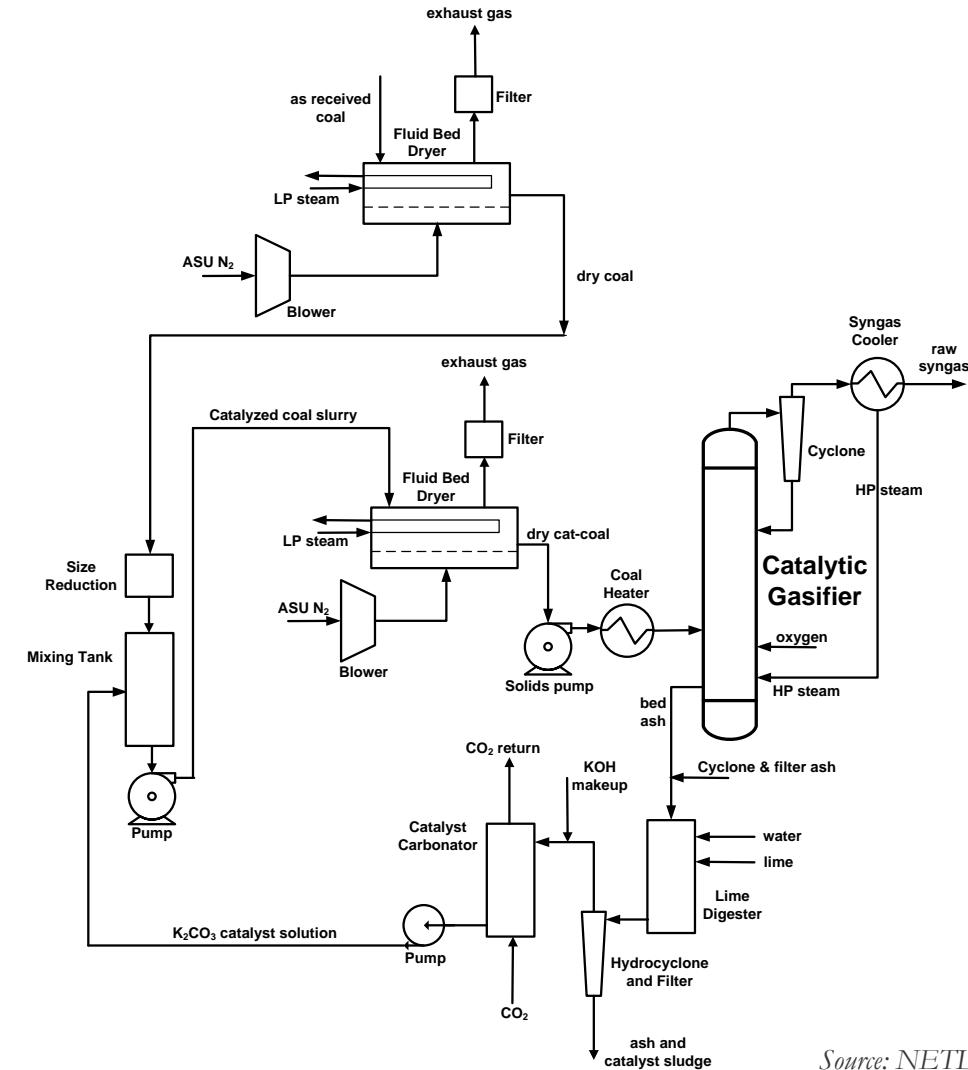
<sup>2</sup> Weiland, N.T., and White, C.W., "Techno-economic Analysis of an Integrated Gasification Direct-Fired Supercritical CO<sub>2</sub> Power Cycle," *Fuel*, **212**:613-625, 2018.

# Screening Study

# Catalytic Gasifier Model

## Assumptions and Limitations

- Catalytic gasifier modeled as near equilibrium reactor
- Steady-state operation
- Heat loss = 2% coal feed HHV
- Coal dried to 5% moisture
- 95% carbon conversion
- No transport gas
- O<sub>2</sub>:coal mass ratio to attain 704 °C temperature
- Steam:coal mass ratio = 1.45 (variable)
- Gasifier pressure = 67.2 bar

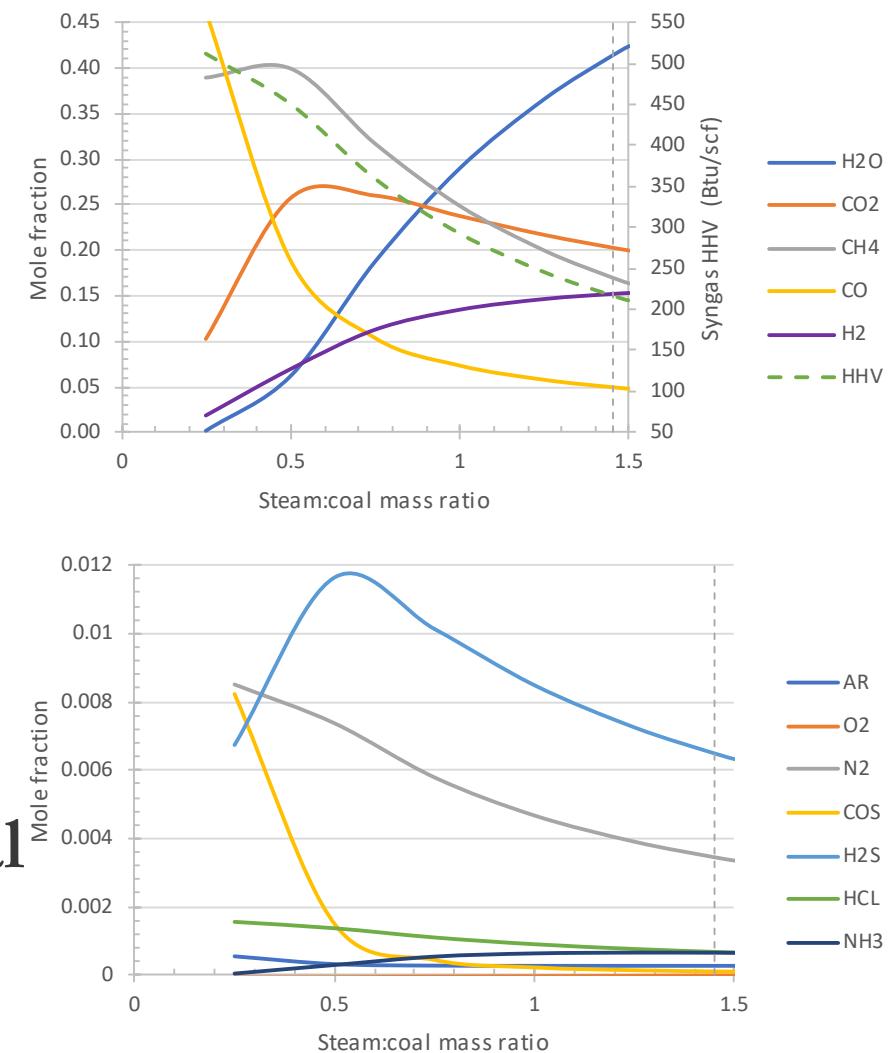


Source: NETL

# Screening Study

Syngas composition versus Steam:Coal mass ratio

- **Top Figure shows major syngas components and HHV**
  - $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{CO}$ ,  $\text{H}_2$
- **Bottom Figure shows minor syngas components**
  - Ar,  $\text{O}_2$ ,  $\text{N}_2$ , COS,  $\text{H}_2\text{S}$ ,  $\text{HCl}$ ,  $\text{NH}_3$
- Vertical dashed line corresponds to Steam:Coal mass ratio of 1.45



Source: NETL

# Screening Study

Catalytic Gasifier .vs. Shell Gasifier



- Table shows raw syngas mole fractions from:
  - Catalytic gasifier, steam:coal mass ratio = 1.45
  - Shell gasifier from: NETL Coal-Fired Gasifier Direct-Fired sCO<sub>2</sub> Study<sup>1,2</sup>
- Methane mole fractions on a dry syngas basis:
  - Catalytic gasifier = 0.291
  - Shell gasifier = 0.0001
- Dry syngas LHV:
  - Catalytic gasifier = 363 Btu/scf
  - Shell gasifier = 293 Btu/scf

Syngas Property	Catalytic Gasifier	Shell Gasifier
Mole %		
H <sub>2</sub> O	39.07	5.90
Ar	0.04	0.16
CO <sub>2</sub>	21.82	4.00
O <sub>2</sub>	0.00	0.00
N <sub>2</sub>	0.37	0.53
CH <sub>4</sub>	17.73	0.01
CO	5.43	62.21
COS	0.01	0.09
H <sub>2</sub>	14.71	26.12
H <sub>2</sub> S	0.69	0.82
HCl	0.07	0.10
NH <sub>3</sub>	0.06	0.07
Total	100.00	100.01

<sup>1</sup> Weiland, N.T., Shelton, W., Shultz, T., White, C.W., and Gray, D. "Performance and Cost Assessment of a Coal Gasification Power Plant Integrated with a Direct-Fired sCO<sub>2</sub> Brayton Cycle," Report: NETL-PUB-21435, 2017.

<sup>2</sup> Weiland, N.T., and White, C.W., "Techno-economic Analysis of an Integrated Gasification Direct-Fired Supercritical CO<sub>2</sub> Power Cycle," *Fuel*, 212:613-625, 2018.

# Screening Study

## Impacts of High-methane Syngas

- **Impact on Gasifier**

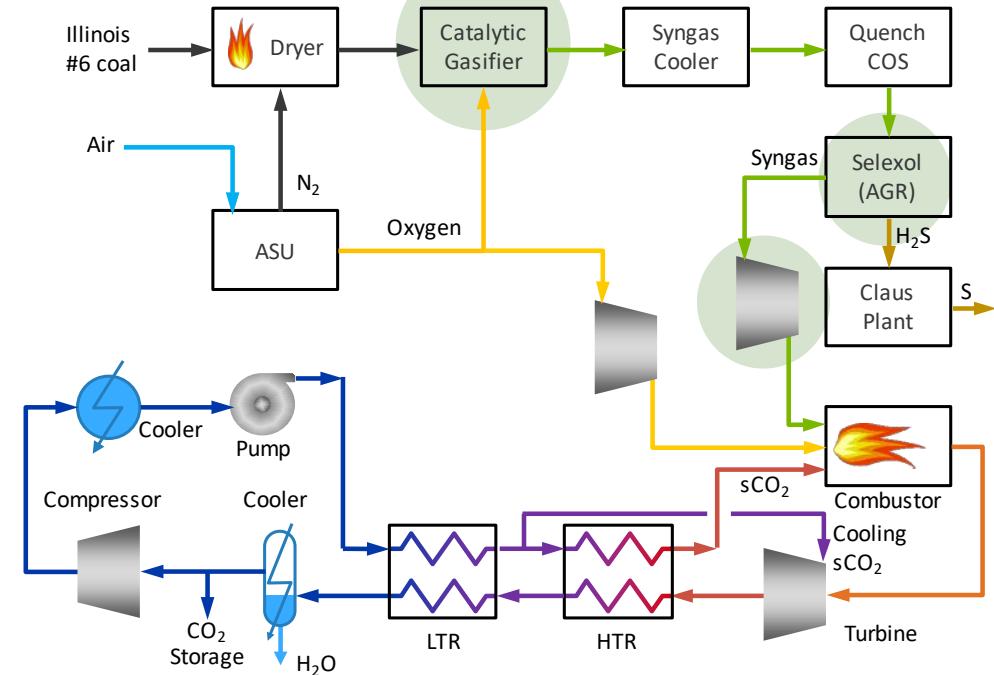
- More compact and lower cost
- Elimination of refractory lining

- **Impact on sCO<sub>2</sub> power cycle**

- Reduced syngas compressor power requirement

- **Impact on BOP**

- Higher cold gas efficiency
- Reduced syngas volumetric flow rate



Source: NETL



# Process Trade-offs

## Auxiliary Power Requirements

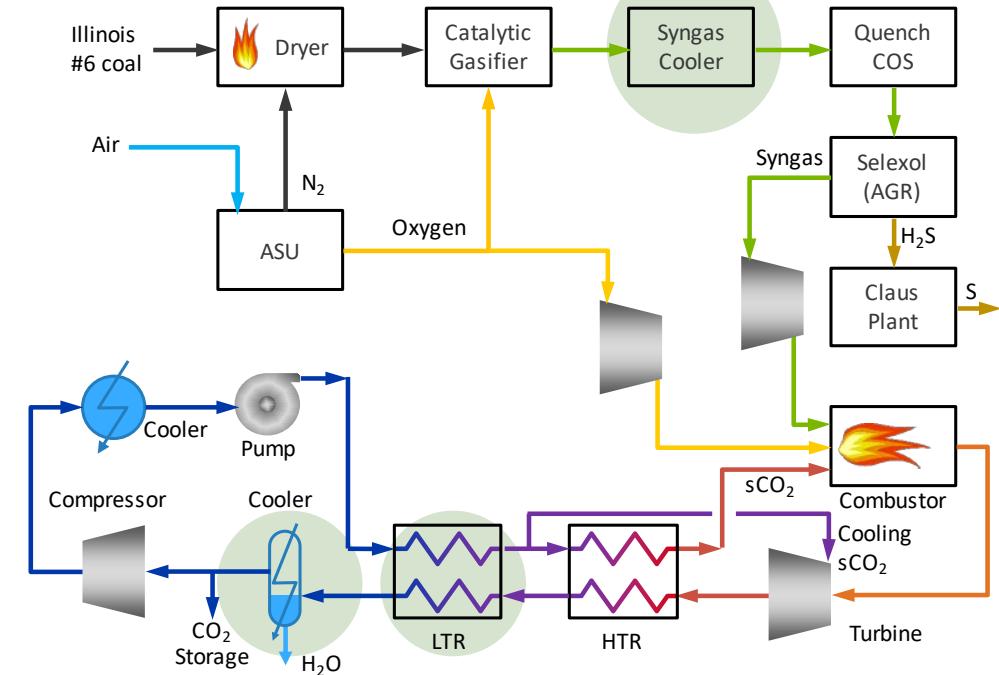


Process Section	Auxiliary Power Dependency	Catalytic Gasifier compared to Shell
ASU	Oxygen production rate	
Gasifier Island	Coal feed rate, Gasifier type	
Syngas Cooling	Syngas temperature, Flow rate	
Syngas Clean-up	Syngas flow rate, S capture process	
Steam Plant	Steam demand	
CPU	CO <sub>2</sub> generated	
sCO <sub>2</sub> Power Cycle	Oxygen, syngas feed rate	
Miscellaneous	Coal feed rate, plant efficiency	
Total		

# Process Trade-offs

## sCO<sub>2</sub> Power Cycle Performance

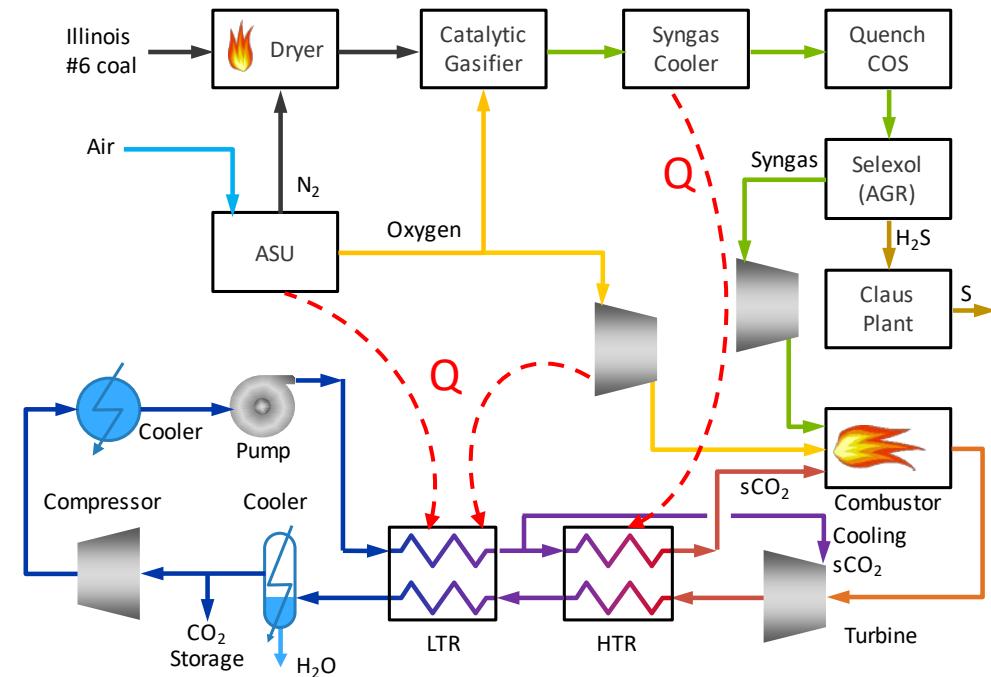
- Impact on thermal input to cycle
  - Less heat available from syngas coolers
  - Net thermal input from gasifier depends on carbon conversion and gasifier heat loss
- Impact on cycle losses and recuperation
  - Increased cooling requirement for H<sub>2</sub>O knock-out
  - Reduced LTR effectiveness due to condensation
- Impact on turbine output
  - No impact on TIT, turbine efficiency, cooling requirement, pressure ratio
  - Impact on net output will depend on net impact to cycle thermal input



Source: NETL

# Options for Thermal Integration

- sCO<sub>2</sub> power cycle efficiency can be increased if process heat can be harvested in the cycle
- Best locations for supplemental heating in the sCO<sub>2</sub> Recompression Brayton Cycle:
  - LTR – cold side, cold end – Helps overcome the higher thermal capacitance of the high pressure CO<sub>2</sub>
    - Potential sources include waste heat from ASU main air compressor and sCO<sub>2</sub> cycle oxygen compressor
  - HTR downstream – cold side – Allows more recycle CO<sub>2</sub> to be heated to turbine inlet temperature, increasing cycle output
    - Potential source is syngas cooling train but low gasifier temperature and high steam demand limit the amount of available high quality heat

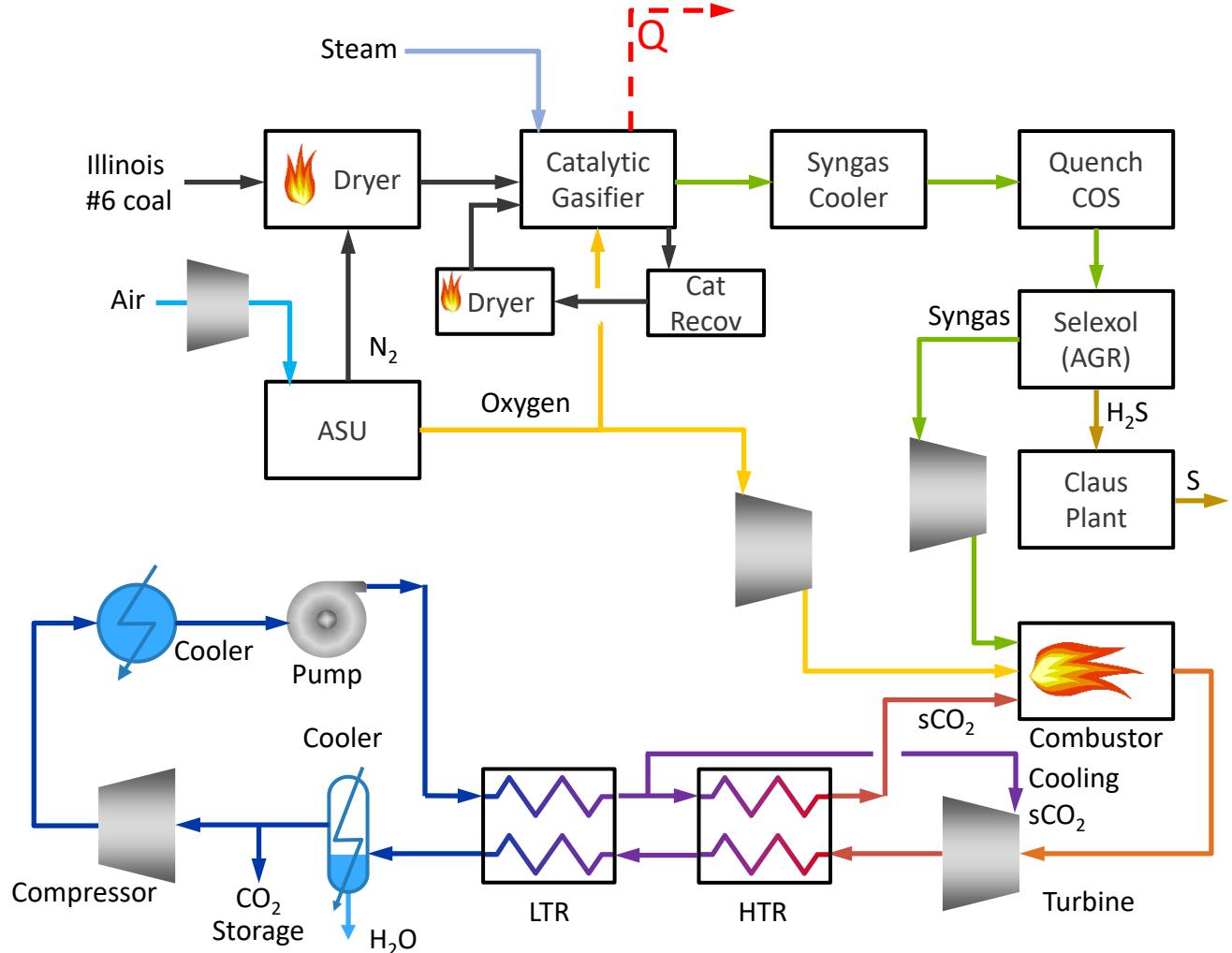


Source: NETL

# Cases/Configurations

## Baseline Configuration

- **Basic Recuperated, Condensing sCO<sub>2</sub> Brayton Cycle with:**
  - Coal drying to 5%
  - Steam:coal mass feed ratio 1.45
  - 95% carbon conversion in gasifier
  - 2% loss in gasifier



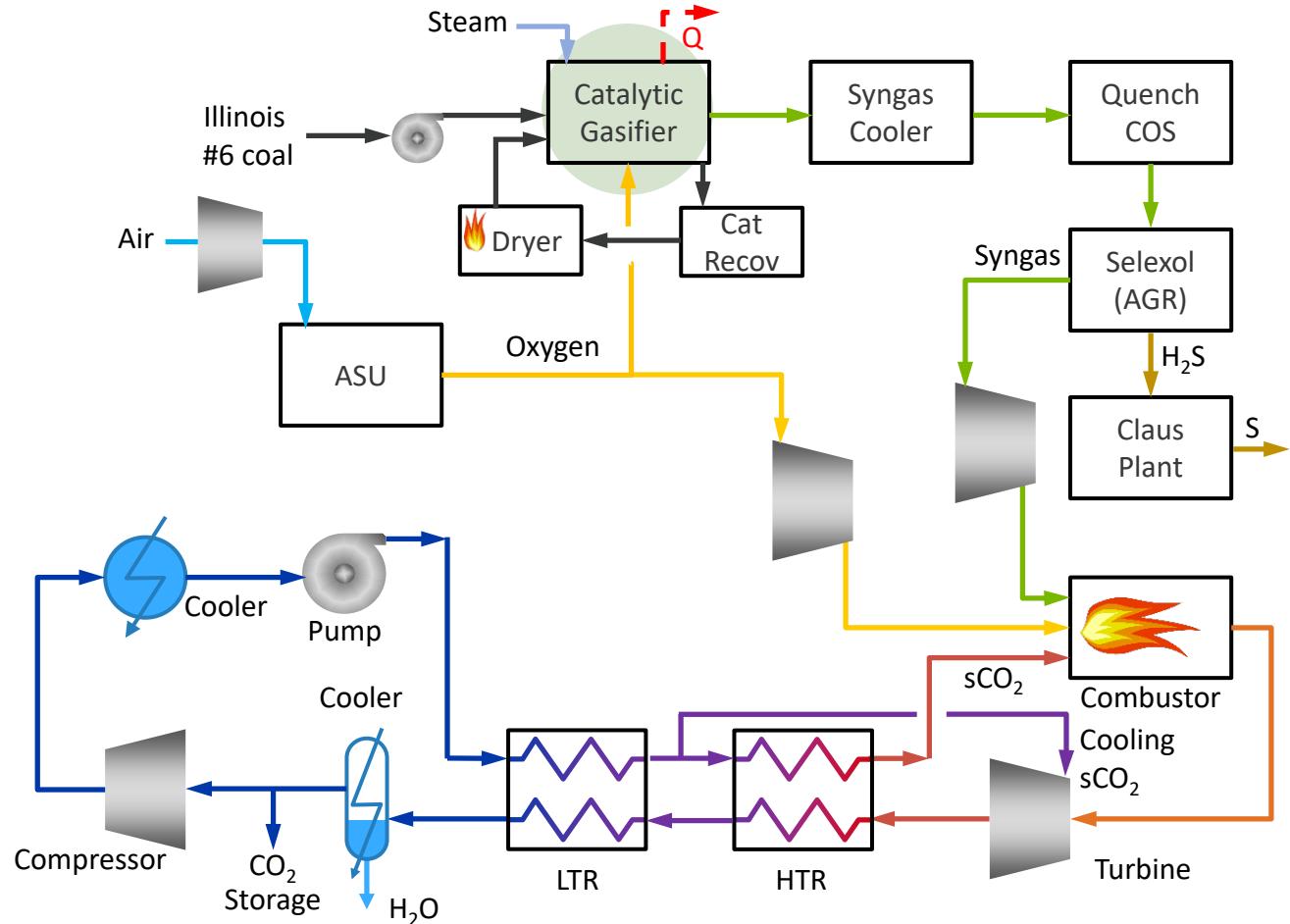
Source: NETL

# Cases/Configurations

# Advanced Catalytic Gasifier Configuration



- Similar to Baseline configuration with Basic Recuperated, Condensing sCO<sub>2</sub> Brayton Cycle, except:
  - No coal drying
  - Dry feed pump
  - Low steam feed to gasifier (0.25)
  - Higher carbon conversion in gasifier (99.5%)
  - Lower heat loss in gasifier (0.75%)

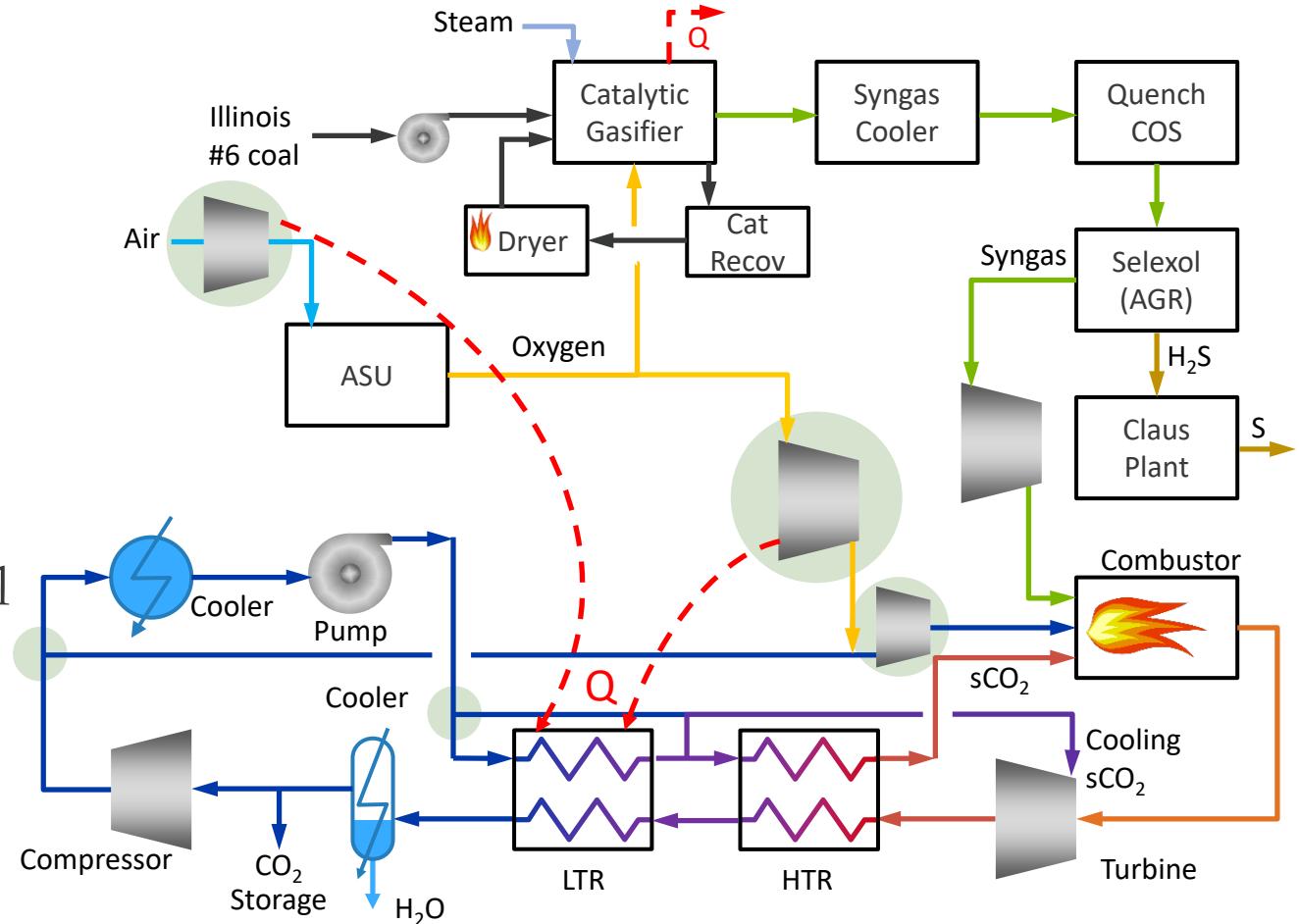


Source: NETL

# Cases/Configurations

Advanced Catalytic Gasifier with (low quality thermal integration)

- Same gasifier and BOP as in Advanced Catalytic Gasifier Configuration
- Recompression, Condensing sCO<sub>2</sub> Brayton Cycle with:
  - Low quality heat harvested from compressors
  - Improved turbine blade cooling model



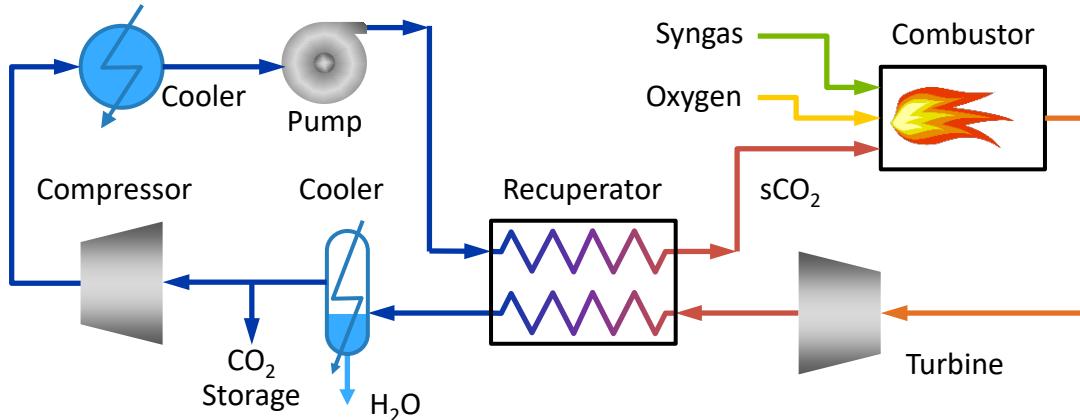
Source: NETL

# Techno-economic Analysis Methodology

# Direct-fired sCO<sub>2</sub> Power Cycle Performance Estimation



- System models for each case to be created using Aspen Plus®
- Steady-state lumped parameter models
- Physical property methods:
  - LK-PLOCK for sCO<sub>2</sub> power cycle
  - PENG-ROB for BOP
- When possible, Aspen models tuned to vendor performance data
- sCO<sub>2</sub> power cycle unit operations based on performance targets and discussions with turbomachinery and HX vendors



Source: NETL

Section	Parameter	Baseline sCO <sub>2</sub> Cycle
Combustor	O <sub>2</sub> purity	99.5%
	Excess O <sub>2</sub>	1%
	Pressure drop	689 kPa (100 psid)
	Heat loss	Zero
Turbine	Inlet temp	1204 °C (2200 °F)
	P <sub>inlet</sub>	30.0 MPa
	PR, P <sub>exit</sub>	10.2, 2.94 MPa
	Blade cooling	4.7%
Recuperator	Max temp	760 °C (1400 °F)
	Min T <sub>app</sub>	10 °C (18 °F)
	Pressure Drop	0.14 Mpa (20 psid) per side
CO <sub>2</sub> Cooler	Cooler/condenser	26.7 °C (80 °F)
	Cooling source	Cooling tower
Recompression	CO <sub>2</sub> bypass	18.1%
Compressor	P <sub>inlet</sub>	2.81 MPa
	P <sub>exit</sub>	7.93 MPa
	Isentropic efficiency	85%
	Stages	4 (3 intercooled)
CO <sub>2</sub> Pump	P <sub>exit</sub>	30.82 MPa
	Isentropic efficiency	85%
	Stages	2 (no intercooling)
CPU	Impurities	10 ppm O <sub>2</sub> max.



# Preliminary Performance Results

Baseline and Advanced Configurations

- **Baseline Case** shows a significant drop in process efficiency compared to Shell case due to:
  - Large steam demand for gasifier
- **Advanced Case** shows a 1.1 percentage point increase in process efficiency compared to Shell case due to:
  - Low steam demand for gasifier
  - Elimination of coal drying
- **Advanced Case with Thermal Integration**
  - In progress



Parameter	Shell	Catalytic Gasifier	
	Case 2	Baseline	Advanced
Coal flow rate (kg/hr)	198,059	198,059	198,059
Oxygen flow rate (kg/hr)	394,234	378,884	394,384
Cold gas efficiency (%HHV)	81.8	90.7	95.6
sCO <sub>2</sub> flow rate (kg/hr)	7,734,832	7,116,774	7,693,562
Carbon capture fraction (%)	99.4	94.4	98.9
Captured CO <sub>2</sub> purity (mol% CO <sub>2</sub> )	99.80	99.81	99.81
<b>Net plant efficiency (HHV %)</b>	<b>40.6</b>	<b>38.4</b>	<b>41.7</b>
Carbon conversion (%)	99.5	95.0	99.5
Power summary (MW)			
Coal thermal input (HHV)	1,493	1,493	1,493
sCO <sub>2</sub> turbine power output	988	933	996
sCO <sub>2</sub> pre-compressor power	76	70	77
sCO <sub>2</sub> pump power	72	64	70
Gross power output*	828	787	837
Total auxiliary power load	222	214	214
Net power output	606	573	623

\*Includes 1.5% generator loss

# Preliminary Conclusions

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- The catalytic gasifier appears to show no advantage over coal-fired direct-fired plant based on Shell gasifier when the catalytic gasifier is operated at the same feed conditions as used in the IGFC (Integrated Gasification Fuel-Cell Combined Cycle) TEA (Baseline Configuration)
  - High steam demand offsets potential benefits
- If the steam:coal ratio can be reduced to ~0.25, an efficiency improvement for the Baseline Catalytic Gasifier Case of up to 2 percentage points may be possible (Advanced Configuration)
- Thermal Integration (advanced case with low quality heat integration) may further increase efficiency by 0.5 – 1 percentage points
- Other potential improvements would also apply to all direct-fired sCO<sub>2</sub> systems (not unique to the catalytic gasification configuration)
- Performance does not appear to warrant additional work on catalytic gasification configurations (low TRL with no active R&D taking place)

Questions?  
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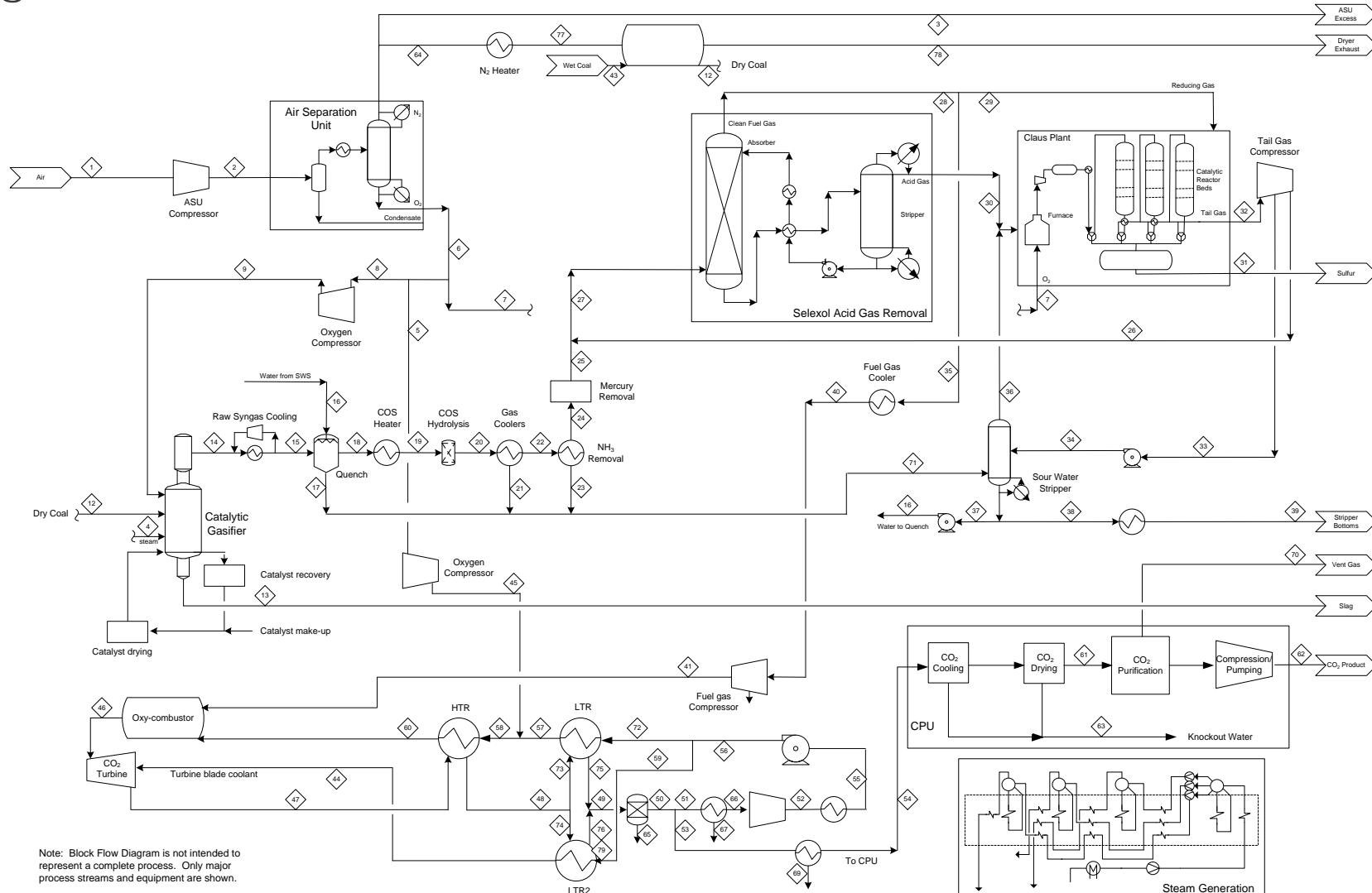


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# Detail Slides

# Configuration Options

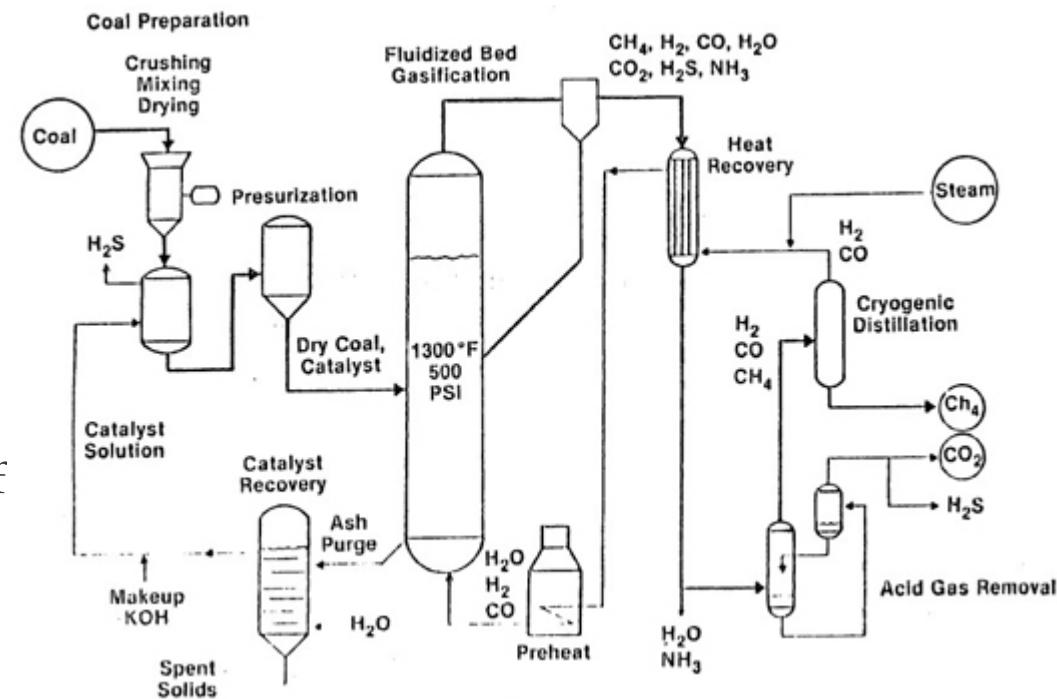
# Baseline Configuration



Note: Block Flow Diagram is not intended to represent a complete process. Only major process streams and equipment are shown.

## Catalytic Gasification Development

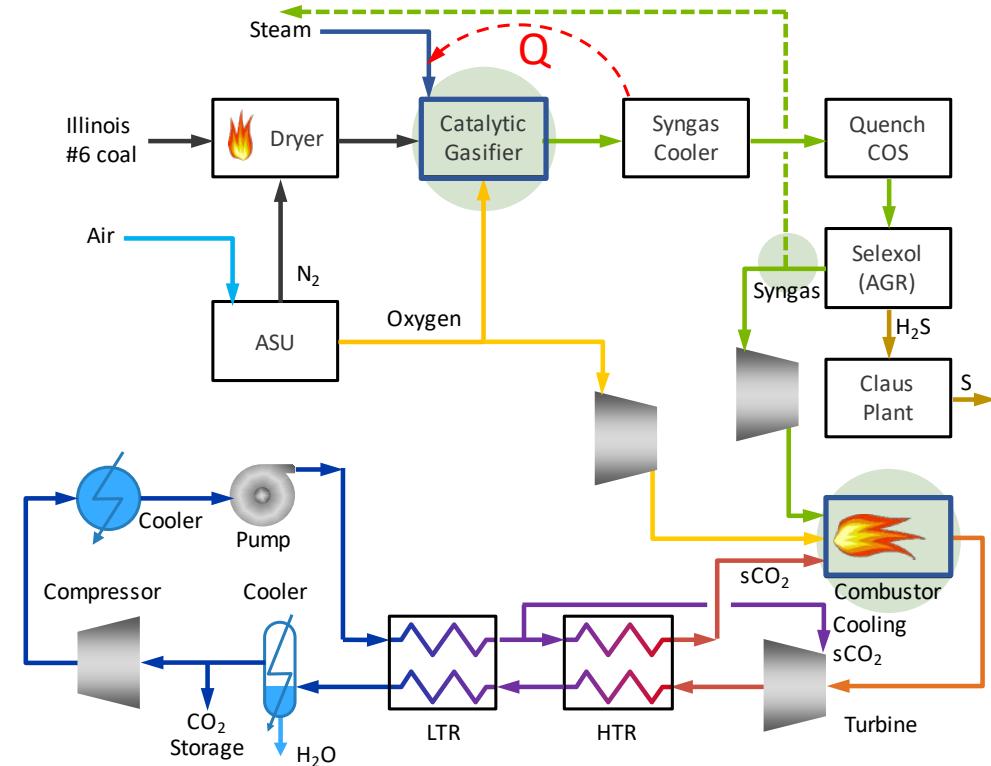
- Potentially attractive process that reacts:
  - Fossil fuel (e.g. coal or petcoke) +  $H_2O$  → High heating value syngas (> 30% methane)  
→ Pipeline-grade natural gas (> 99% methane)
  - High heating value syngas option uses oxy-fired gasifier
  - Pipeline-grade natural gas uses a high hydrogen recycle stream
- Primary development work (Pipeline-grade NG) by EXXON (1971-1982) included:
  - Lab studies to determine a catalyst ( $K_2CO_3$  with KOH makeup)
  - Some reaction rate models
  - Pilot plant testing
  - Planned demonstration unit (Holland) that was cancelled
- GreatPoint Energy (GPE) formed ~2005
  - Continued EXXON approach to commercialize the gasification of fossil fuel into a pipeline-grade natural gas (bluegas<sup>TM</sup>)
  - Projected market cost of bluegas:
    - \$3.92/MMBtu (PRB Coal)
    - \$3.34/MMBtu (Petcoke)
  - At the time (~2007), US natural gas cost was \$6-8/MMBtu
  - Due to changes in US natural gas prices, GPE efforts appear to cease ~2010



(source: Fischer-Tropsch Archive)

# Options for Steam Heat Sources

- **Syngas coolers**
  - Already being used to maximum extent
- **Catalytic gasifier water wall**
  - Increases gasifier O<sub>2</sub> demand and reduces syngas methane content
- **Oxy-combustor water wall**
  - Significantly reduces sCO<sub>2</sub> turbine output
- **Syngas-fired HP boiler**
  - Direct reduction in fraction of heat recovered by power cycle
- **Catalytic gasifier water wall appears to be best option from thermodynamic considerations**



Source: NETL

# Impacts on Process Efficiency ( $\eta_p$ )

Qualitative Assessment



- $\eta_R$  is fraction of fuel heating value absorbed by power cycle – depends on:
  - Gasifier cold gas efficiency
  - Syngas heat and mass recovery
  - Oxy-combustor heat losses
  - Gasifier carbon conversion
- $\eta_c$  is power cycle efficiency – depends on:
  - Turbine inlet temperature
  - Cycle pressure ratios (working fluid, fuel, and O<sub>2</sub>)
  - Recuperator effectiveness
  - Working fluid composition
  - Compressibility of working fluid, fuel, and O<sub>2</sub>

$$\eta_p = \frac{HHV_{coal} * \eta_R * \eta_c - P_{aux}}{HHV_{coal}}$$

$$\eta_p = \eta_R * \eta_c - \frac{P_{aux}}{HHV_{coal}}$$

# Impacts of High-methane Syngas on $\eta_R$

## • Impact on Gasifier

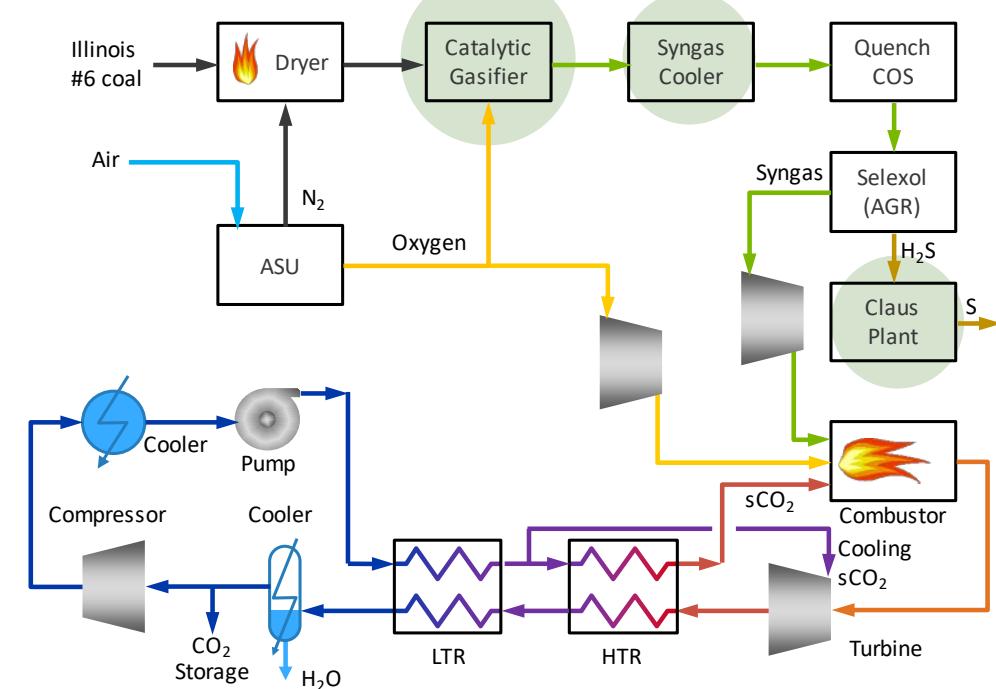
- Higher cold gas efficiency
- Higher heat loss
- Higher steam demand
- Lower carbon conversion

## • Impact on sCO<sub>2</sub> power cycle

- No impact on combustor heat loss
- No impact on combustion efficiency

## • Impact on BOP

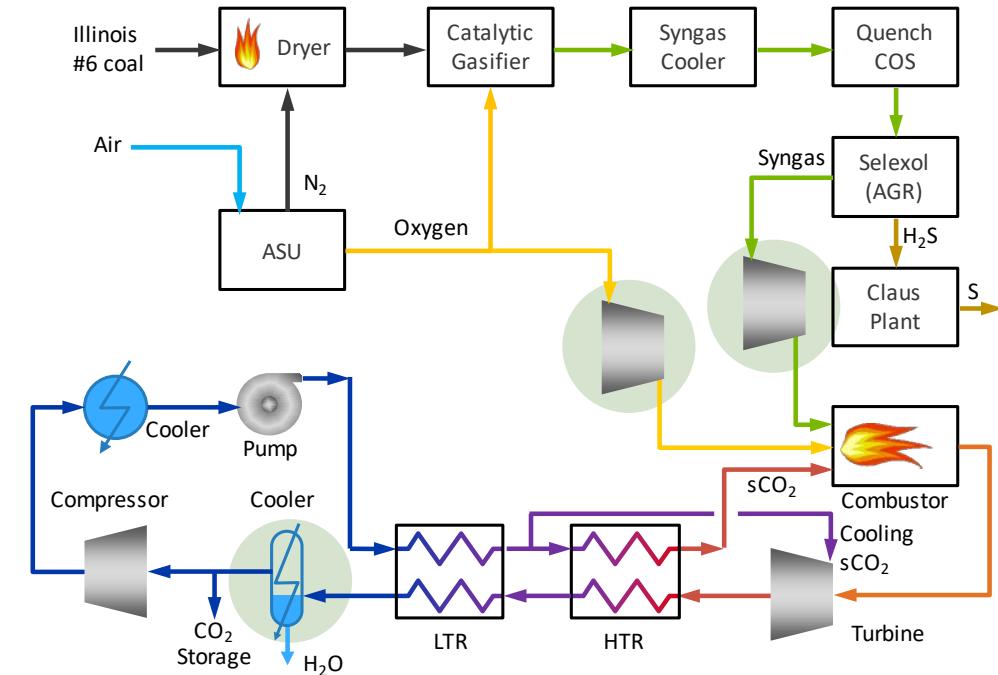
- Lower syngas heat recovery
- Increased syngas loss in sulfur recovery



Source: NETL

# Impacts of High-methane Syngas on $\eta_c$

- Lower syngas compressor power demand
  - Lower pressure ratio
  - Greater compressibility
- Greater O<sub>2</sub> compressor power demand
  - Greater O<sub>2</sub> requirement in oxy-combustor
- Increased H<sub>2</sub>O content in combustor effluent
- Lower LTR effectiveness due to condensation
- No impact on turbine:
  - Inlet temperature, efficiency, cooling requirement, pressure ratio
- Increased cooling requirement for water knock-out



Source: NETL



# Impacts of High-methane Syngas on $P_{aux}$

Compared to CFDF Case 2 with Shell gasifier



Process Section	Auxiliary Power Dependency	Catalytic Gasifier compared to Shell
ASU	Oxygen production rate	↓
Gasifier Island	Coal feed rate, Gasifier type	↓
Syngas Cooling	Syngas temperature, Flow rate	↓
Syngas Clean-up	Syngas flow rate, S capture process	↑
Steam Plant	Steam demand	↑
CPU	CO <sub>2</sub> generated	↓
sCO <sub>2</sub> Power Cycle	Oxygen, syngas feed rate	↑
Miscellaneous	Coal feed rate, plant efficiency	↓
<b>Total</b>		↓

# Impacts on Process Efficiency ( $\eta_p$ )

## Quantitative Assessment



- $\eta_R$  is estimated to increase 0 – 4%
  - Using IGFC conditions and assumptions
  - Impact depends strongly on steam:coal ratio
- $\eta_c$  is estimated to decrease by 7 – 10 %
- $P_{aux}$  is estimated to decrease by 7 – 15%
- $\eta_p$  is estimated to decrease by 0 – 4 percentage points

$$\eta_p = \frac{HHV_{coal} * \eta_R * \eta_c - P_{aux}}{HHV_{coal}}$$

$$\eta_p = \eta_R * \eta_c - \frac{P_{aux}}{HHV_{coal}}$$

# Screening Study Preliminary Conclusions



- The catalytic gasifier appears to show no advantage over coal-fired direct-fired plant based on Shell gasifier when the catalytic gasifier is operated at the same feed conditions as used in the IGFC TEA
  - High steam demand offsets potential benefits
- If the steam:coal ratio can be reduced to ~0.25, an efficiency improvement for the Baseline Catalytic Gasifier Case of up to 2 percentage points may be possible