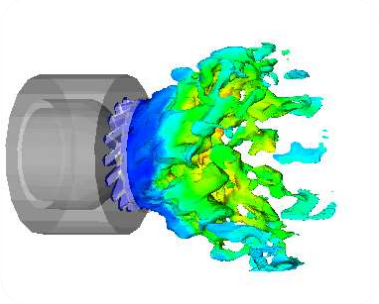
Effect of Impurities on Supercritical CO_2 Combustion

K R V Manikantachari (**Raghu**)[1,2], Scott Martin[3], Subith Vasu[1]



[1]Mechanical and Aerospace Engineering, University of Central Florida, Orlando, FL
[2]Power Systems Manufacturing, LLC, Jupiter, FL
[3]Eagle Flight Research Center, Embry-Riddle Aeronautical University, Daytona beach, FL

Supercritical CO_2 Symposium 2022
Virtual presentation

Outline

- Introduction
- Objective
- Approach
- Results and Discussion
- Conclusions

Introduction

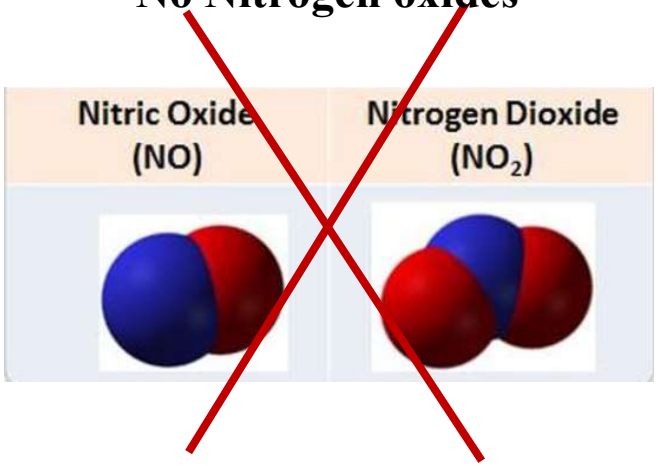
(Why to think about impurities?)

Important features of direct-fired sCO_2 cycle

CO_2 capture

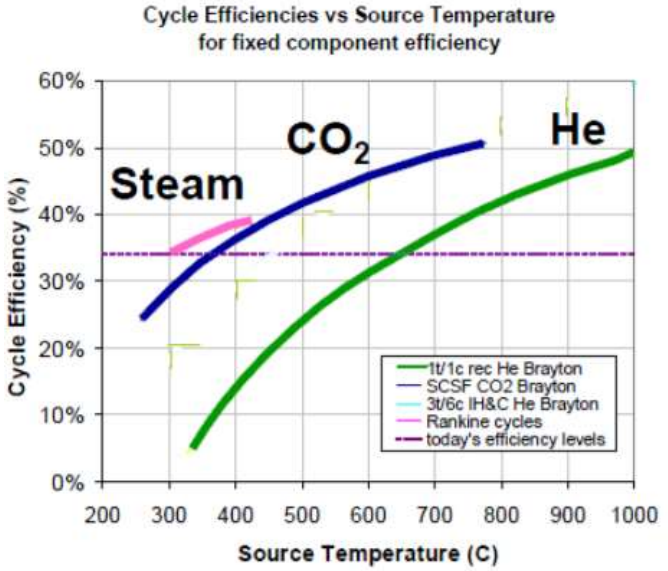
Picture source: http://www.21stcentech.com/environment-update-carbon-capture-technique-revealed/

No Nitrogen oxides



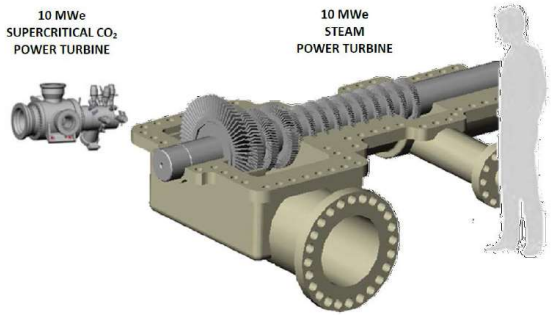
Picture source: https://www.colorado.edu/aqiq/resources/nitrogen-oxides/

Higher efficiency



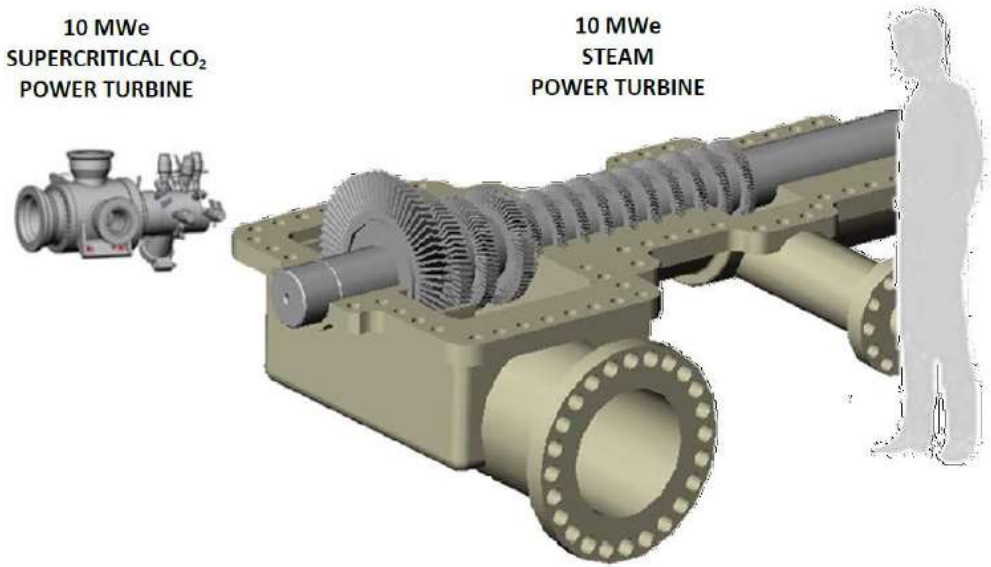
Source: Jason Wilkes, SwRI tutorials (sCO2 symposium'18)

Compactness



Source: Persichilli et al. (2012) and SwRI tutorials (sCO2 symposium'16)

Reason 1: Need of smaller combustors



Source: Persichilli et al. (2012) and SwRI tutorials (sCO2 symposium'16)

If turbine design is scaled down from existing ones, combustor may need to be scaled down (for alignment and compatibility).

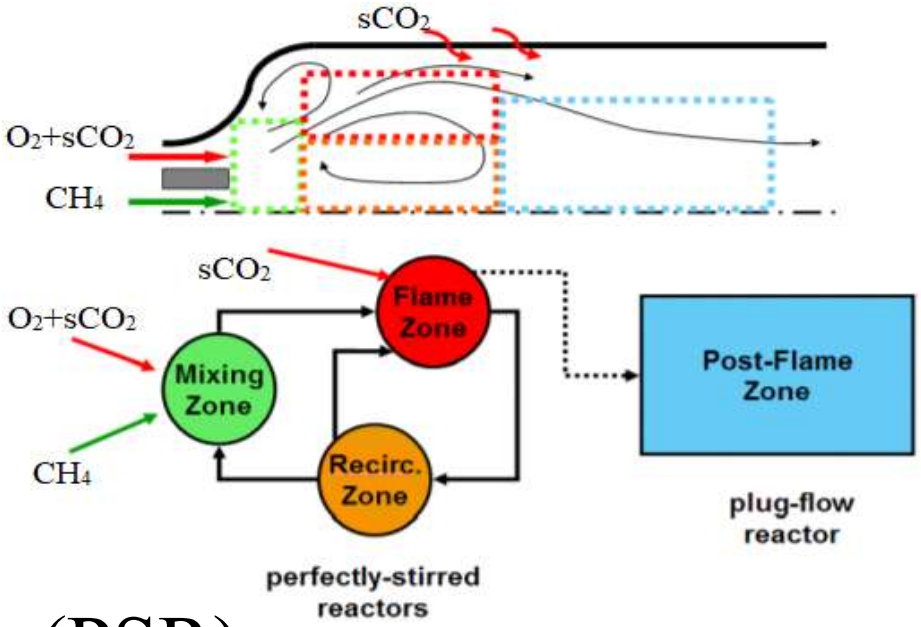
Relation between smaller volume and impurities

- Both the volume and recirculation design determines total residence time of combustion mixture

- As we reduce the residence time, complete oxidation of fuel becomes challenging.

A reactor network analysis

- PSR (also known as WSR) and PFR modeling was extensively used in 1950s to develop gas turbine combustors.



- Perfectly-Stirred Reactor (PSR) accounts the time associated with the molecules to enter and exit the reactor, called reactor residence time.

Reactor network modeling

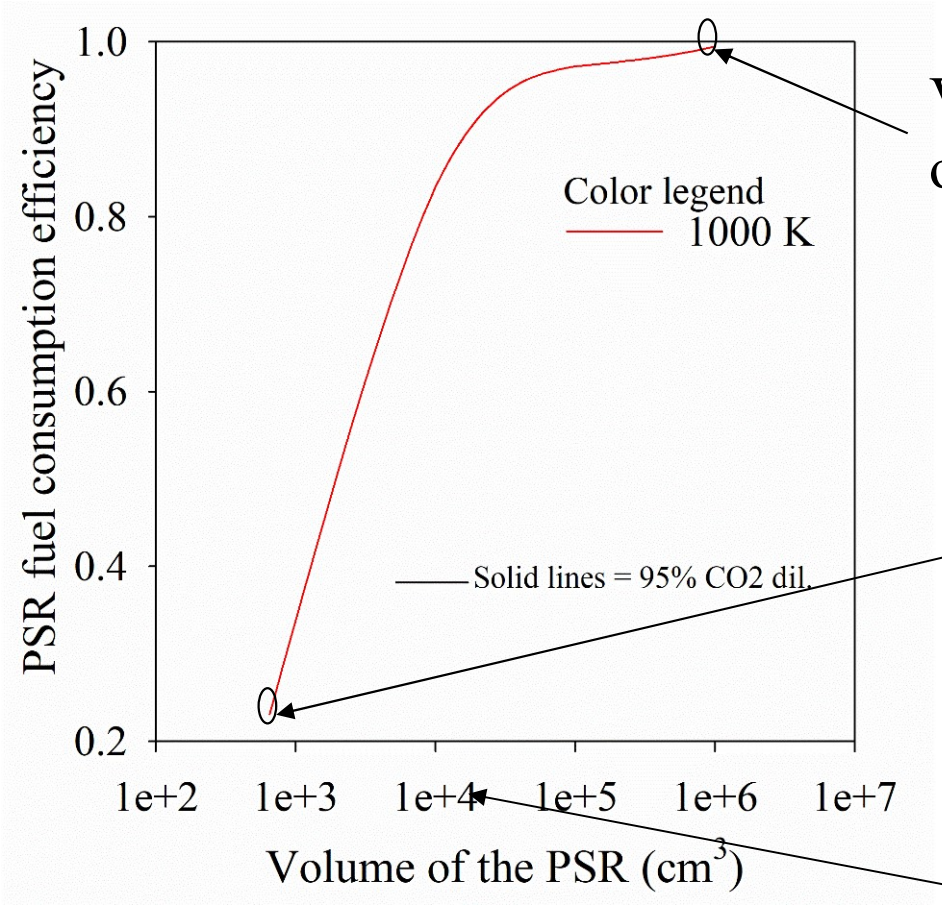
- The UCF 1.1 (derived from Aramco 2.0 and updated with MD reaction rates) mechanism is used.
- All real gas corrections are incorporated through CHEMKIN PSR and PFR models.
- Soave-Redlich-Kwong (SRK) equation of state is used based on our prior work[2].

1. Schmitt, R., Butler, P., and French, N. B., 1993, "CHEMKIN Real Gas," UIME PBB, pp. 93-006.

2. Manikantachari, K., Martin, S., Bobren-Diaz, J., and Vasu, S., 2017, "Thermal and transport Properties for the simulation of Direct-Fired sCO2 Combustor," Journal of Engineering for Gas Turbines and Power. GTP-17-1210, 139(12), 121505.

Volume of sCO_2 reactor Vs Fuel oxidation

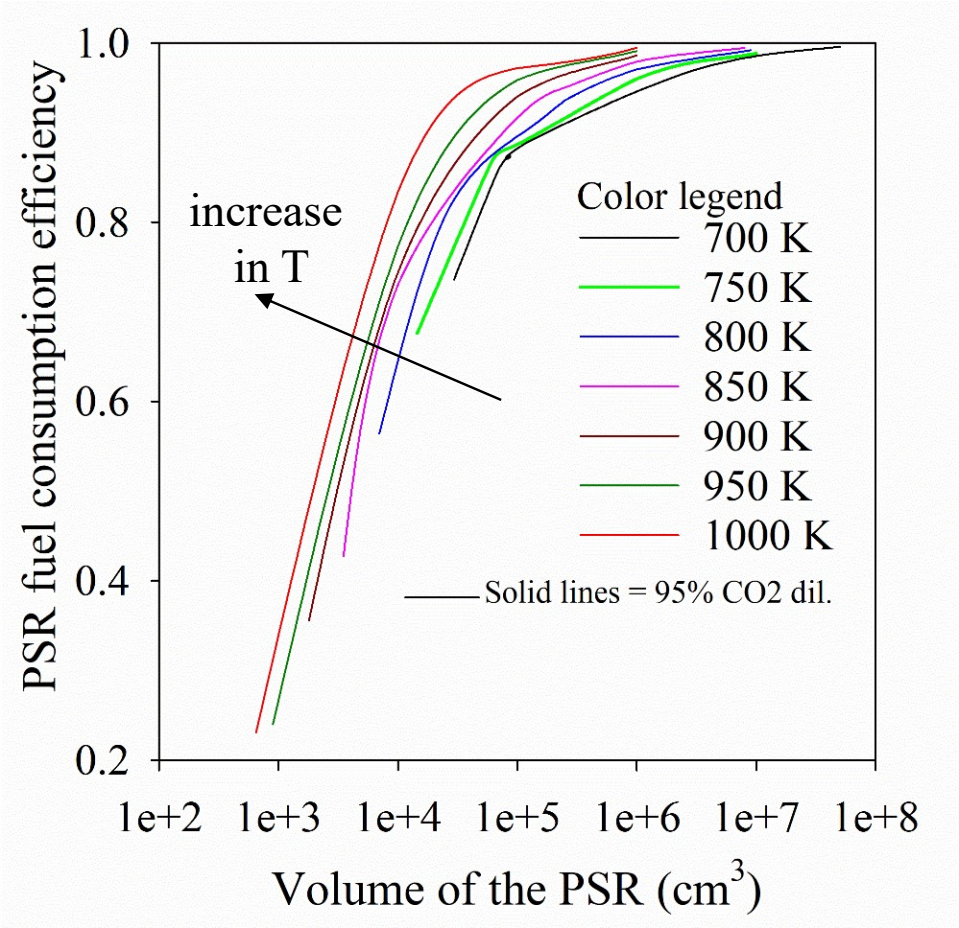
At 95% primary dilution



- Burning final trace of fuel needs large reactor volume.

Volume of sCO_2 reactor Vs Fuel temperature

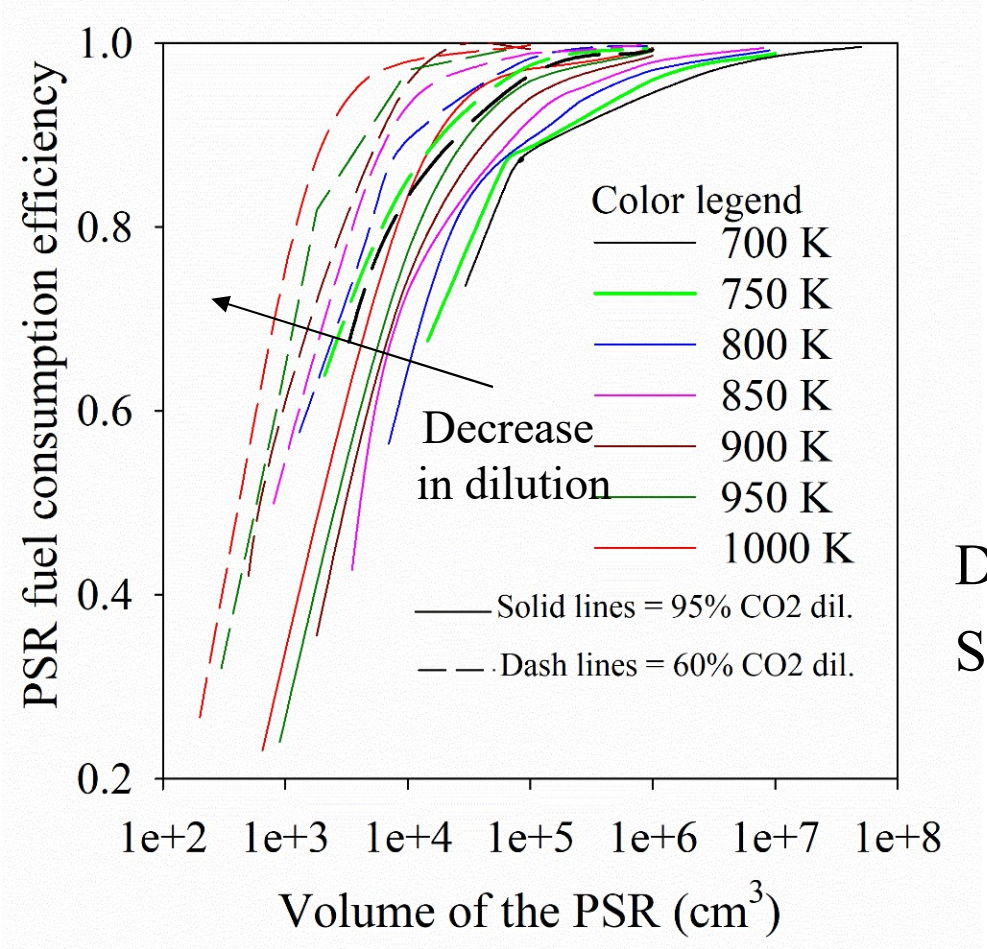
At 95% primary dilution & Various reactant temperatures



- As the reactant temperature increases the required blow-out volume and required reactor volume decreases.

Volume of sCO_2 reactor Vs sCO_2 fraction

Influence of primary dilution level of combustor volume

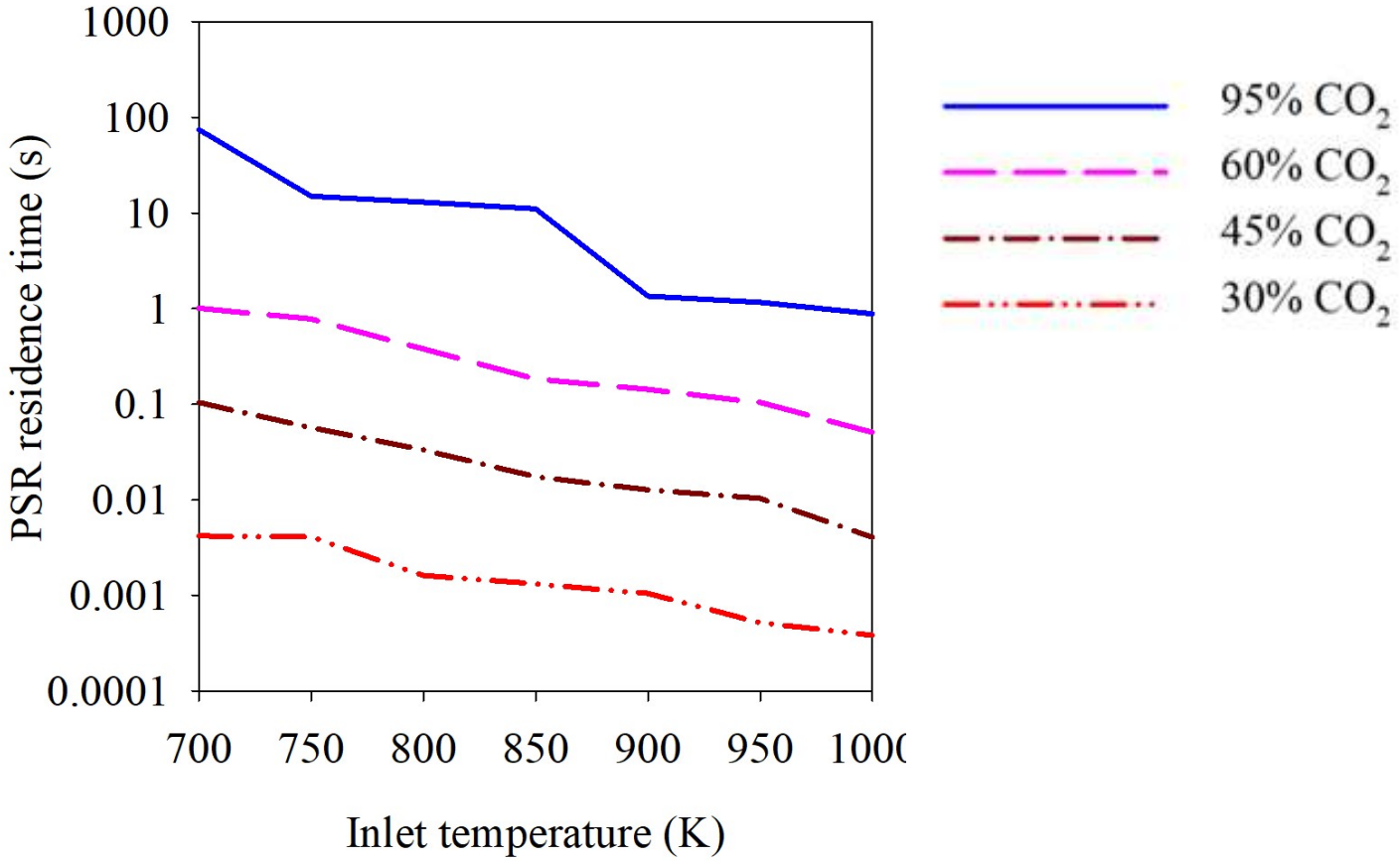


Dash lines → 60% dilu.

Solid lines → 95% dilu.

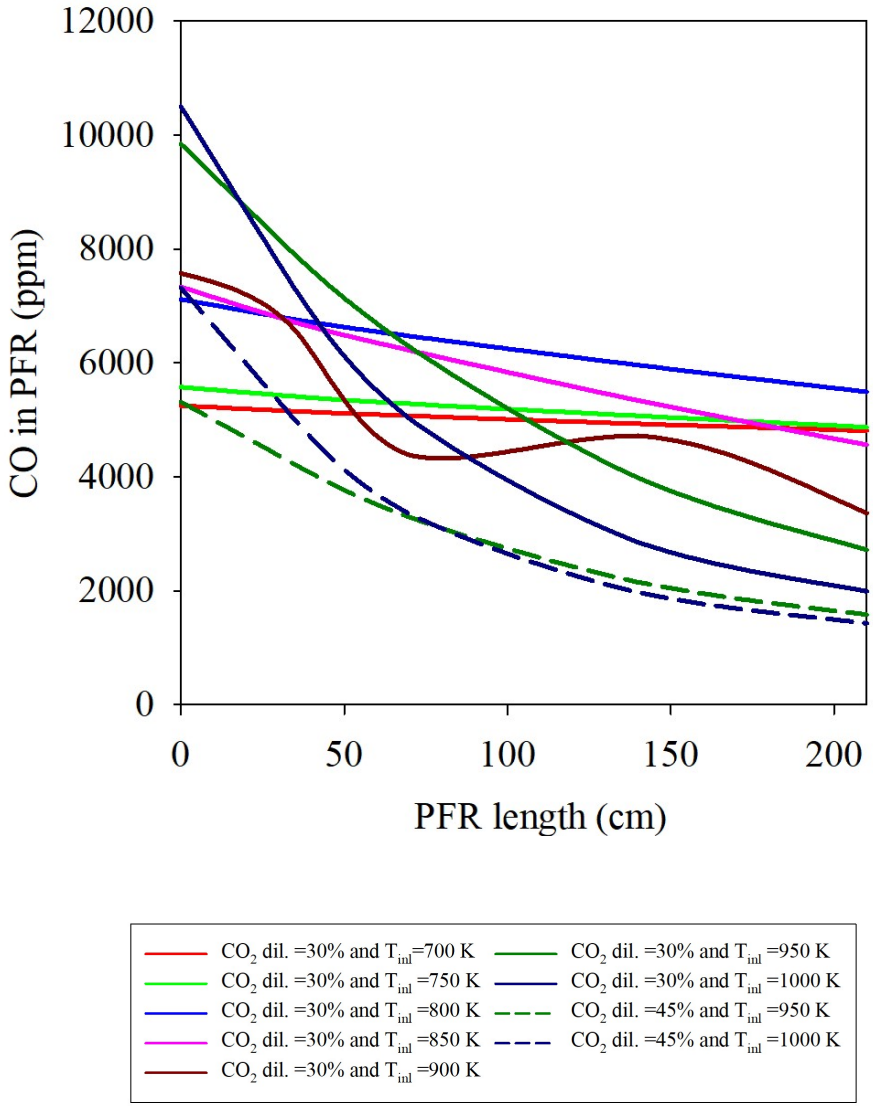
- Lesser primary dilution is more advantageous during cold start.

Residence time requirement



- With 95 % CO_2 dilution it is not practical to burn methane within reasonable residence time

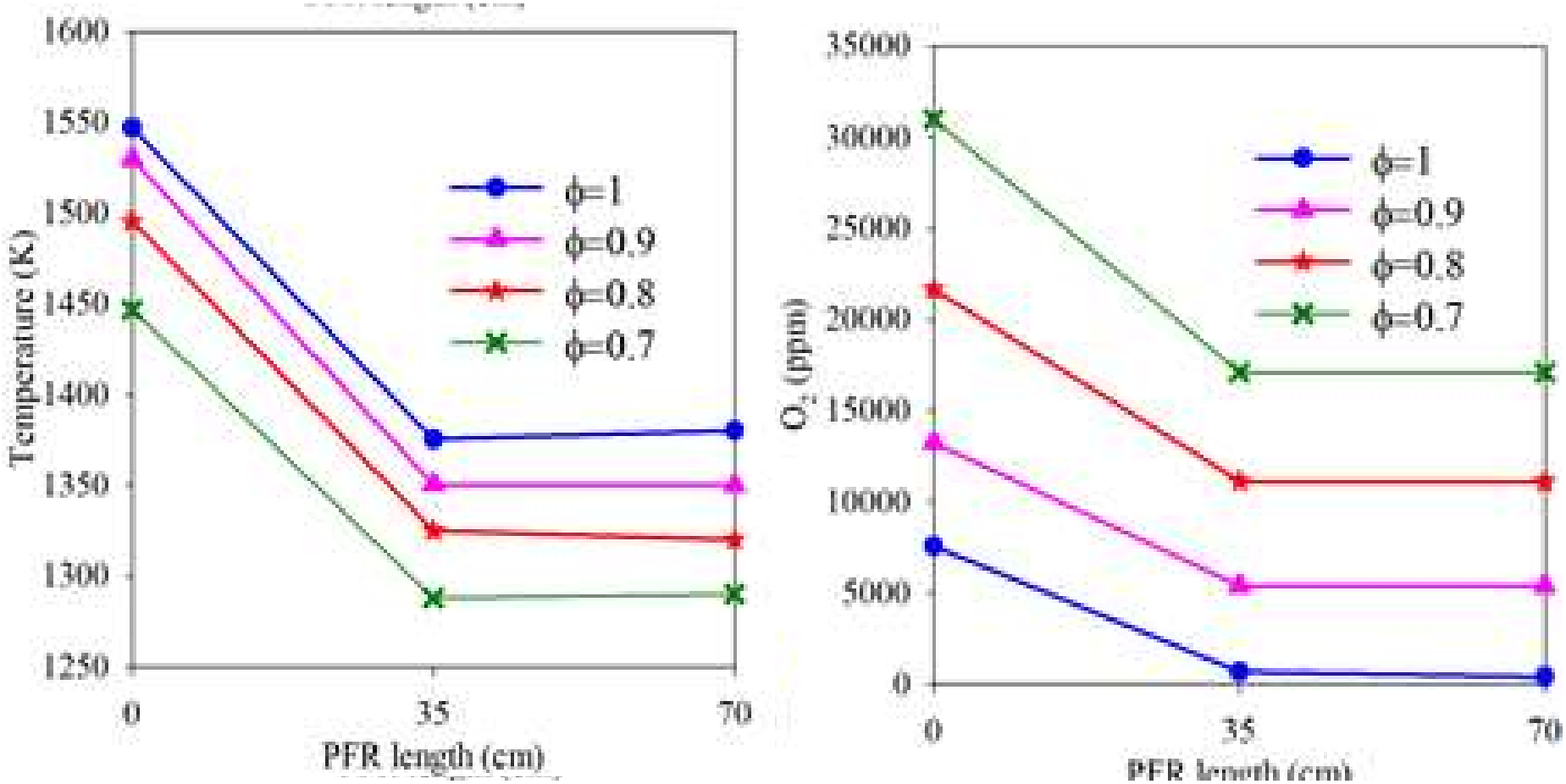
Emissions at the combustor exit



- CO can be a major concern when we try to scale down sCO_2 combustor

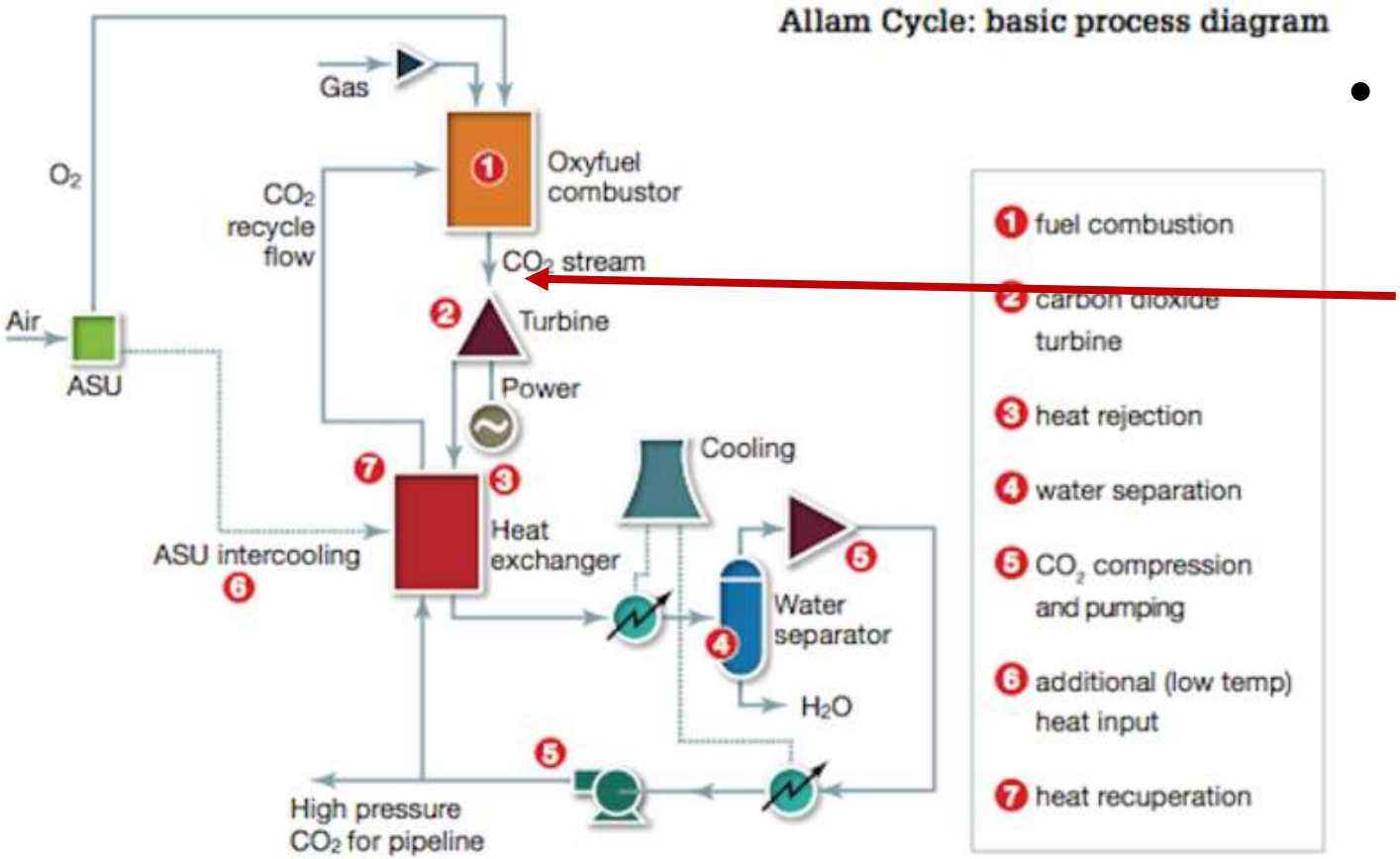
Complete oxidation of CO with lean strategy

The effect of lean combustion on CO



- If CO is oxidized with excess O2, then O2 will remain at the exit

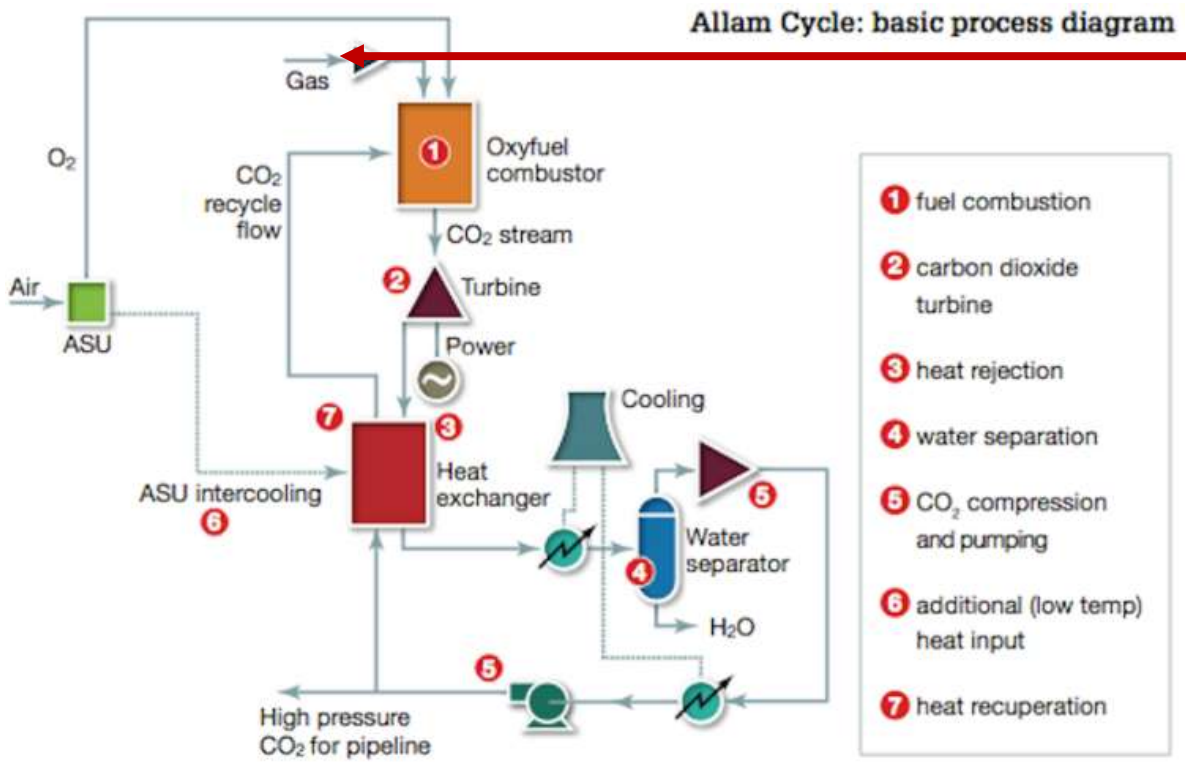
Emissions can become impurities



- Emissions other than pure H_2O and CO_2 in the exhaust must be treated as impurities in a semi closed loop operation

Reason 2: Impurities in fuel

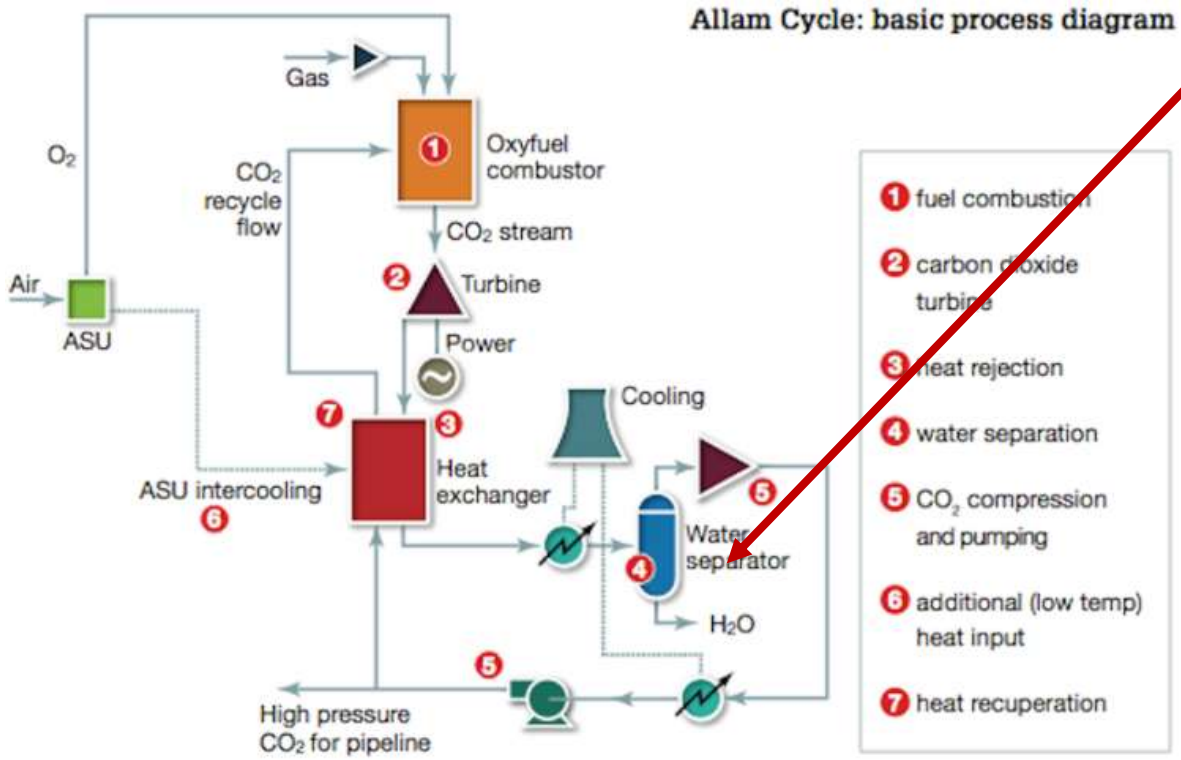
- Natural gas can have impurities such as H_2S, H_2O, N_2, CO_2 etc. and they can



Fuel impurities

Reason 3: Inefficient water sepration

- Natural gas can have impurities such as H_2S, H_2O, N_2, CO_2 etc. and they can



Inefficient water separation can also add traces of H_2O to incoming CO_2

Objective

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High-pressure operation is the major challenges for these combustor development.

Experimentation is expensive, time consuming and even dangerous at these pressures. Therefore, high fidelity simulation tools play a major role in the initial development of this combustor.

High fidelity LES simulations are performed to understand the influence of impurities on sCO2 combustion

Cases Considered

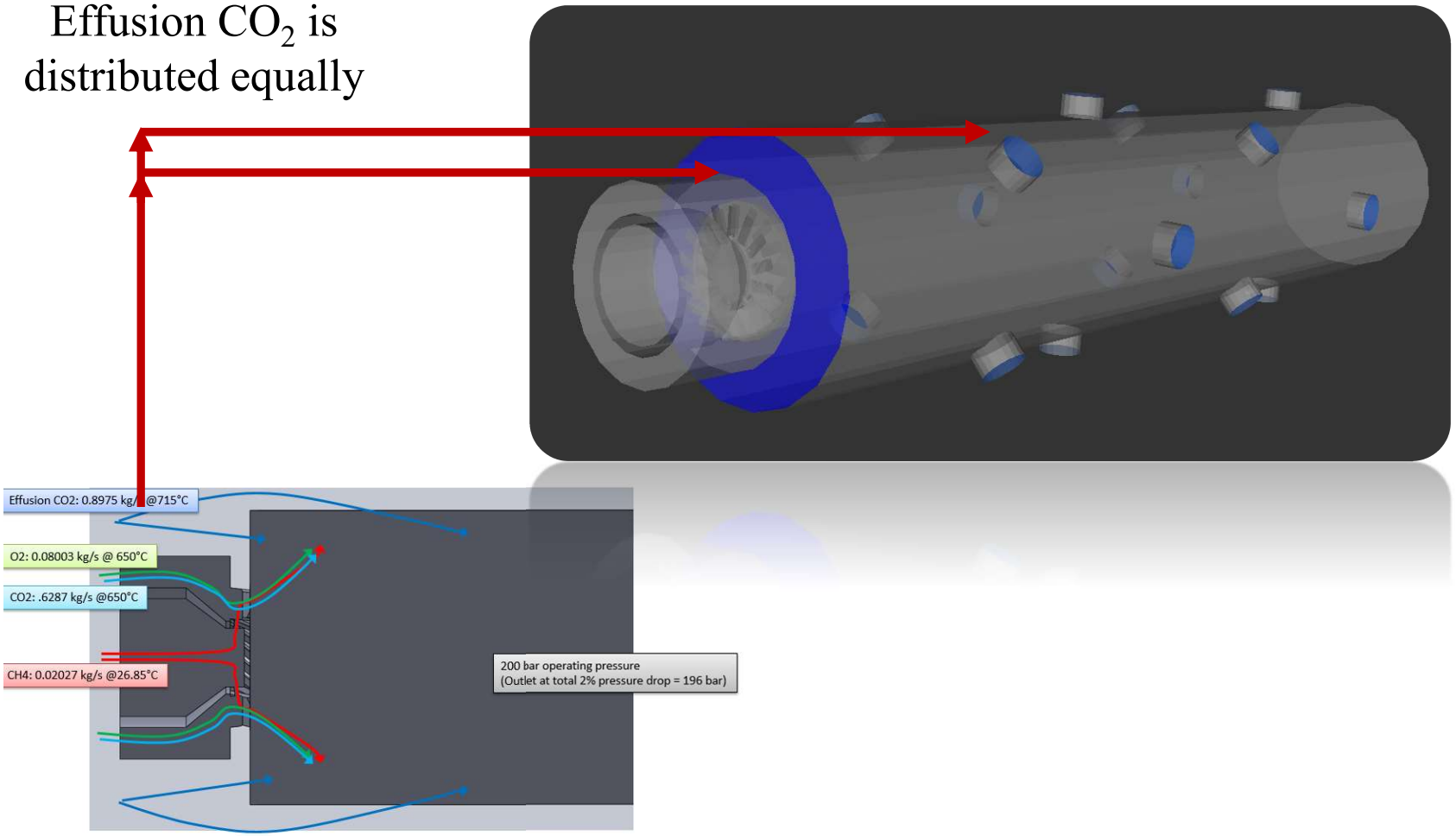
Cases investigated in this study	What does the case represent?
Case-1	The re-cycled stream consists of pure CO_2.
Case-2	The re-cycled CO_2 stream consists of O_2 impurity by 5000 ppm
Case-3	The re-cycled CO_2 stream consists of H_2O impurity by 5000 ppm

Approach

Geometry

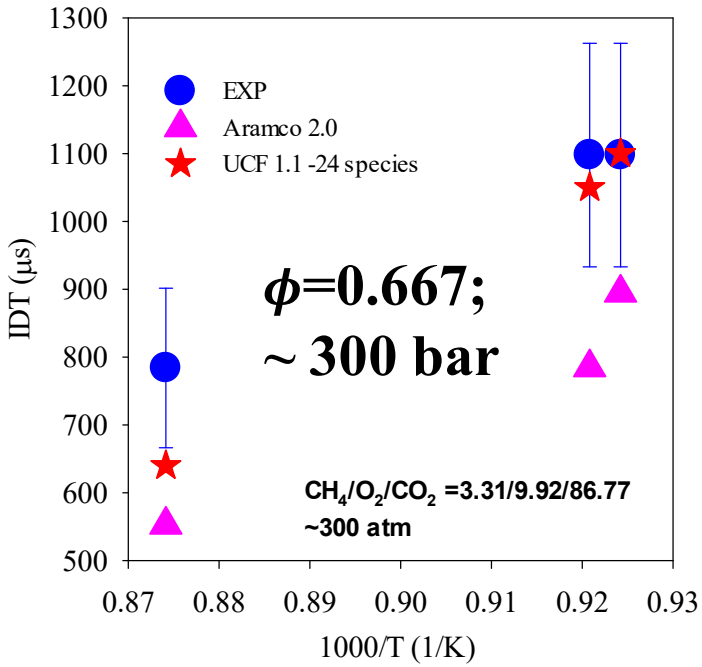
- SwRI sCO_2 combustor design is used

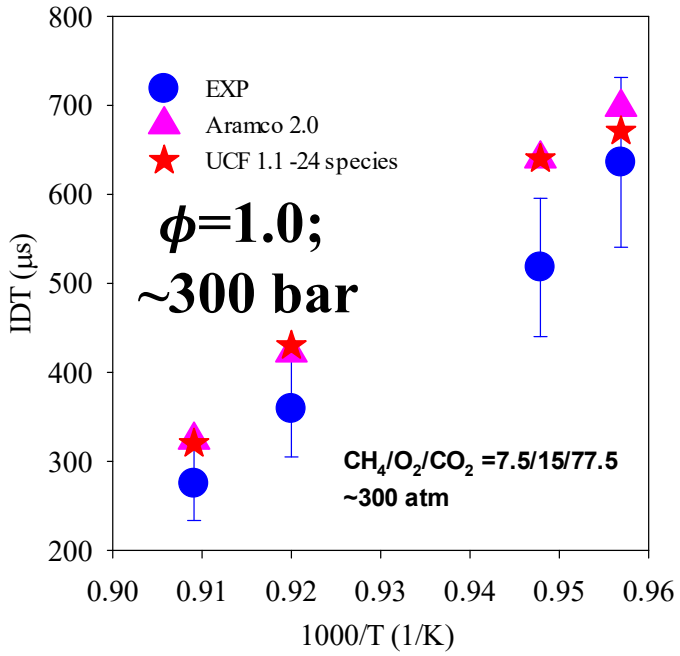
Effusion CO_2 is distributed equally



Chemical Kinetic Mechanism

High pressure Ignition Delay Times:





- The UCF 1.1 mechanism (Raghu et al., 2018)

→ based on **Aramco 2.0**

→ has important reaction rates calculated by **molecular level simulations**.

EOS implementation in Converge

- To consider thermodynamic quantities such as internal energy, enthalpy, entropy and specific heats as functions of both temperature and pressure:

Ideal gas		Real gas		Departure function
$U^0(T)$		$U(T,p)$		$\Delta U(T,p)$
$H^0(T)$		$H(T,p)$		$\Delta H(T,p)$
$S^0(T)$	=	$S(T,p)$	=	$\Delta S(T,p)$
$C_v^0(T)$		$C_v(T,p)$		$\Delta C_v(T,p)$
$C_p^0(T)$		$C_p(T,p)$		$\Delta C_p(T,p)$

- These departure functions are correlated, can be conveniently evaluated through departure function for Helmholtz energy: $\Delta A(T,p) = \int_{\infty}^{V} \left(p - \frac{RT}{v}\right) dv + RT ln \frac{v}{v^0}$

$$\Delta S(T,p) = -\frac{\partial}{\partial T}\Delta A(T,p)$$

$$\Delta U(T,p) = \Delta A(T,p) + T\Delta S(T,p) \qquad \Delta C_v(T,p) = \frac{\partial}{\partial T}\Delta U(T,p)$$

$$\Delta H(T,p) = \Delta A(T,p) + T\Delta S(T,p) - RT(Z-1) \qquad \Delta C_p(T,p) = \frac{\partial}{\partial T}\Delta H(T,p)$$

Source: Converge manual

Inputs

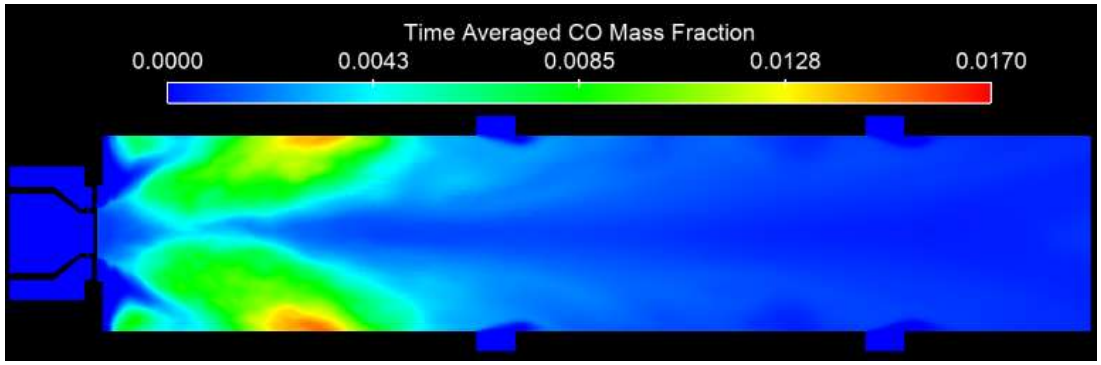
- Converge ® is used for simulations

Modeling	Parameter /model chosen
Turbulence modeling	Large-eddy simulation → Viscous One Equation. This model uses sub-grid kinetic energy in modeling the turbulent viscosity
Wall heat transfer modeling	O'Rourke and Amsden
Combustion modeling	SAGE detailed chemistry (all species transport equations are solved).
Number of cells	Approximately six million cells (Adaptive mesh refinement is used)
Equation of state	Soave-Redlich-Kwong equation of state
Viscosity and Thermal conductivity	Pure CO_2 properties between 800 -1600 K from REFPROP are used.
Chemical kinetic mechanism	A UCF 1.1 (23-species) mechanism derived from Aramco 2.0
Simulation time	6 follow-through times

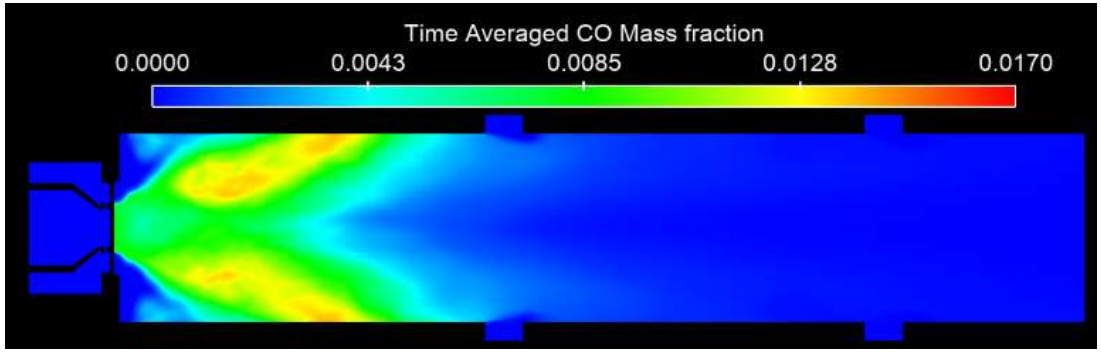
Results and Discussion

Time averaged CO mass fraction

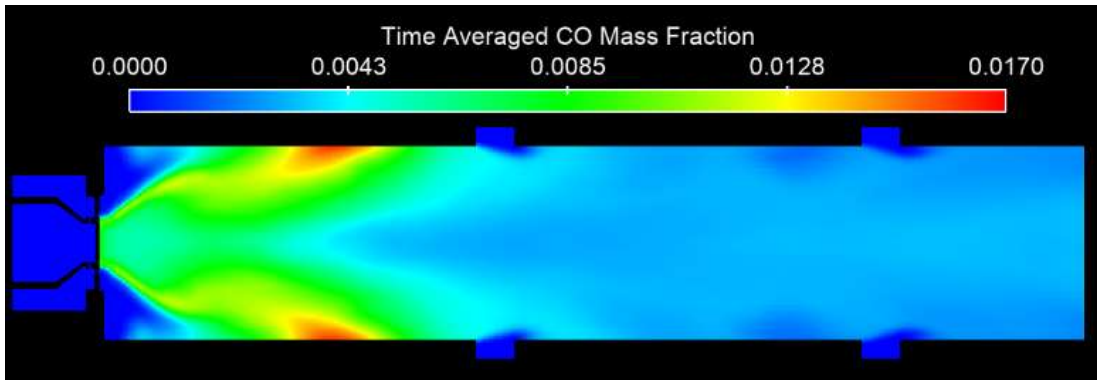
Pure CO_2



O_2+CO_2



H_2O+CO_2



Moles at the Combustor Exit

	CO (ppm)	O2 (ppm)	CH4 (ppm)	Temperature (K)
CO_2	1194	351	0	1402.3
CO2+O_2	185	2000	0	1415.9
CO2+H_2O	1782	248	0	1408.4

Conclusions

Conclusions

- Complete oxidation of fuel is challenging while scaling down the size of combustor
- Small impurities can influence the flame structure
- Not much impact on the exit temperature (if sufficient residence time is given)
- Having excess O_2 (5000 ppm) can oxidize CO and minimize CO at the outlet

Acknowledgments

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Questions

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