High Inlet Temperature Combustor for Direct Fired Supercritical Oxy-Combustion

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Outline

- Project Overview
  - Project Objectives
  - sCO2 Background
  - Technical Challenges
- Selected Progress Update
  - Cycle Evaluation
  - Kinetic Models
  - Supercritical Oxy-Combustor Design

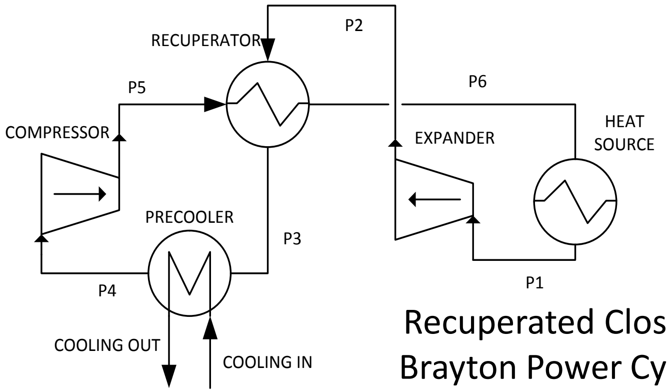
PROJECT OVERVIEW

Project Objectives

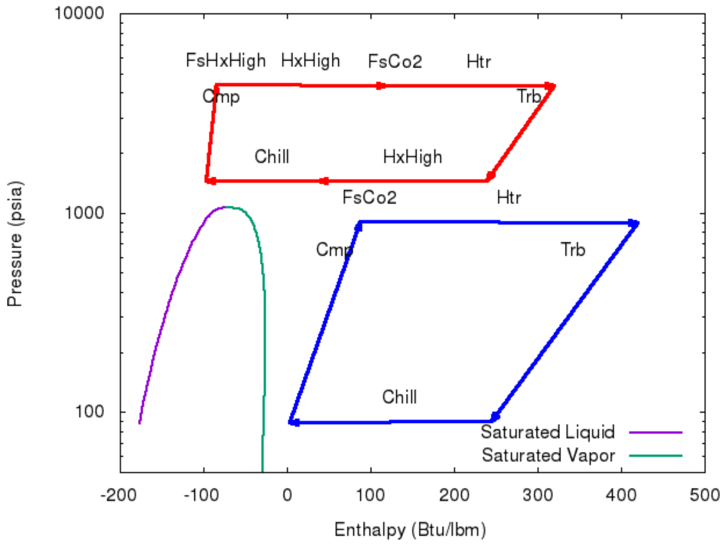
- Optimize the supercritical CO2 power cycle for direct fired oxy-combustion
  - Target plant conversion efficiency is 52% (LHV)
- Technology gap assessment for direct fired plant configurations
- Develop a high inlet temperature oxy-combustor suitable for the optimized cycle
  - Target fuels are Natural Gas and Syngas

What is a sCO2 cycle?

- Closed Brayton Cycle
  - Working fluid is CO2
- Cycle Type
  - Vapor phase
  - Transcritical
  - Supercritical
- Supercritical CO2 has:
  - High fluid density
  - High heat capacity
  - Low viscosity

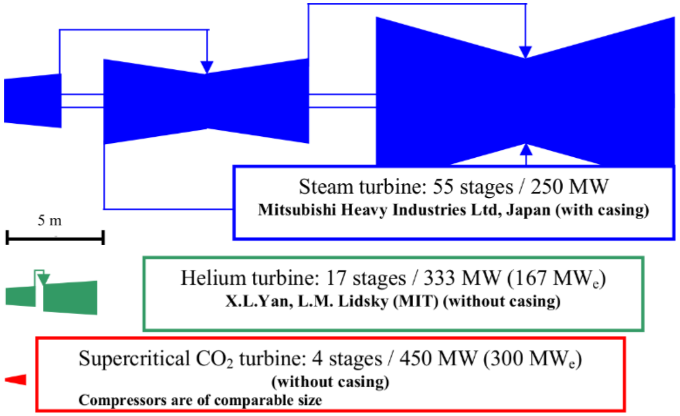


Recuperated Closed Brayton Power Cycle



Why sCO2 Power Cycles?

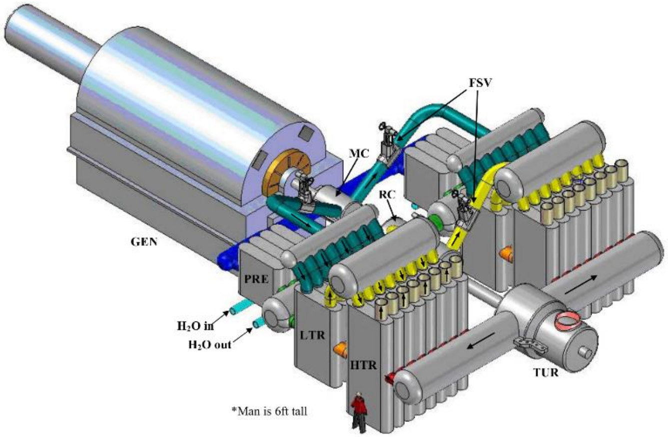
- Offer +3 to +5 percentage points over supercritical steam for indirect coal fired applications
- High fluid densities lead to compact turbomachinery
- Efficient cycles require significant recuperation
- Compatible with dry cooling techniques



Steam turbine: 55 stages / 250 MW
Mitsubishi Heavy Industries Ltd, Japan (with casing)

Helium turbine: 17 stages / 333 MW (167 MW_e)
X.L.Yan, L.M. Lidsky (MIT) (without casing)

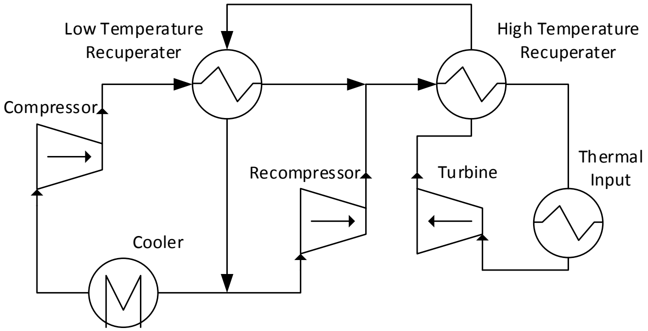
Supercritical CO_2 turbine: 4 stages / 450 MW (300 MW_e)
(without casing)
Compressors are of comparable size

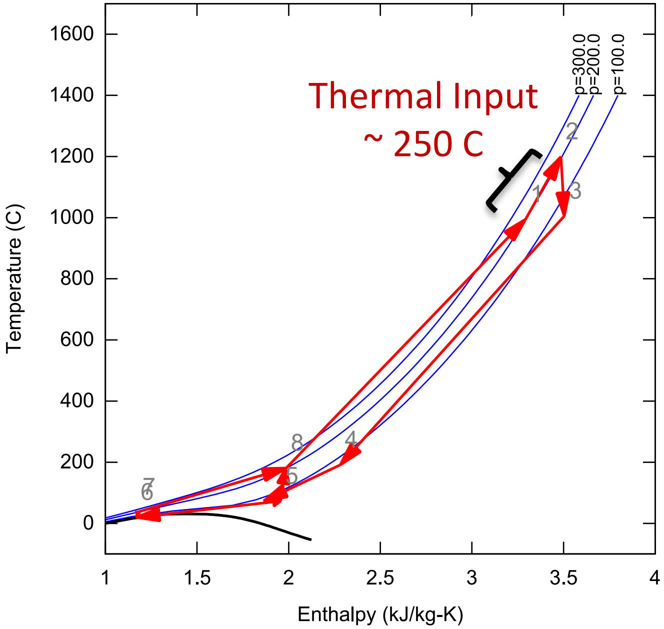


Third Generation 300 MWe S-CO2 Layout from Gibba, Hejzlar, and Driscoll, MIT-GFR-037, 2006

Why Oxy-Combustion?

- High efficiency cycles are highly recuperated
  - Unique thermal integration challenges
- Direct fired configurations remove at least two heat exchangers
- Supercritical oxy-combustion is well suited for integrated CCS





Flavors of Oxy-Combustion

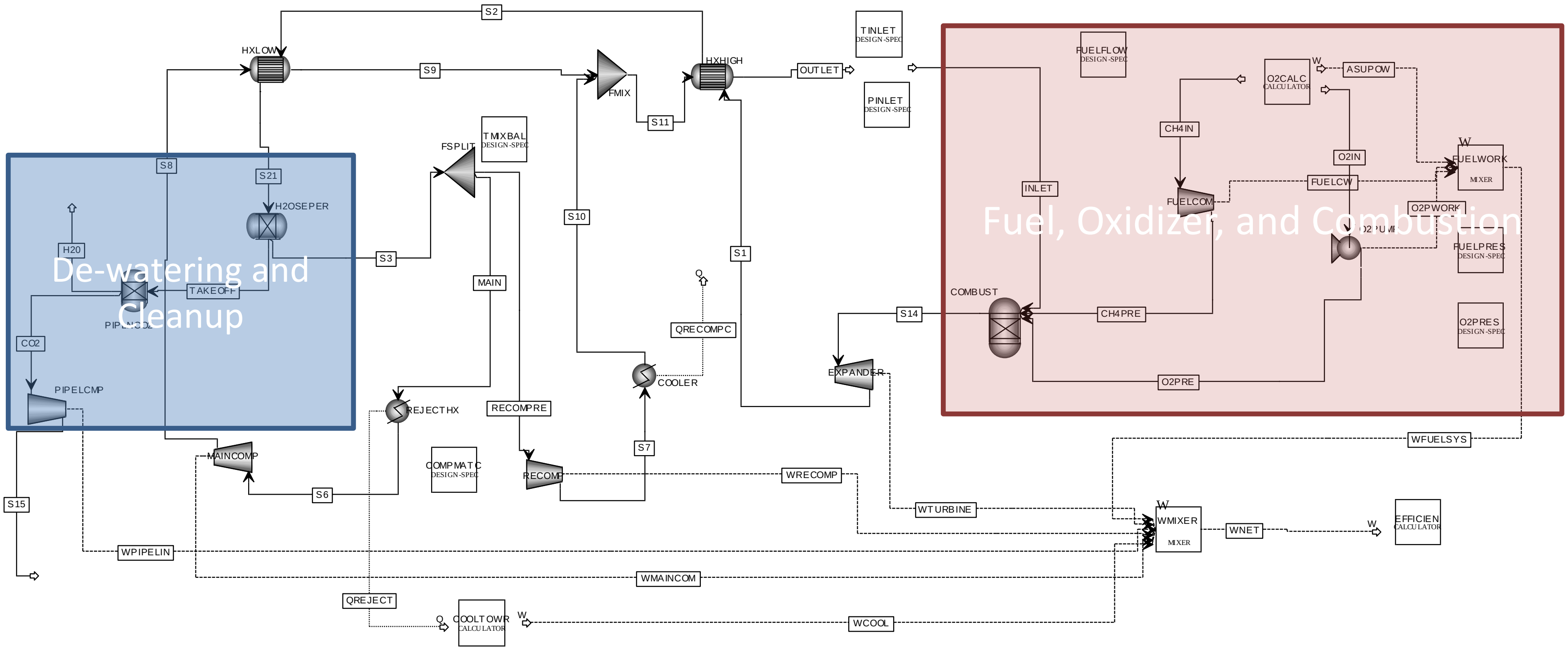
- Flue Gas Recirculation
  - Combustion at near ambient pressures
  - Recycled flue gas is mixed with incoming air
  - Increases flame temperatures
  - Increases CO2 concentration for CCS
- Pressurized Oxy-combustion
  - Combustion at elevated pressure (~ 10 bar)
  - Latent heat is recoverable and heat transfer rates are increased
  - Minimizes air in-leakage
- Supercritical Oxy-combustion
  - Combustion occurs at supercritical pressures (>74 bar)
  - Required for direct fired sCO2 cycles, compatible with indirect cycles
  - CO2 acts as a solvent in dense phase, accelerating certain reactions
  - Compression requirements drive closed combustion solutions
  - Flue gas cleanup and de-watering at pressure may be challenging

Progression

- System Design and Thermodynamic Analysis
  - Evaluate cycles to determine combustor design parameters
- System level Technology Gap Assessment
- Kinetics Models
  - Evaluate kinetic models to determine applicability
  - Initial kinetic evaluation at combustor inlet conditions
- Combustor Concept
  - Material constraints at 1000 C 200 bar inlet, 1200 C 200 bar outlet conditions
- Combustor demonstration

SYSTEM ENGINEERING DESIGN AND THERMODYNAMIC ANALYSIS

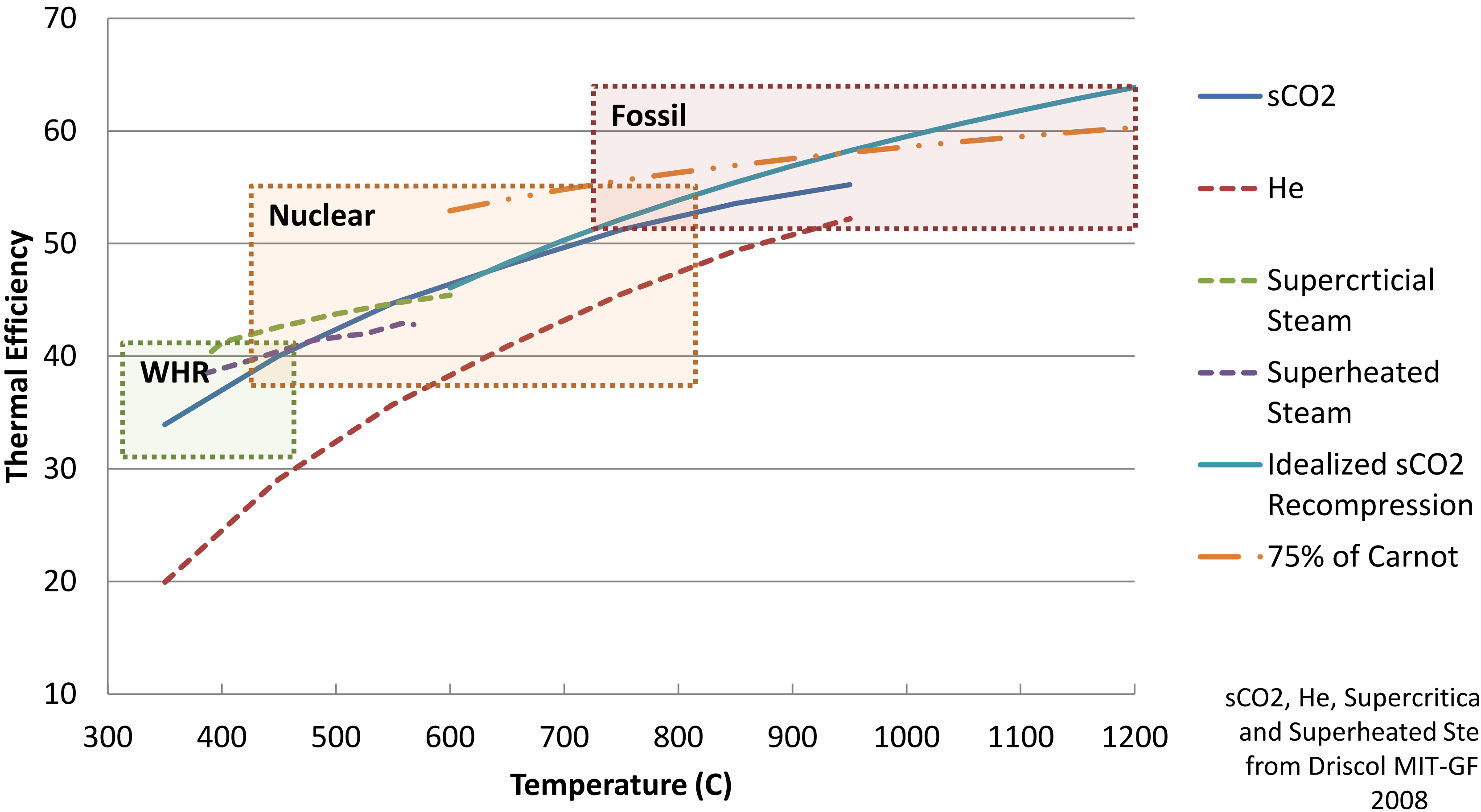
Oxy-Combustion Plant Model



Direct Fired Supercritical Oxy-Combustion

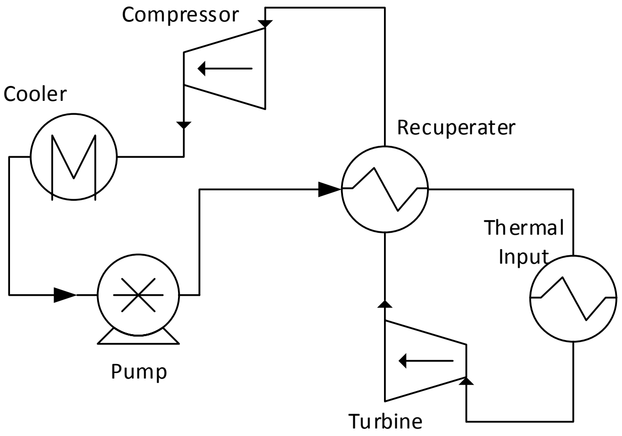
- Plant evaluation factors power cycle layout, environmental conditions, component performance, and secondary systems
- Plant optimization focused on thermal efficiency
  - *Target 52% plant efficiency to compete with NGCC*
  - Drives 64% power cycle thermal efficiency
  - *Turbine inlet near 1200°C*

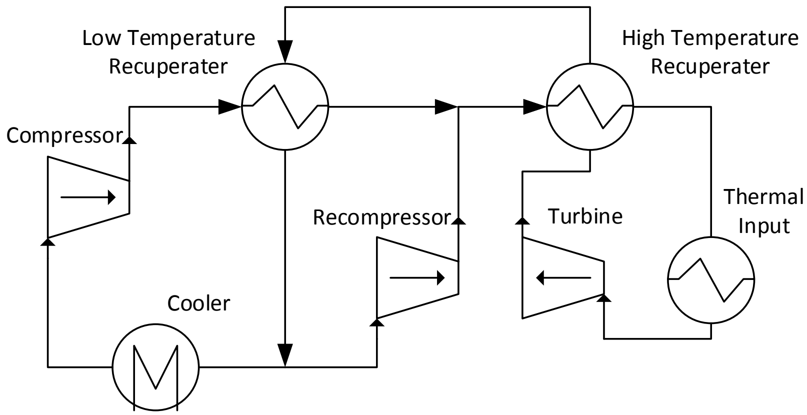
Representative Cycle Efficiencies

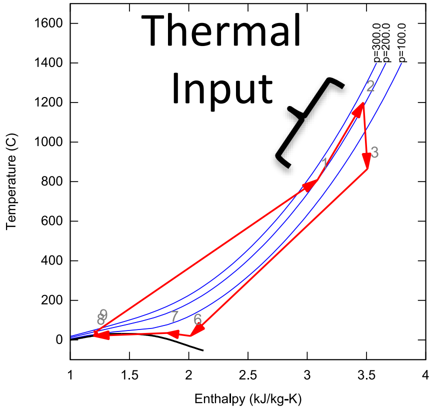


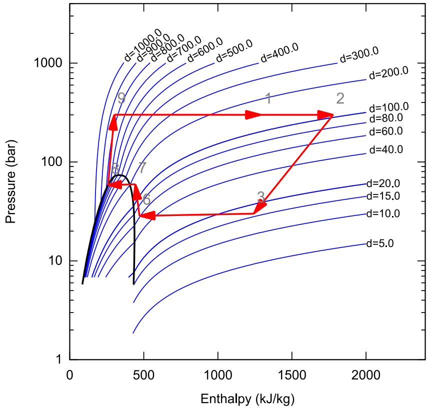
sCO2, He, Supercritical Steam, and Superheated Steam are from Driscol MIT-GFR-045, 2008

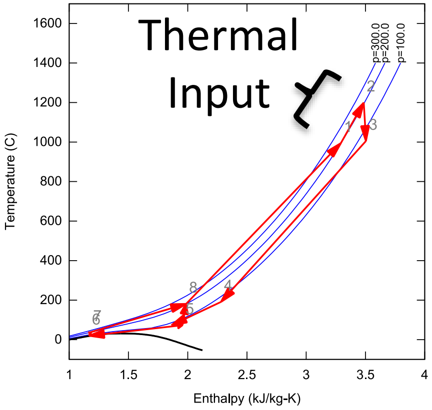
Partial Condensation and Recompression Cycles

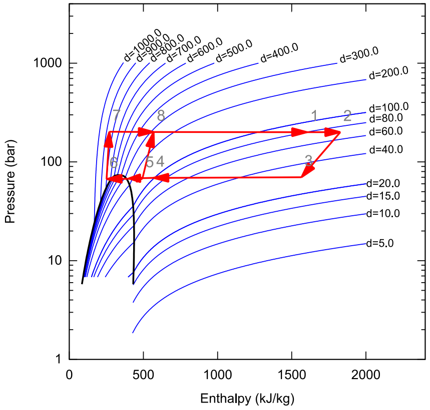












Cycle Comparison

	Single Recuperator Condensation	Single Recuperator Condensation	Recompression	Recompression
Net fuel to bus bar plant efficiency	54.03%	51.60%	56.73%	53.44%
Total Recouperation (kW)	989.91	1078.16	1163.44	1205.34
HE Duty per Net Power Ratio (kW/kW)	2.48	3.21	4.34	6.55
Power per Mass Flow Ratio (kJ/kg)	399.06	335.38	268.08	183.92
Combustor Inlet Temp. (°C)	755.18	808.60	918.16	994.37
Combustor Inlet Pres. (bar)	300.00	200.00	300.00	200.00

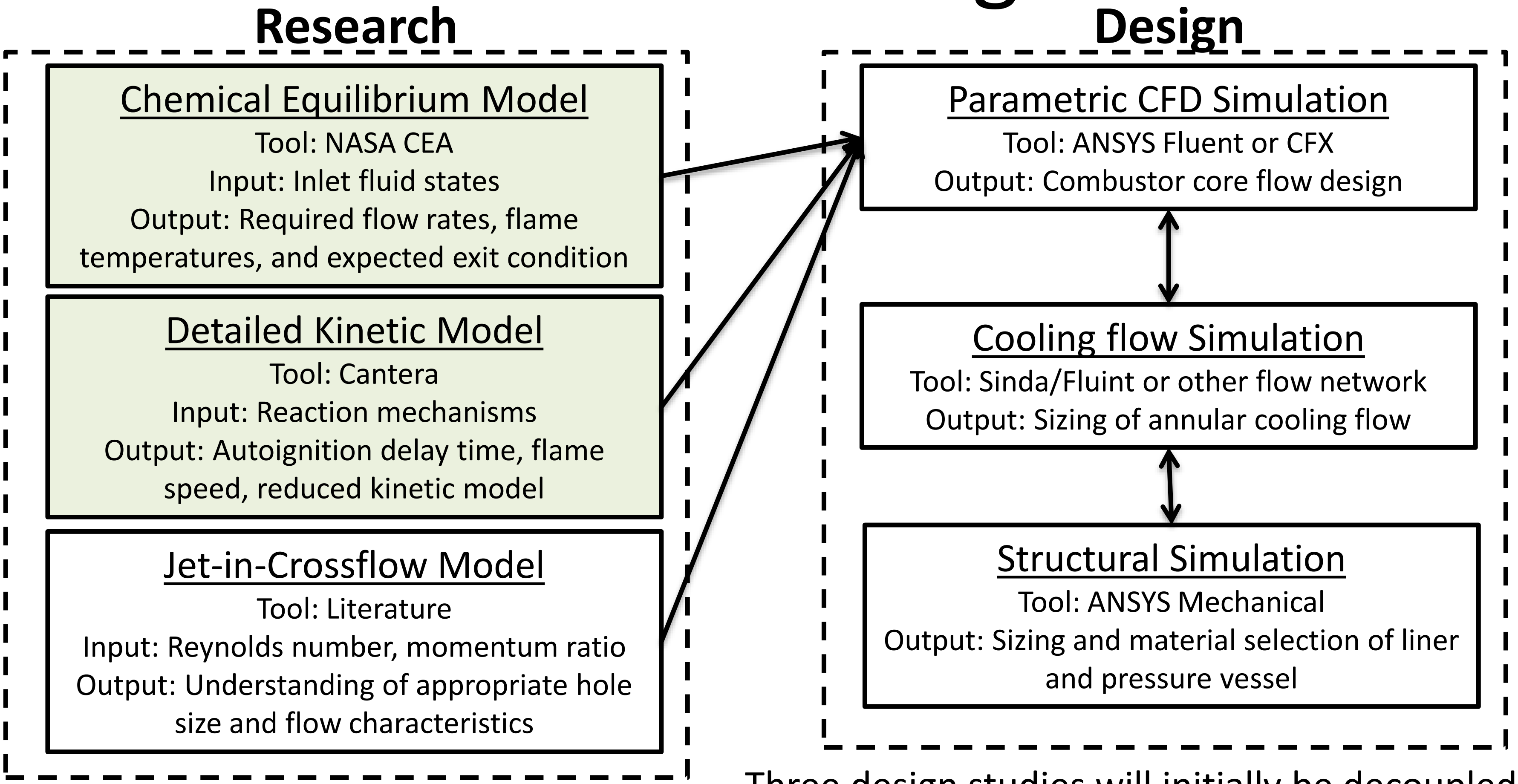
** Cycles evaluated at 1200°C Turbine Inlet Temperature and unit 1 kg/s mass flow

Cycle Analysis Results

- Recompression cycle has highest efficiency by 1.8% at 200 bar, 2.7% at 300 bar
- Condensation cycle is superior in all other metrics
  - Reduced recuperation (~ 50%)
  - Lower combustor inlet temperature
  - Higher power density (power output / flow rate)
- Both cycle configurations are compatible with an *auto-ignition* style combustor for 1200 C Turbine inlet temperatures.

COMBUSTION KINETICS

Research and Design Path



Research

Chemical Equilibrium Model
Tool: NASA CEA
Input: Inlet fluid states
Output: Required flow rates, flame temperatures, and expected exit condition

Detailed Kinetic Model
Tool: Cantera
Input: Reaction mechanisms
Output: Autoignition delay time, flame speed, reduced kinetic model

Jet-in-Crossflow Model
Tool: Literature
Input: Reynolds number, momentum ratio
Output: Understanding of appropriate hole size and flow characteristics

Design

Parametric CFD Simulation
Tool: ANSYS Fluent or CFX
Output: Combustor core flow design

Cooling flow Simulation
Tool: Sinda/Fluint or other flow network
Output: Sizing of annular cooling flow

Structural Simulation
Tool: ANSYS Mechanical
Output: Sizing and material selection of liner and pressure vessel

Three design studies will initially be decoupled, but may be performed iteratively or become fully coupled if needed.

Kinetic Model: Motivation

- The fundamental size of the combustor is governed by the timescale of chemical reactions
- The chemical reaction kinetics determine how fast fuel oxidation occurs
  - A detailed chemical kinetic model is required to size the combustor
  - A reduced chemical kinetic model is required for detailed flow-field design in CFD

Chemical Mechanisms

Sample Methane Oxidation Mechanisms for Same Overall Reaction

Species: 4 Reactions: 1

$CH_4 + 2\ O_2 \rightarrow 2\ H_2O + CO_2$ $\qquad r = AT^n e^{-\frac{E_a}{RT}}[CH_4]^a[O_2]^b$

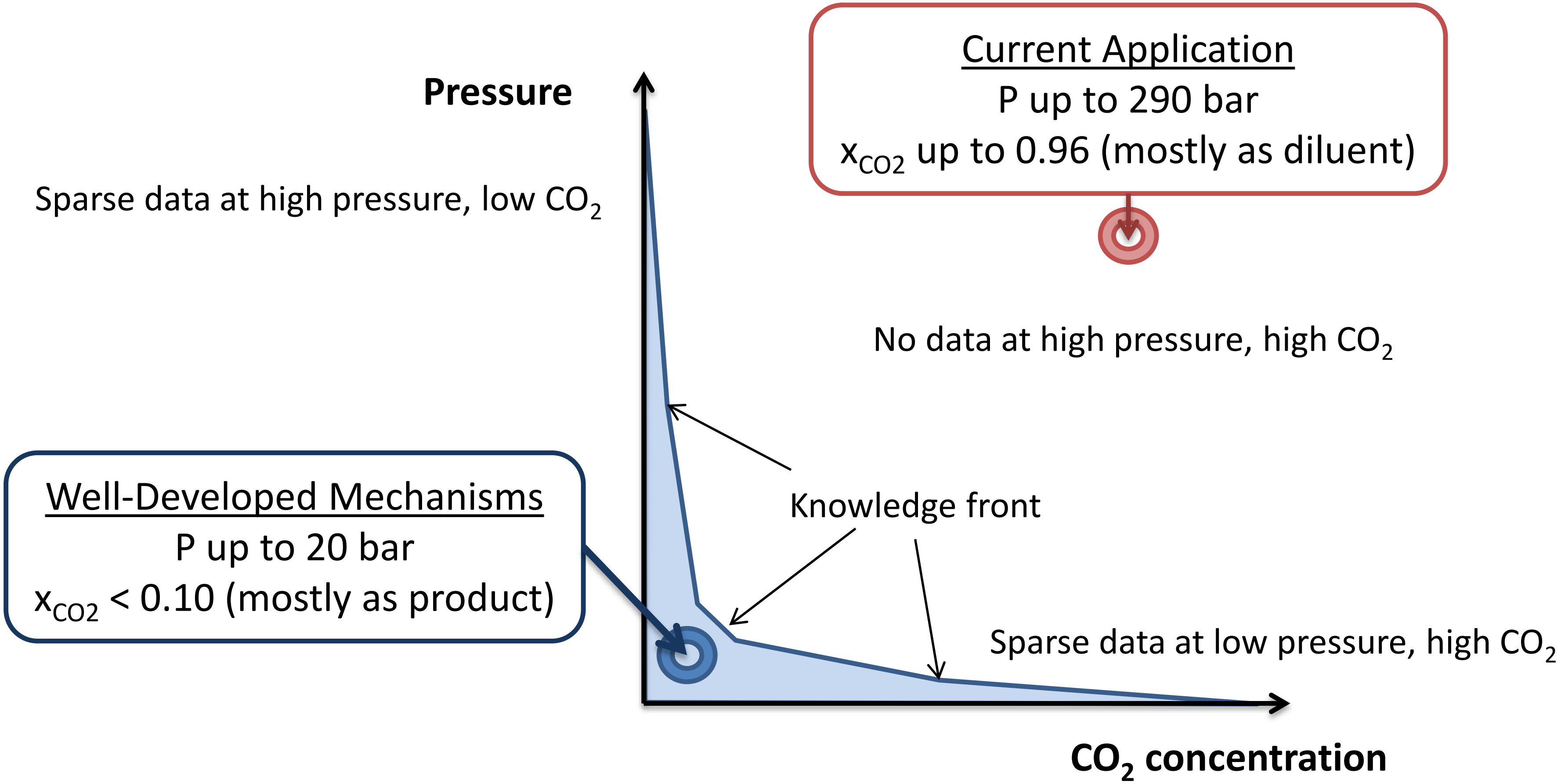
Species: 5 Reactions: 2

$CH_4 + 1.5\ O_2 \rightarrow 2\ H_2O + CO$ $\qquad r_1 = A_1T^{n1} e^{-\frac{E_{a_1}}{RT}}[CH_4]^{a1}[O_2]^{b1}$

$CO + 0.5\ O_2 \rightarrow CO_2$ $\qquad r_2 = A_2T^{n2} e^{-\frac{E_{a_2}}{RT}}[CO]^{a2}[O_2]^{b2}$

- A set of species, chemical equations, and reaction rate equations is called a mechanism
  - Reaction rate is a function of temperature and reactant concentrations
- Actual hydrocarbon combustion is complex process involving a multitude of intermediate reactions and species
  - Modeling the complete process is not practical
  - Mechanisms in the literature are approximations that use a subset of species and reactions
  - Adding species and reactions improves predictions and provides more information, but with non-linear increase to computational cost

Kinetics Knowledge Base



Pressure

Sparse data at high pressure, low CO_2

Current Application

P up to 290 bar

x_{CO2} up to 0.96 (mostly as diluent)

No data at high pressure, high CO_2

Well-Developed Mechanisms

P up to 20 bar

$x_{CO2} < 0.10$ (mostly as product)

Knowledge front

Sparse data at low pressure, high CO_2

CO_2 concentration

No data available at conditions relevant to this application.

Modeling Strategy

- No available kinetic model is validated for this application
  - Forced to use extrapolation
- Select a set of detailed models that are validated for low pressure and low CO_2 concentration
  - Other mechanism criteria
    - $> 10^2$ reactions: More detailed models may have better extrapolation capability
    - $< 10^3$ reactions: Too large of a mechanism will be impractical to validate and execute in design studies
  - Mechanisms evaluated

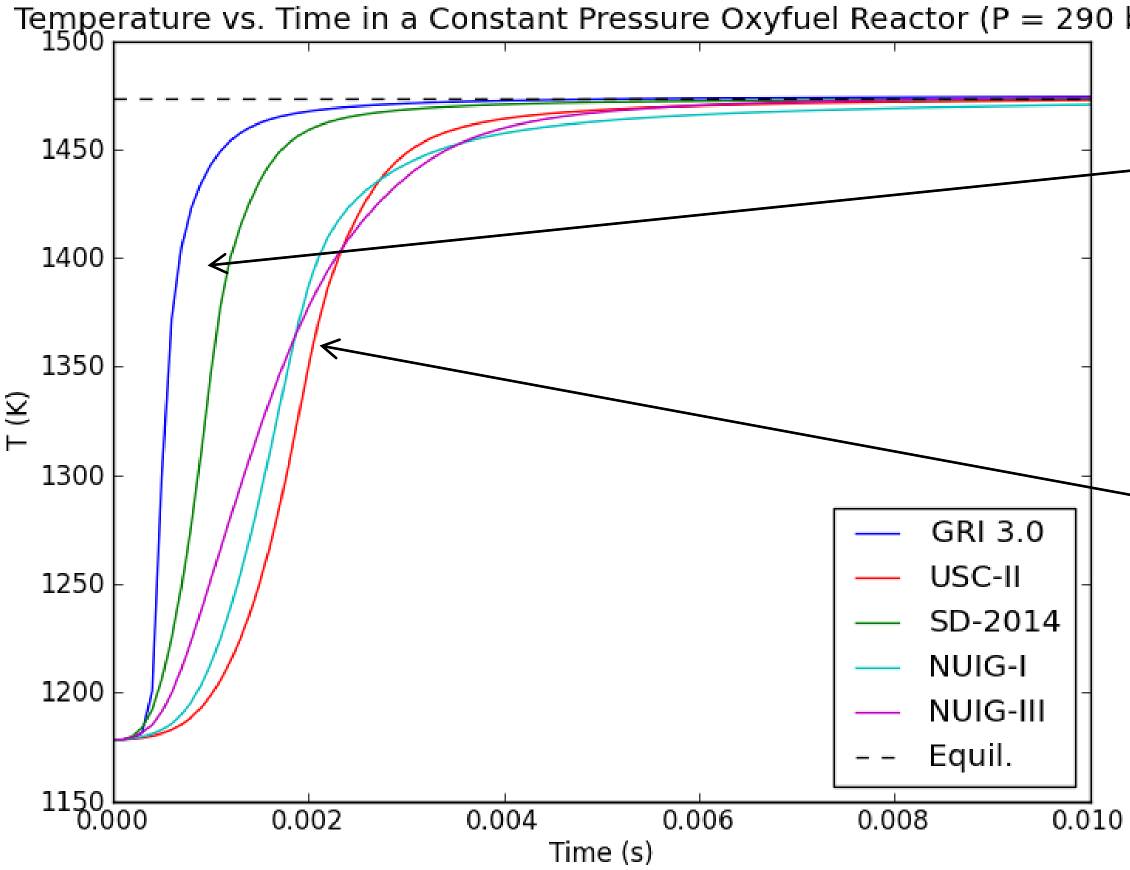
Mechanism	Species Count	Reaction Count
GRI-Mech 3.0 [1]	53	325
USC-II [2]	112	784
San Diego 2014-10-04 [3]	50	247

- Compare model predictions at validated conditions
  - Autoignition, flame speed, and residual CO
- Compare model results at supercritical oxyfuel combustor conditions
- Select best performer for use in this project with appropriate uncertainty range
- Cantera 2.1.2 is used as the modeling environment

Chemical Kinetic Model Performance Summary

- High pressure in air
  - Autoignition
    - Mechanisms generally perform similarly
    - Performance is similar to that at low pressure
    - GRI 3.0 has an advantage when predicting peak [OH] concentration
    - USC-II is most accurate at the conditions relevant to the supercritical oxyfuel combustor concept
  - Flamespeed:
    - USC-II is most accurate at 60 atm and consistently runs between 10% and 20% average error
    - Other mechanisms are very accurate at pressures up to 40 atm but have error around 40% at 60 atm
- Low pressure in CO_2
  - Flamespeed
    - GRI 3.0 and USC-II both perform well
  - [CO] in an isothermal reactor
    - SD-2014 is best but USC-II is also acceptable
- In general, high pressure appears to be a greater extrapolation risk than high CO_2

Comparison of Predictions at Supercritical Oxyfuel Conditions



GRI 3.0 and SD-2014 track together and demonstrate faster kinetics.

USC-II, NUIG-I, and NUIG-III track together and demonstrate slower kinetics.

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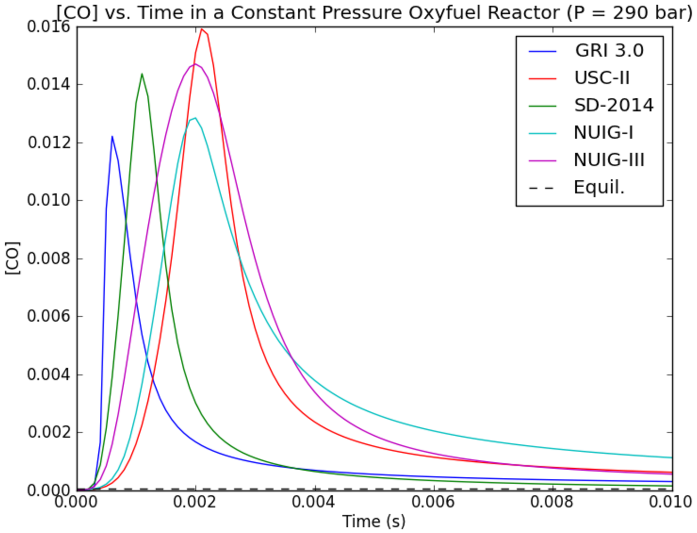
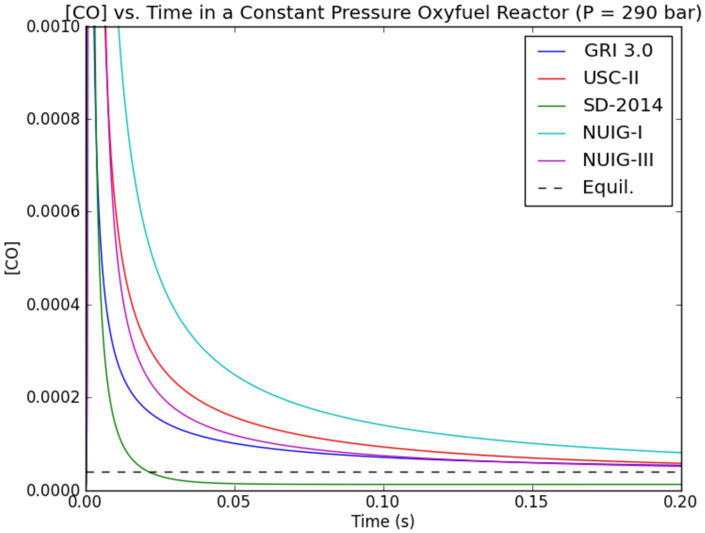

[CO] vs. Time in a Constant Pressure Oxyfuel Reactor (P = 290 bar)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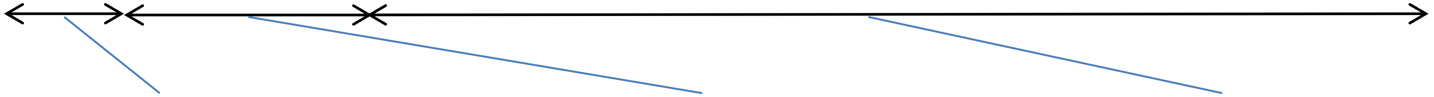


Initial phase
(CH_4 consumption
and CO production)
2 ms

Second phase
(majority of
CO consumption)
2-6 ms

Third phase
(remaining
CO consumption)
> 6 ms

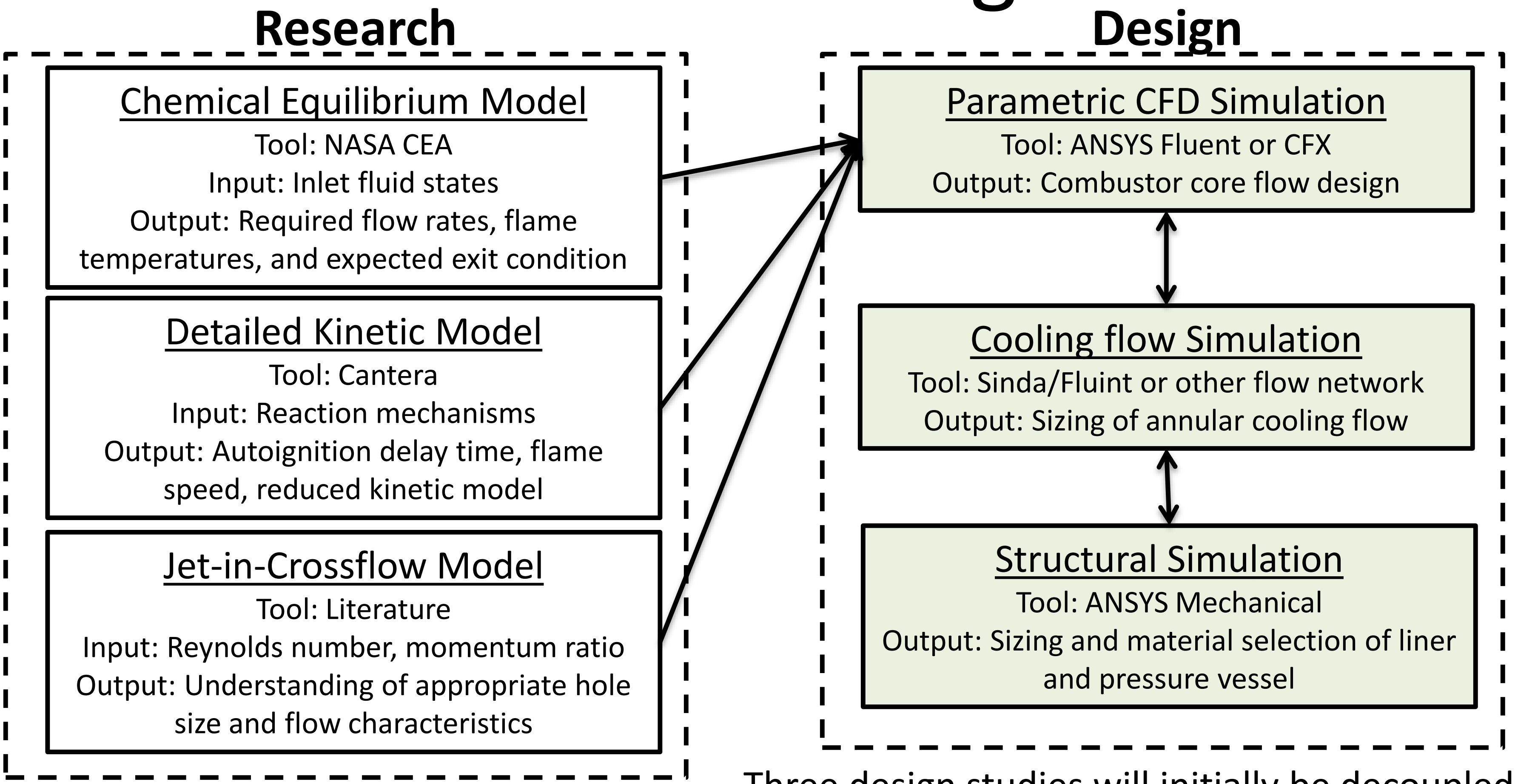
Mechanism Selection

- Primary selection criterion is accurate prediction of the overall reaction time scales
  - Drives the combustor design
  - More important than other details such as peak concentration values
- USC-II is the clear choice based on this criterion
  - Most accurate in highest pressure flamespeed and autoignition validation comparisons
- USC-II also had good to adequate performance in low pressure CO_2 studies
- USC-II predictions should carry +/- 50% uncertainty in this application

Reduced Order Model

- For incorporation into a CFD model a reduced order model was developed
- Equations based on Arrhenius rate equation were tuned to match USC-II model predictions
  - Match autoignition delay
  - Match residual CO levels
  - Overall time to complete reaction

Research and Design Path



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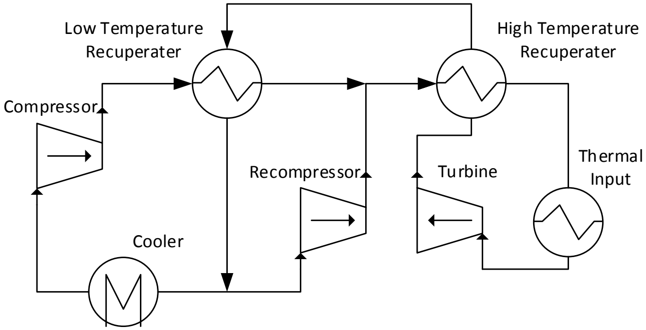
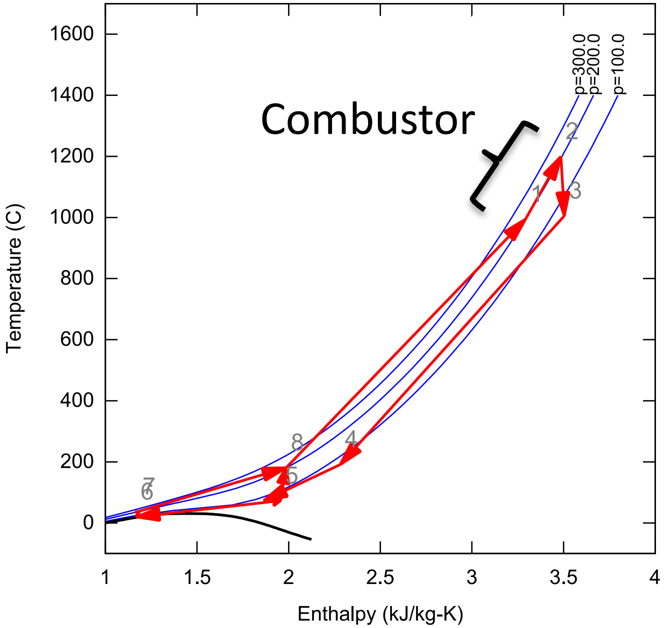
Three design studies will initially be decoupled, but may be performed iteratively or become fully coupled if needed.

COMBUSTOR DEVELOPMENT

Operating Requirements

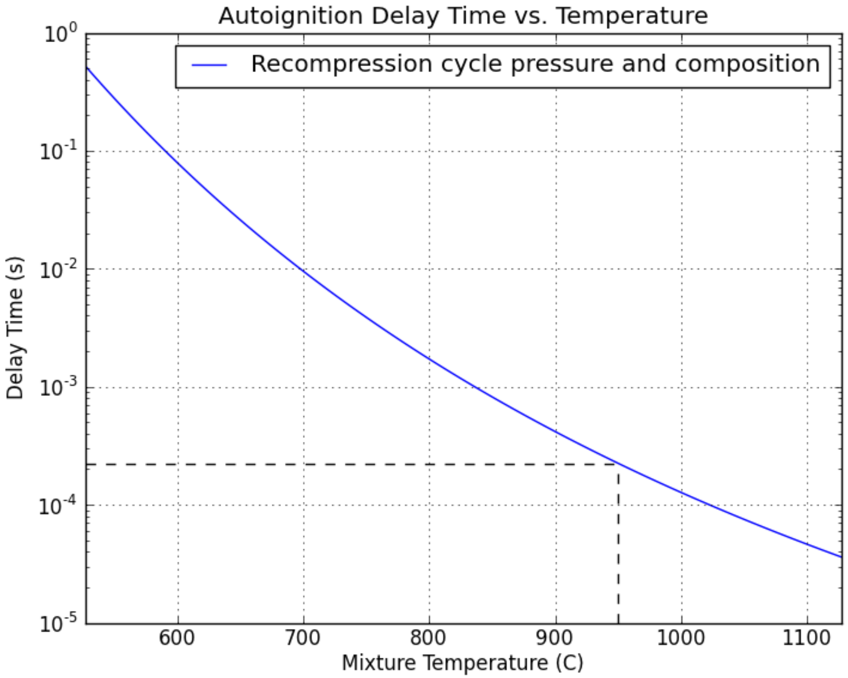
- Combustor inlet conditions
  - – 200 to 300 bar
  - – 750 to 1000 C
- Natural Gas or Syngas with CO2 diluent
  - – Not concerned about NOx





Auto Ignition Flame Stabilization

- Conventional low temperature combustors require submerged components
  - Fuel/air pre-mixing
  - Flame stabilization
- Requirements do not apply to high inlet temperature oxy-combustors
  - NOx emissions are not a concern
  - Inlet temperature above the fuel's autoignition temperature
- Autoignition can be used to stabilize the flame without submerged components
  - Fuel/O2 will spontaneously ignite after a short delay time
  - No recirculation zones are required
- Additional research is needed to verify autoignition properties at high pressure with CO2 diluent



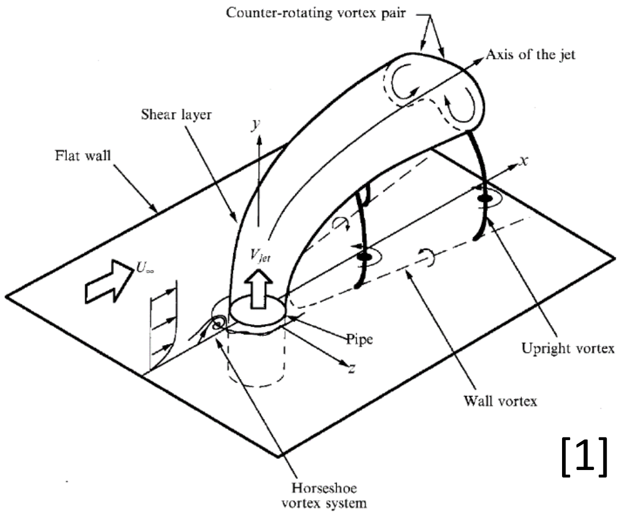
Based on correlation from [1]

References

1. L. J. Spadacinni and M. B. Colket, "Ignition Delay Characteristics of Methane Fuels," *Progress in Energy and Combustion Science*, Vol. 20 No. 5, pp. 431-460, 1994.

Mixing Theory

- Fuel and oxidizer must thoroughly mix
  - Homogenous output condition
- The tee mixer, or jet-in-crossflow (JICF) is a simple, highly effective, and well-documented mixing device without submerged parts
  - Counter-rotating vortex pair entrains fluid
- Flow physics for JICF is complicated by turbulent structures
  - Steady RANS was used for modeling
  - Known deficiency in modeling the unsteady behavior



[1]

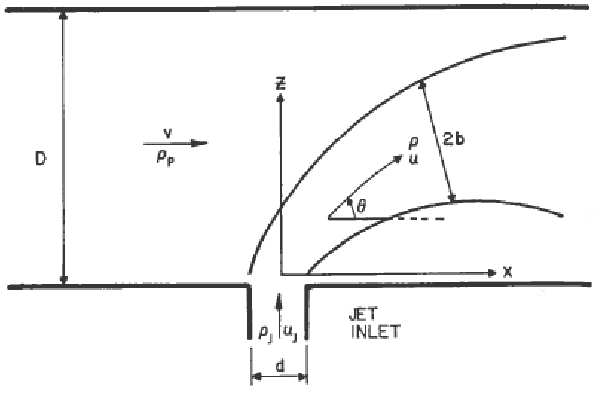


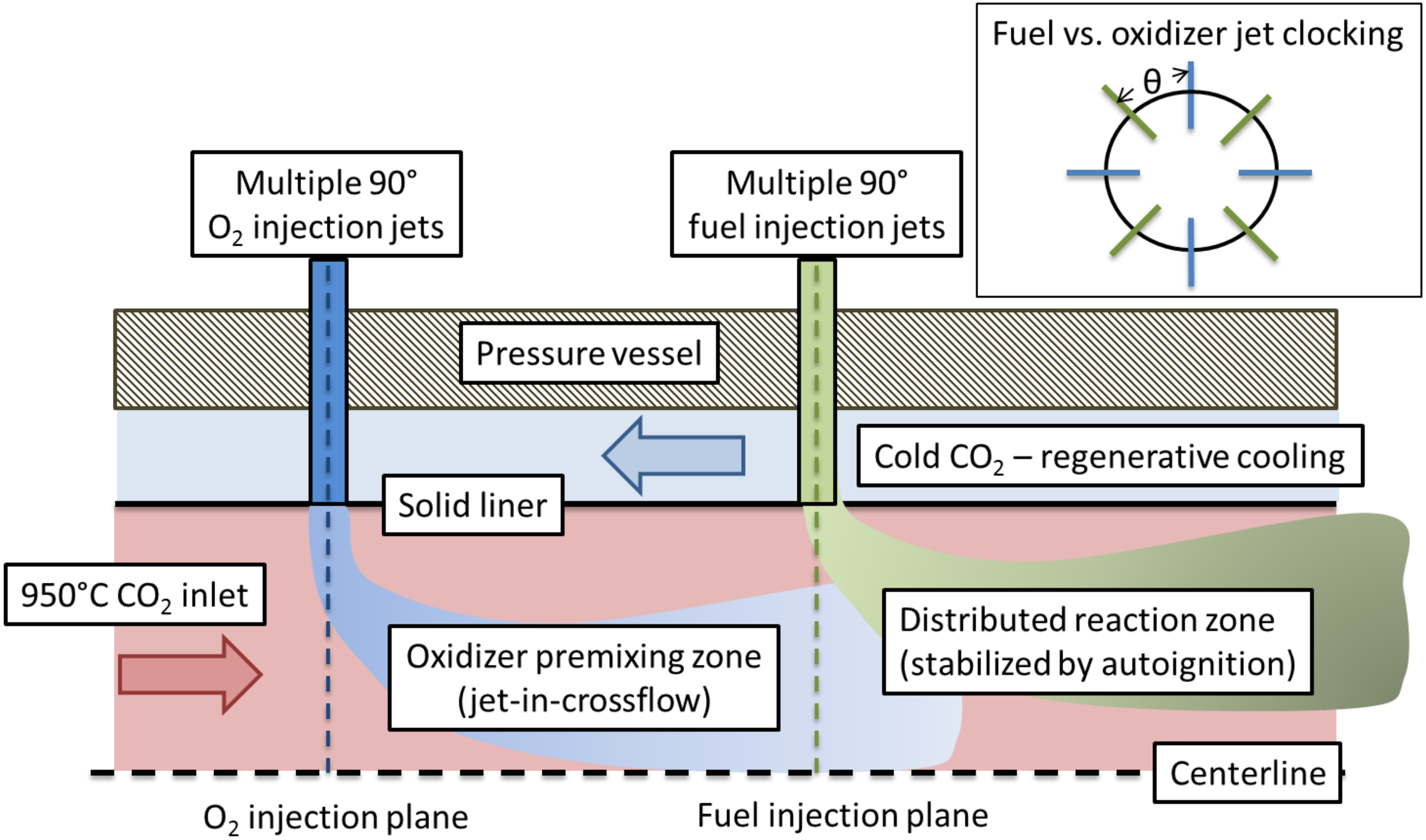
Figure 1. Schematic of a single jet mixer.

[2]

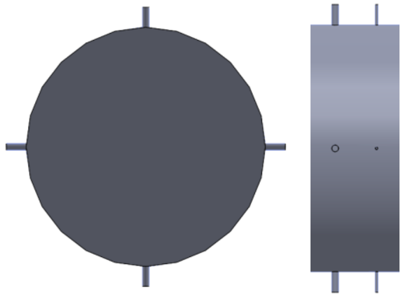
References

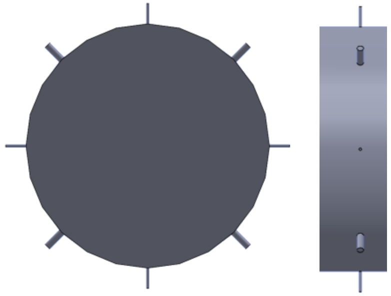
1. Kelso, et al. "An experimental study of round jets in cross-flow," J. Fluid Mech, vol. 306, 111-144, 1996.
2. "Jet Injection for Optimum Pipeline Mixing," Encyclopedia of Fluid Mechanics, vol. 2, Ch. 25, Gulf Publishing, 1986.

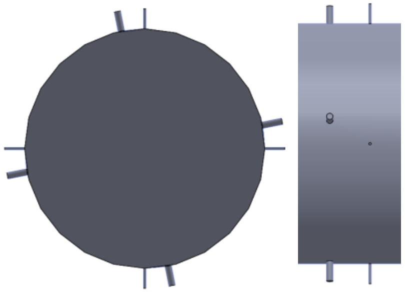
Initial Combustor Concept



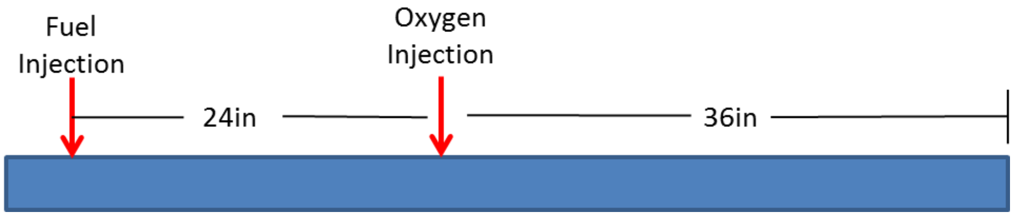
CFD Geometries


4 Hole Aligned


4 Hole 45° Clocked

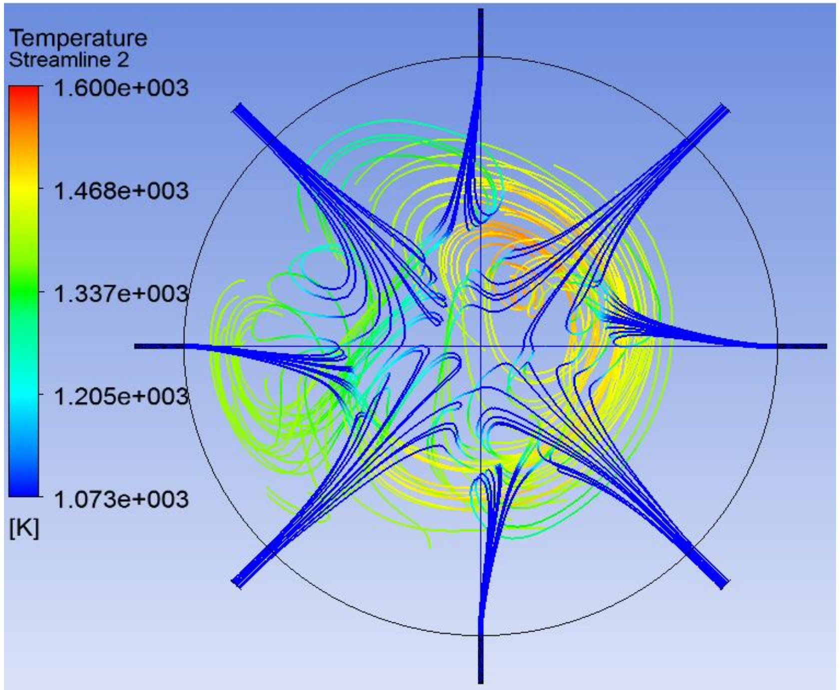

4 Hole 11.25° Clocked

- CFD simulation using reduced reaction mechanism
- Explore injector hole location, velocity, and size
  - Thermal conditions inside the combust
  - Instrumentation placement



Injector Hole Sizing

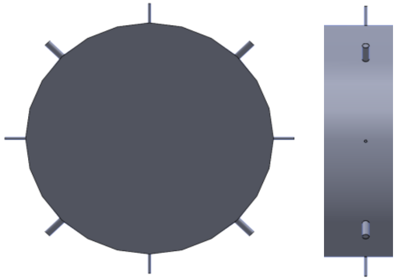
- Injector hole sizing dictated by momentum of fluid being injected
- Fuel flow and density dictates a much smaller hole that Oxygen
- Keeps combustion zone in center of combustor



	Fuel	Oxygen
2-Hole Diameter (inch)	0.055	0.15
4-Hole Diameter (inch)	0.027	0.075

Sample Result: 45° Clocked

- Four fuel, four oxygen injectors, 45° angle between ports
- High max temperature
  - Highest temperature are located away from the walls
- Rapid combustion, relatively good mixing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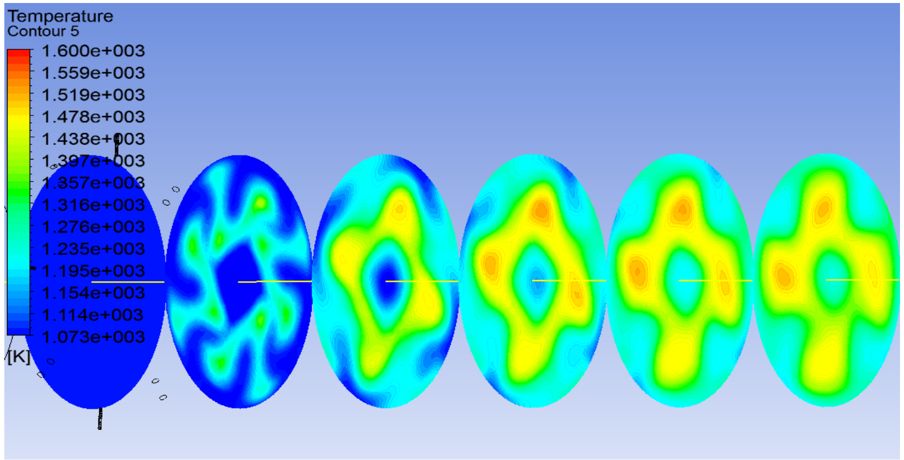
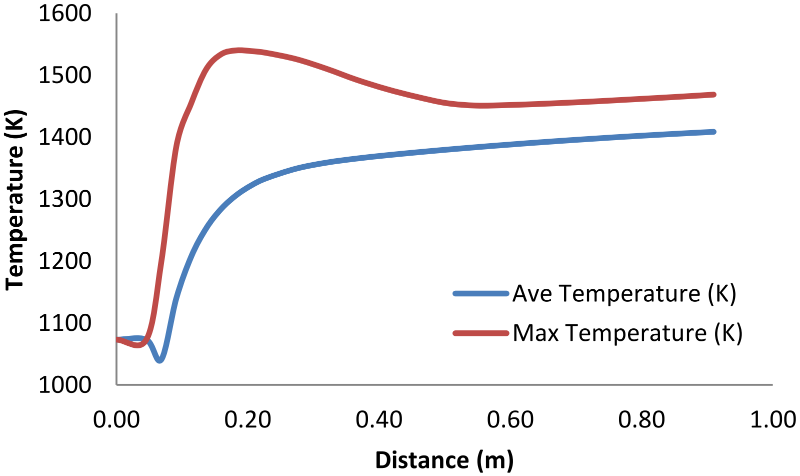
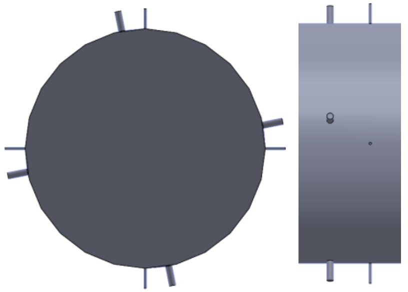
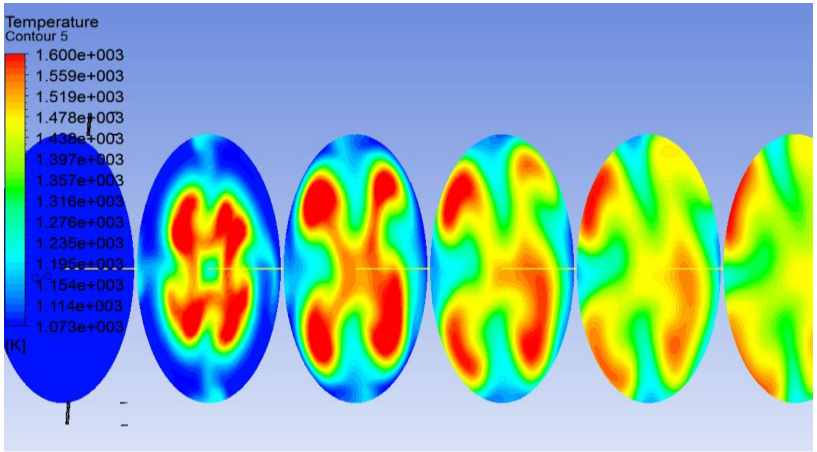


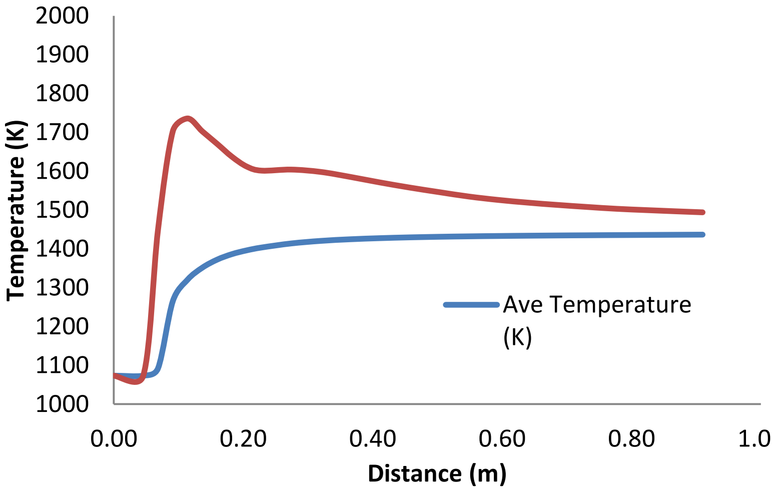


Sample Result: 11.25° Clocked

- Four fuel, four oxygen injectors, 11.25° angle between ports
- Very high max temperature, which is in contact with walls

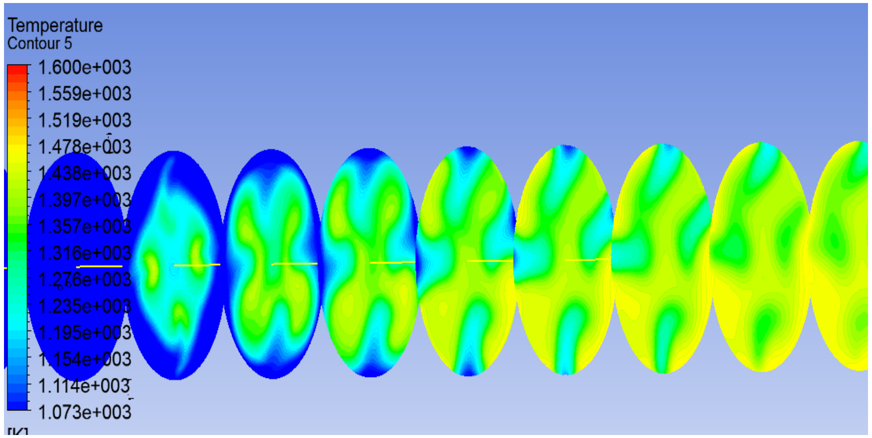

4 Hole 11.25° Clocked

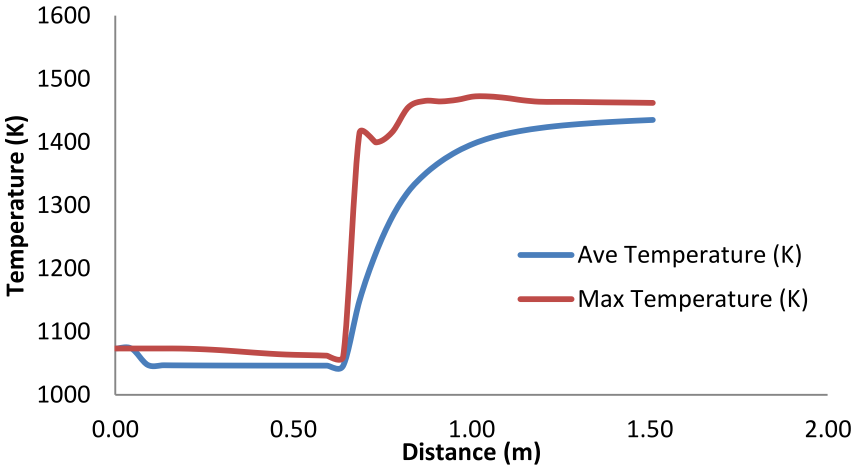




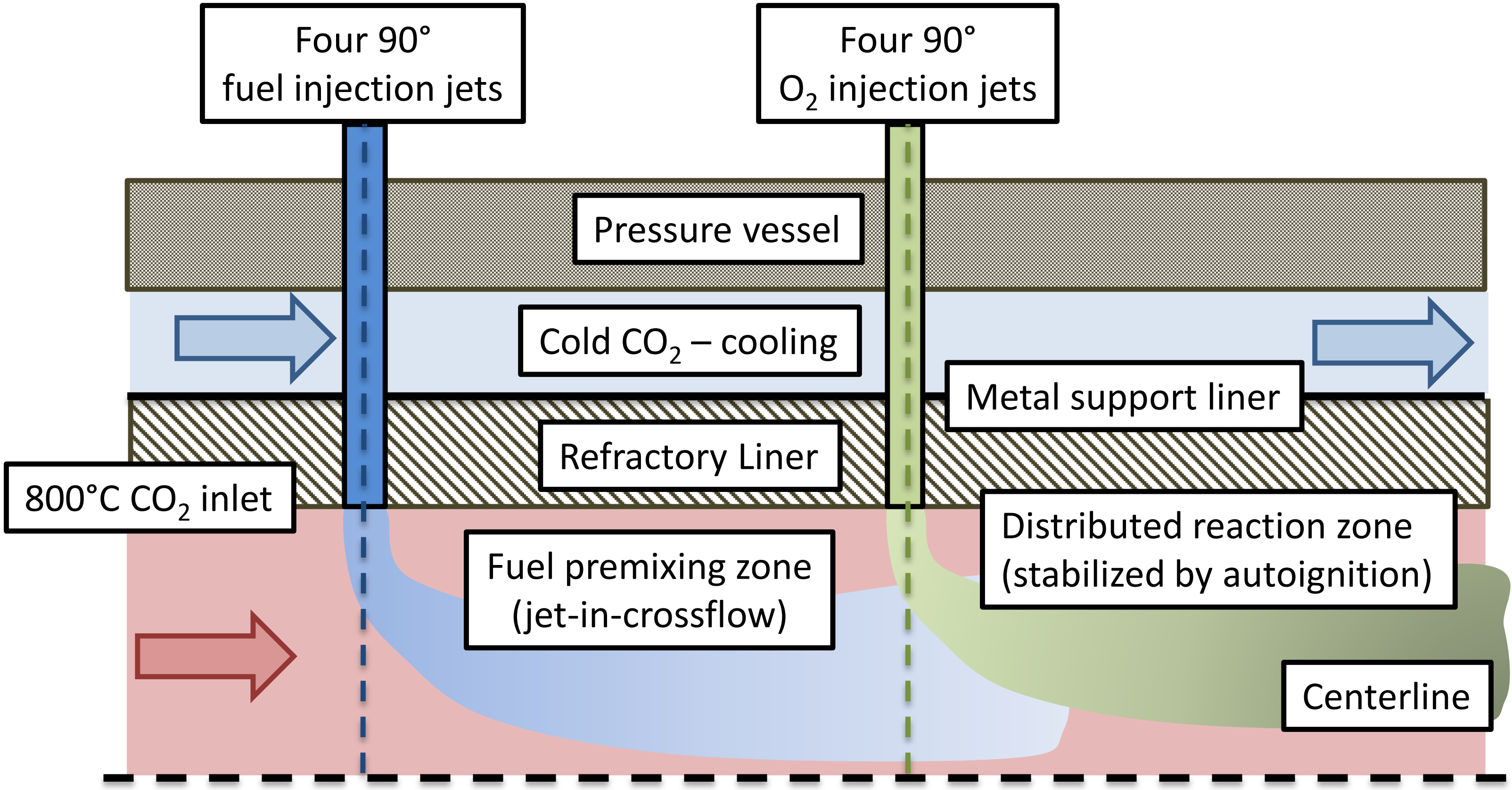
Refined Design: Fuel Injection 24in Upstream

- Fuel well mixed throughout combustor before oxygen
- Allows hydrocarbon "cracking" before oxygen injection
- Cool max temperatures
- Very good mixing at outlet
- Very low unburnt fuel percentage





Refined Design Concept



Four 90°
fuel injection jets

Four 90°
O_2 injection jets

Pressure vessel

Cold CO_2 – cooling

Metal support liner

Refractory Liner

800°C CO_2 inlet

Fuel premixing zone
(jet-in-crossflow)

Distributed reaction zone
(stabilized by autoignition)

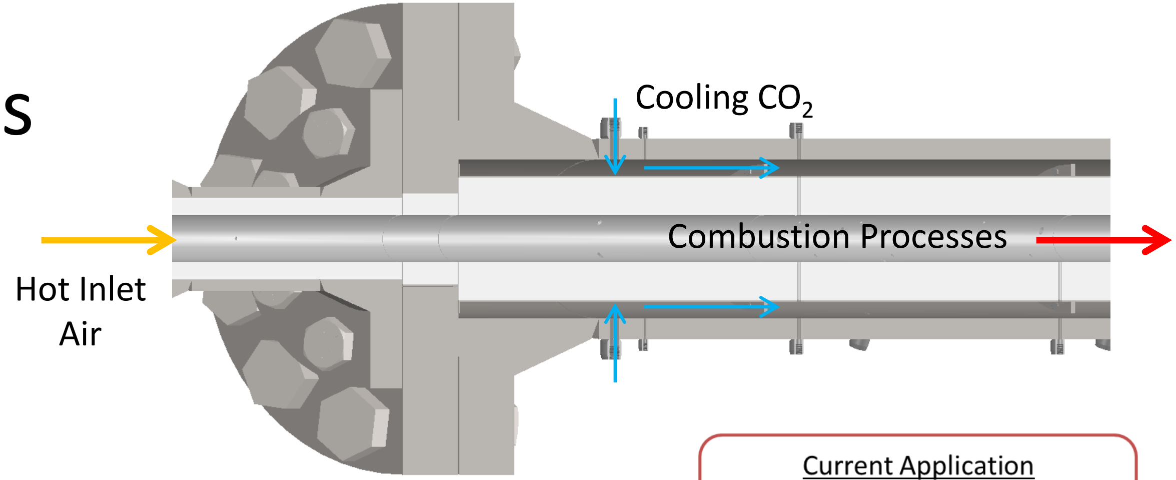
Centerline

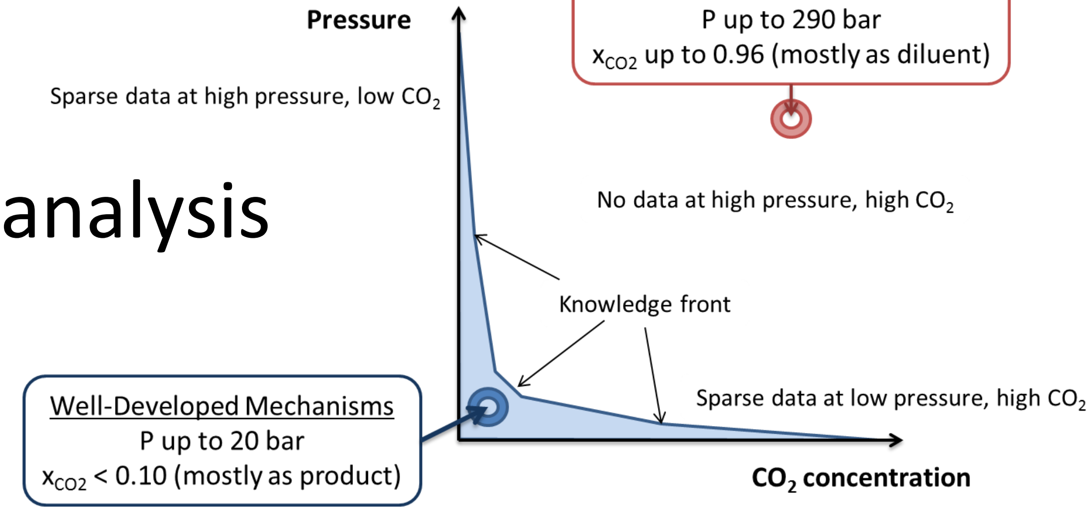
Fuel injection plane

O_2 injection plane

Instrumentation

- Thermocouples
- Pressure
  - Static
  - Dynamic
- Optical access
- Gas sampling and analysis





Current Application
P up to 290 bar
x_{CO2} up to 0.96 (mostly as diluent)

Well-Developed Mechanisms
P up to 20 bar
$x_{CO2} < 0.10$ (mostly as product)

WRAPUP

Status Summary

- Program Objectives
  - Advance fossil based sCO2 power cycles
  - Reduce technical risk for direct fired oxy-combustion
- Progress to Date
  - System Design and Thermodynamic Analysis
  - Kinetic Models
  - Bench Scale Testing
  - Auto-ignition based Combustor Design
- Moving Forward
  - Additional Combustor Concepts
  - Phase II Demonstration Concept

QUESTIONS?

Component Specifications

Component	**Specifications**
Compressor	Polytropic η: 0.85, Mechanical η: 0.95
Isothermal Compressor	3 stage Isothermal Compressor, T Ratio: +5°C/stage
Refrigeration	% Carnot: 0.45, Ambient Temp: 15°C
Cryo-Pump	Pump η: 0.55, Mechanical η: 0.95
CO2 Pump (Non Cryo)	Pump η: 0.75, Mechanical η: 0.95
Heat Exchanger	Pinch ΔT: 10°C, ΔP: -1 bar
CH4 Delivery Compressor	Polytropic η: 0.85, Mechanical η: 0.98
O2 Pump	Pump η: 0.55, Mechanical η: 0.94
ASU	ASU ~300 kW-hr/ton if Liquid, ~250 kW-hr/ton if gas
Turbine	Isentropic η: 0.92, Mechanical η: .99
Pipe Line CO2 Compressor	Polytropic η: 0.85, Mechanical η: .98
Cooling Tower	Cooling tower: 0.06 kW/Ton, Minimum Temp: 20°C
Water Chiller	Cooling: 0.6kW/Ton