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# Study of the effect of CO addition in a Direct Fired Oxy-Fuel Combustor for sCO2 Power Cycles using Direct Detailed Chemistry and Adaptive Mesh Refinement

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# Introduction

- Supercritical $CO_2$ ($sCO_2$) power cycle is an emerging technology which has the potential to address both environmental concerns and energy demands
- Operating pressures at supercritical condition are in 200-300atm range
- At these extreme pressure conditions, experiments are expensive. Therefore, CFD modeling would play an ever-important role
- Managing impurities in the cycle is another foreseen stumbling block for successful operation
- Vasely *et al.* [1] showed that, impurities could significantly influence $sCO_2$ cycle performance
- Hence, it is **very crucial to understand the effect of impurities on sCO2 combustion**
- Sources of impurities in $sCO_2$ combustion:
  - Impurities in fuel, inefficiency of air-separation unit before combustor, inefficiency of water separation unit after heat exchanger.
  - Ineffective air-separation unit may not filter Ar and $N_2$ entirely.
  - **Water separation unit may not separate $\boldsymbol{CO}, \boldsymbol{H_2O}$ and other minor combustion products which are coming from the exhaust stream.**

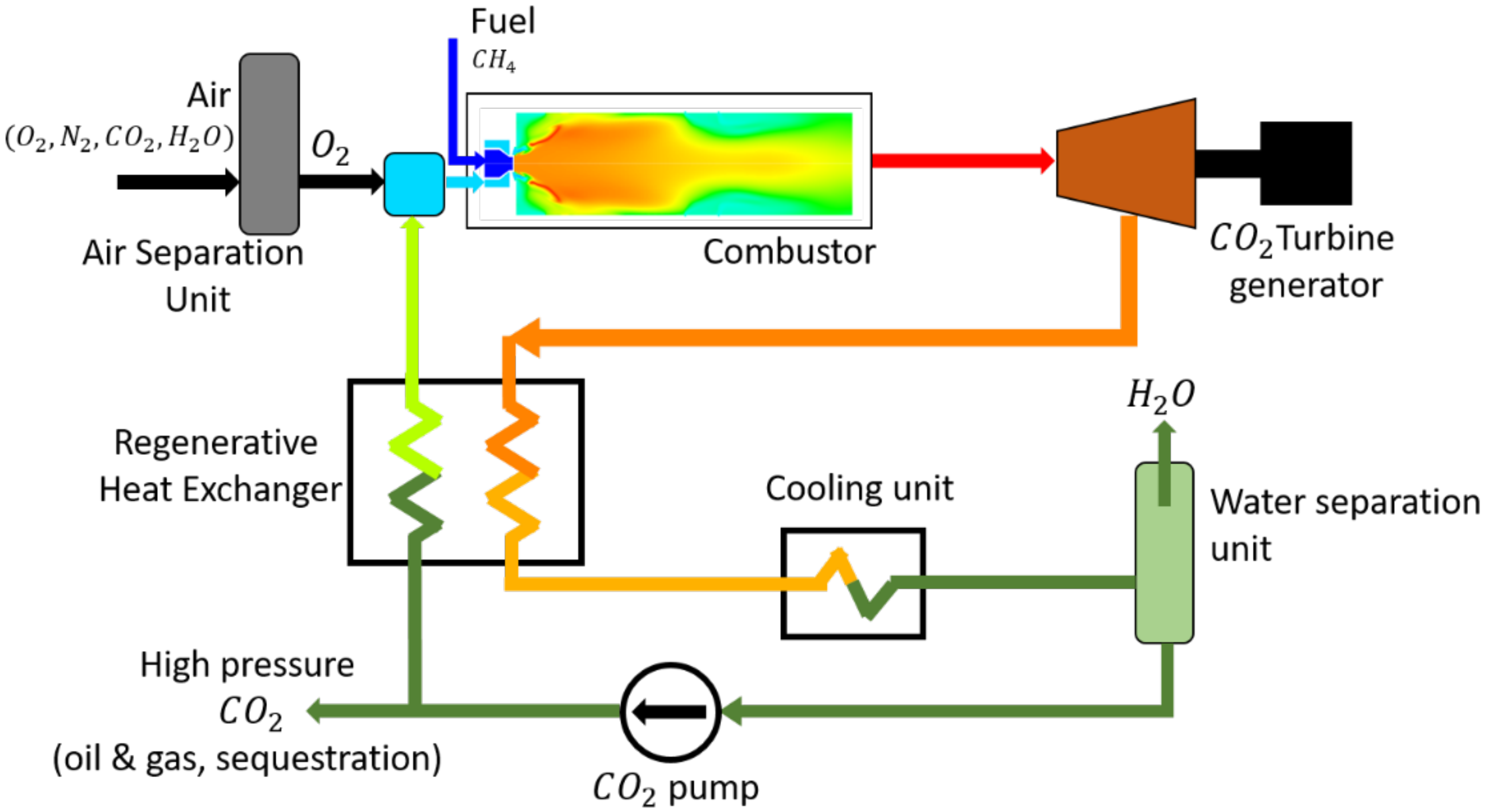
[1] Vesely, L., Manikantachari, K. R. V., Vasu, S., Kapat, J., Dostal, V., and Martin, S., 2018, "Effect of Impurities on Compressor and Cooler in Supercritical CO2 Cycles," Journal of Energy Resources Technology, 141(1), pp. 012003-012003-012008.

# Goal of the Study

- $sCO_2$ combustors work in a semi-closed loop
- Exhaust $CO_2$ is reintroduced in combustion chamber after removing water and other impurities
- Not all CO is removed and a significant part of it can make its way back into the combustion chamber
  - Pathways: mainstream flow, effusion and dilution flow
- Closed $sCO_2$ loop can become unstable if a positive feedback is established
  - A small amount of CO in inflow stream(s), increases CO at outflow multiple fold

- **Goal: study the effect of CO addition (impurity)**
- **We investigate this problem using two approaches**
  1. *Simplified model:* perfectly stirred reactor
  2. *Full 3D CFD modeling* of the combustor

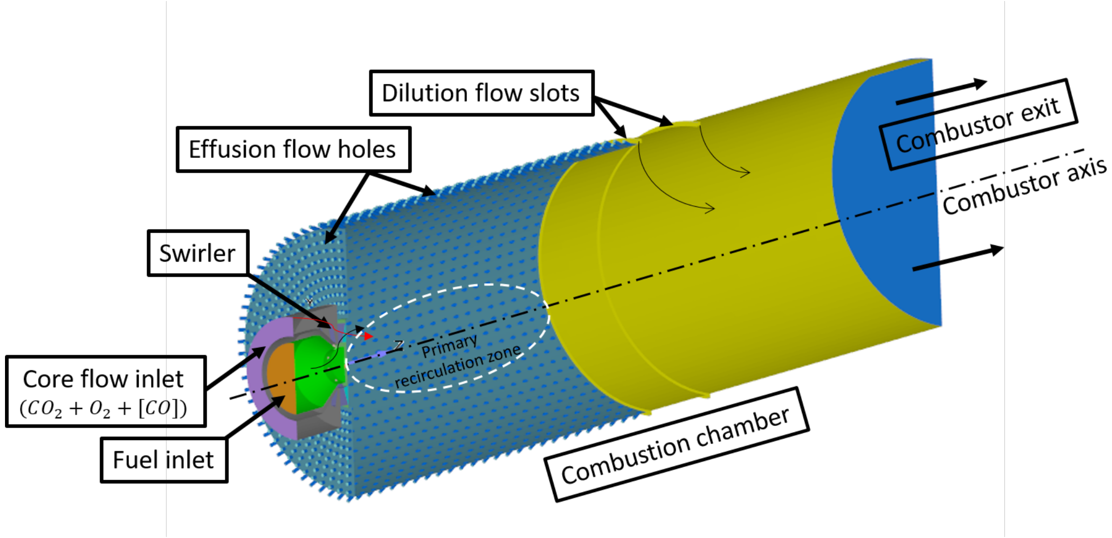
# Supercritical $CO_2$ cycle



*Schematic of Allam cycle which makes the basis for sCO2 combustors*

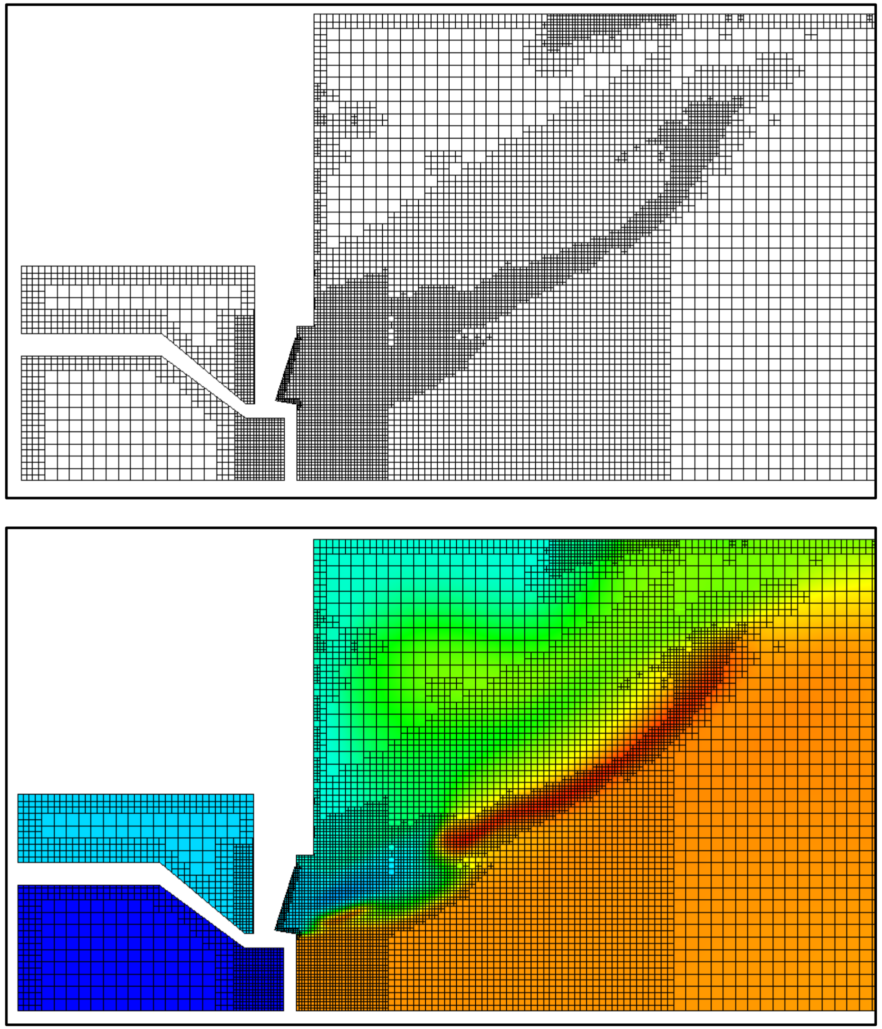
# Geometry

- Concept oxy-fuel combustor geometry created at SWRI (Ref: Jacob Delimont *et al.)*
- Part of design study by SWRI, Thar Energy *et al.* for creating a 1MW (thermal) $sCO_2$ combustor
- Experimental in nature. Similarity with traditional gas fueled single axial combustors
- Simplified in-order to facilitate a parametric design study
- Combustor zones: swirler, primary zone and dilution
- $CO_2$ captured from exit cycled back in combustor through core inflow, effusion holes and dilution slots.
- Core flow composed of $O_2$ (obtained from air-separation unit upstream) premixed with super critical $CO_2 + CO$ impurities
- Fuel $(CH_4)$ injected through circular holes along inner diameter in the swirler.



# Numerical Modeling and Mesh

- Turbulence modeling
  - Realizable $k - \epsilon$ turbulence model
- Chemistry model
  - Cai-2017 (Cai, 2017)
  - Saudi ARAMCO 2.0 (W.K. Metcalfe, 2013)
  - No Adaptive Zone used
- Mesh settings
  - Base mesh: 2mm
  - Fixed refinement on walls
    - $Y^+ \sim 20$
  - AMR max refinement level = 3
    - Smallest cell size = 0.25mm
  - Cell count $4M\ cells$



*Adaptive mesh refinement for temperature in the recirculation zone*

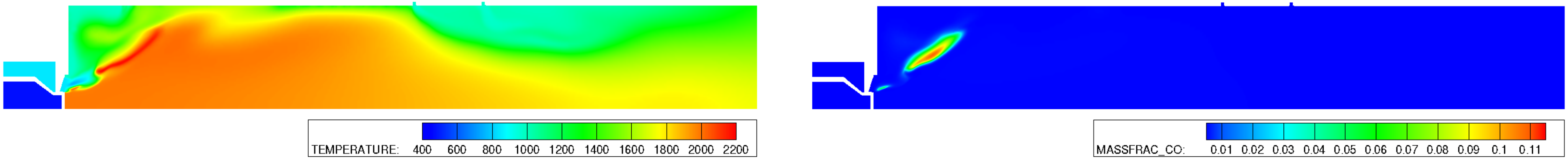
# Effect of Mechanism

We study two mechanisms widely used in the CFD community for $CH_4$ combustion

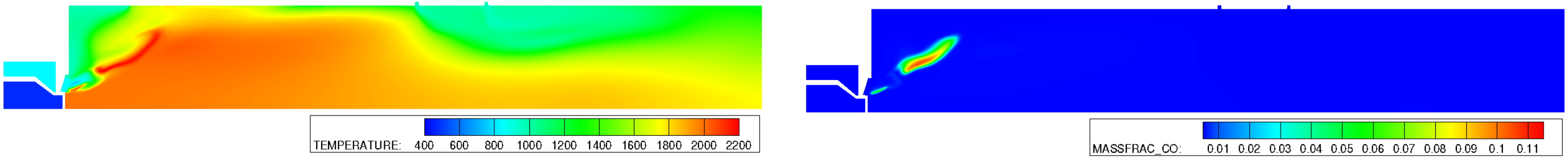
- Cai-2017 (Cai, 2017)
  - Developed at RWTH Achen (Germany)
  - Suitable for oxy fuel combustion at high pressure (~30bar)
- Saudi ARAMCO 2.0 (W.K. Metcalfe, 2013)
  - AramcoMech 2.0 builds upon AramcoMech1.3
  - Developed by Combustion Chemistry Centre ($C^3$) at NUI Galway (funded by Saudi Aramco)
    - *https://www.nuigalway.ie/combustionchemistrycentre/#*
  - Reduced version of this mechanism (73 species) has been used in this work
  - Developed to characterize kinetic and thermochemical properties of large number of $C_1 - C_4$ based hydrocarbon and oxygenated fuels
  - Validated at very high pressures

# Effect of Mechanism

- Goal
  - Qualitatively show difference between two mechanisms for methane combustion
  - Compare prediction of flow field, flame shape and emissions in the concept $sCO2$ combustor
  - For this part, no CO is added to inflow stream
- Conclusion
  - Similar temperature and CO profiles. Some differences in flame shape and temperature in corner recirculation
  - Overall, both mechanisms perform equally well for $sCO_2$ combustion.



Temperature (left), CO (right) distribution from Saudi ARAMCO 2.0

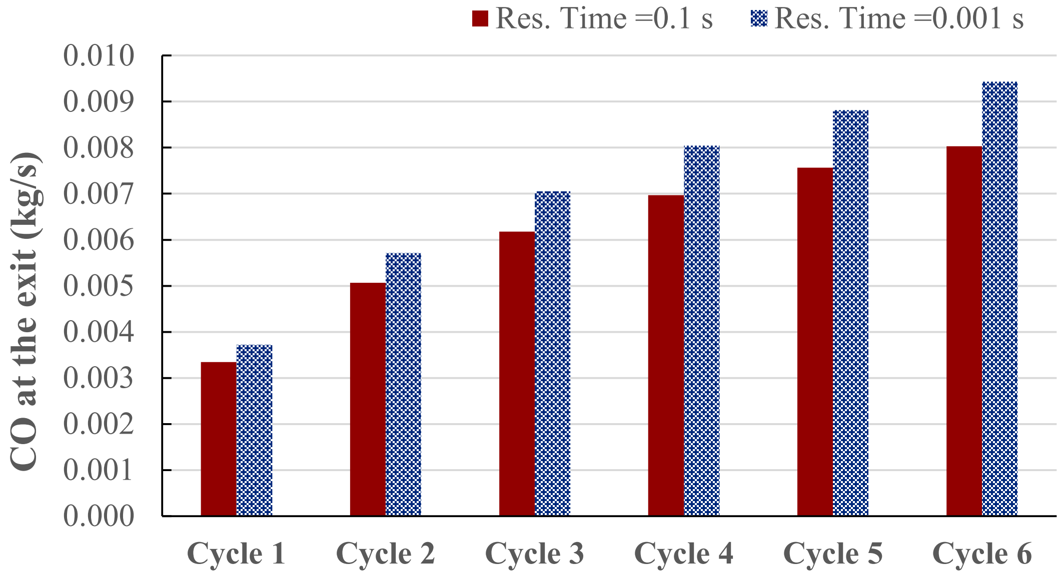


Temperature (left), CO (right) distribution from Cai-2017

# Effect of $CO$ Addition: PSR Modeling

| **PSR inlet species** | **Flow rate** |
|---|---|
| $\boldsymbol{CH_4}$ | $0.02\ kg/s$ |
| $\boldsymbol{O_2}$ | $0.08\ kg/s$ |
| $\boldsymbol{CO_2}$ | $75\%, 90\%$ and $95\%$ |

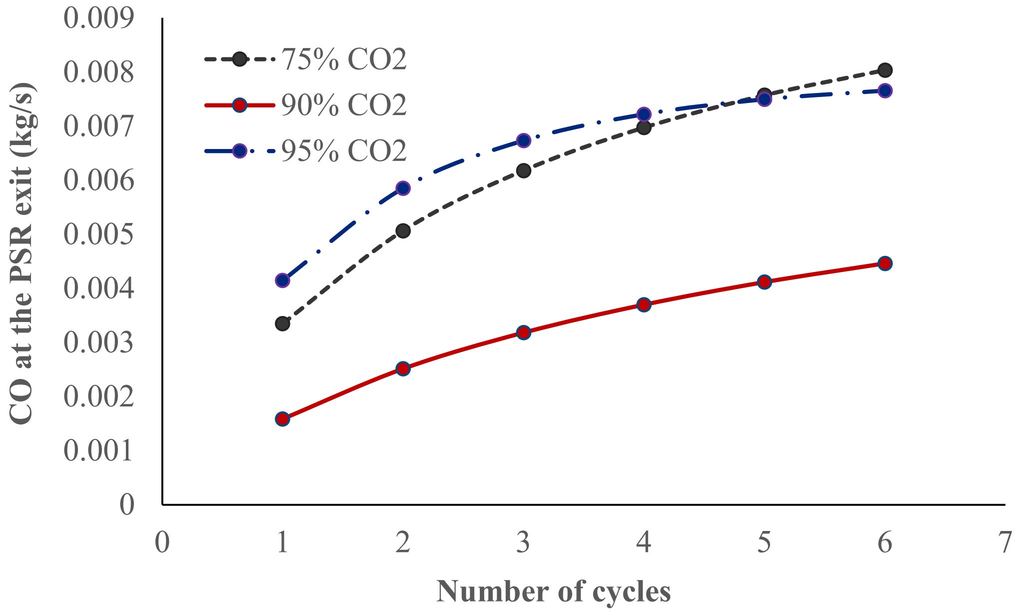
- Perfectly Stirred Reactor (PSR) inflow conditions
- We first study effect of residence time on exit $CO$
  - Case has $75\%$ $CO_2$ dilution
  - Two residence times studied: 0.001s and 0.1s
    - 0.1s $t_{res}$ is representative of typical combustor
  - $CO$ from cycle $N-1$ is introduced in $N^{th}$ cycle
- Growth of $CO$ is faster in low $t_{res}$ PSR
- Expected as expected: in low $t_{res}$ PSR, time not sufficient to oxidize $CH_4$ to $CO_2$
- Remainder of the study: $t_{res}$ PSR = $0.1s$



*CO at PSR exit for different residence time cases*

# Effect of $CO$ Addition on exit $CO$: PSR Modeling

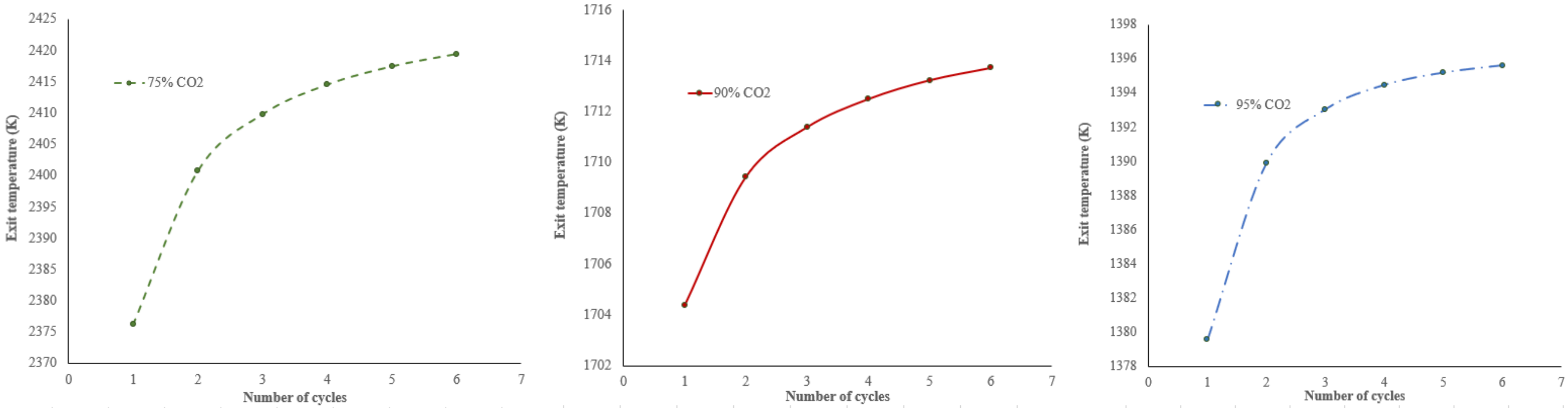
- $sCO_2$ systems work in a semi closed loop → exit $CO$ can come back into combustor through recycled $CO_2$
  - Potential to make $sCO_2$ system unstable
- PSR modeling
  - $N^{th}$ PSR cycle, uses exit $CO$ from $(N-1)^{th}$ cycle. Cycle 1 has no $CO$.
  - Exit $CO$ increases in consecutive cycles for all three $CO_2$ dilution mass-fractions
  - Trend it not exponential, as suspected by some in the $sCO_2$ community
  - Exit $CO$ appears to settle down to a steady value in couple of cycles



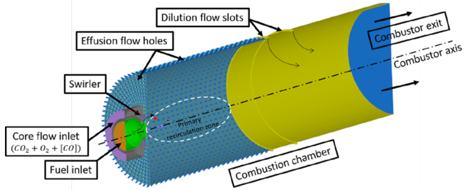
Evolution of exit CO in the PSR for different CO dilution cases. Each cycle uses the exit CO of the previous cycle as inflow condition for CO. Cycle 1 has no CO at inflow.

# Effect of $CO$ Addition on $T_4$ (exit temp): PSR Modeling

- Evolution of exit temperature for different $CO_2$ dilution levels
- As $CO_2$ dilution increases ↑ from 75% → 95%, exit temperature decreases ↓ over all
- For each case, exit temperature shows a trend to reach a steady value which is in-line with the trend in CO as oxidation of CO is the major contributor to overall heat release.



*Evolution of exit temperature with cycles in different $CO_2$ dilution cases.*



# Effect of $CO$ Addition on exit $CO$: 3D CFD Model

- Full 3D CFD using steady RANS and direct detailed chemistry used to simulate SWRI concept combustor
- If measured mass/mole fraction of $CO$ at outflow > CO introduced into the combustor → indicator of a +ve feedback
- Δ increase in CO at exit is **less** compared to what is added to the inflow
- Above argument could be misleading
  - Why? Amount of $CO_2$ at inflow and outflow are different
  - Correction: Look at the ratio of mole fraction of $CO$ to $CO_2$ at the inflow and outflow

| | **Outflow CO (kg/s)** | |
|---|---|---|
| | **ARAMCO 2.0** | **Cai-2017** |
| **Inflow CO** = 0 kg/s | $1.6 \times 10^{-5}\ kg/s$ | $1.6 \times 10^{-6}\ kg/s$ |
| **Inflow CO =** $4.67 \times 10^{-5}\ kg/s$ | $4.1 \times 10^{-5}\ kg/s$ | $4.0 \times 10^{-5}\ kg/s$ |
| **Inflow CO =** $6.1 \times 10^{-5}\ kg/s$ | $4.5 \times 10^{-5}\ kg/s$ | $4.6 \times 10^{-5}\ kg/s$ |

*Mass flux of $CO$ (kg/s) at combustor outflow*

| | **Outflow Xfrac(CO)/Xfrac(CO2)** | |
|---|---|---|
| | **ARAMCO 2.0** | **Cai-2017** |
| **Inflow X(CO)/X(CO2)** = 0 | $7.6 \times 10^{-5}$ | $6.3 \times 10^{-6}$ |
| **Inflow X(CO)/X(CO2) =** $1.9 \times 10^{-4}$ | $1.5 \times 10^{-4}$ | $1.6 \times 10^{-4}$ |
| **Inflow X(CO)/X(CO2) =** $2.5 \times 10^{-4}$ | $1.9 \times 10^{-4}$ | $1.93 \times 10^{-4}$ |

*Ratio of mole fractions of $CO$ to $CO_2$ at outflow*

# Summary

- Numerical framework
  - Perfectly Stirred Reactor (PSR); Full 3D RANS simulation with direct detailed chemistry and Adaptive Mesh Refinement for capturing flame shape and flow gradients
- Two key mechanisms (ARAMCO 2.0 and Cai-2017) studied for $CH_4$ combustion
  - Predicted temperature and CO profile very similar
  - Exit CO prediction also very close
- Investigated effect of $CO$ addition
  - Determine if a concept $sCO_2$ combustor (designed at SWRI) establishes a +ve feedback loop, which would adversely affect the performance of the combustion system
- $CO$ addition in the outflow does not seem to lead the $sCO_2$ combustor (working in a semi closed loop) in a positive feedback loop
- Exit $CO$ tends to reach an equilibrium value (PSR model) or reduce (3D CFD) compared to what is introduced at the inflow end

# THANK YOU!

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