EFFECT OF IMPURITIES IN THE RE-CYCLED CO_2 STREAM ON A SUPERCRITICAL CO_2 COMBUSTOR

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spectroscopy. He is the author of more than 150 journal and conference articles including one article in the prestigious *Science* magazine. He is also a reviewer for numerous journals, session chair for conferences, and has reviewed proposals for federal agencies. He has won several national and international awards given to early career academic researchers. He is the recipient of 2017 American Society of Mechanical Engineers (ASME) and International Gas Turbine Institute's Dilip Ballal Early Career Award and the Society of Automotive Engineers (SAE)'s 2018 Ralph R Teetor Educational Award. Currently, he has ongoing research projects from FAA, NASA, DTRA, DOE, DoD, FSGC, ACSPRF, and several industries.

ABSTRACT

This work provides a short review of sCO_2 combustor design considerations and provides more insights into the effect of impurities in the re-cycled CO_2 stream of the sCO_2 combustor. Two main impurities studied here are, O_2 and H_2O. Incomplete combustion and inefficiency of water separation unit in the Allam cycle [1] may increase the probability of these impurities to re-enter into the combustion chamber.

In this work, Large-Eddy Simulations (LES) are also performed on a sCO_2 combustor by using Converge® CFD tool. Here, realgas corrections are accounted for with the Soave-Redlich-Kwong equation-of-state (SRK EOS) and kinetics are accounted for by an Aramco 2.0 derived 23-species mechanism. The results show that, when the O_2 and H_2O impurities are up to 5000 ppm, the near burner radial reaction zone increases in width. Further, the CO production/oxidation in the primary zone is significantly influenced by these impurities. Also, the CO distribution is observed to be higher at the core of the swirl in the primary zone due to impurities. Under the studied conditions, the H_2O impurity is delaying the CO oxidation. Hence, higher CO levels can be expected at the end of combustor if H_2O impurities are higher in the re-cycled CO_2 stream. However, O_2 impurities support the complete oxidation of CO hence a better thermal efficiency can be achieved.

INTRODUCTION

The supercritical CO_2 (sCO_2) power cycle is an emerging technology which has the potential to address both environmental concerns and energy demands. The well-known features of this power cycle are: 1) the high expected cycle efficiency compared to corresponding HE, AR and steam cycles, 2) compactness of the overall power plant, 3) complete capture of CO_2 and 4) the wide applicability over all power producing applications. This is a closed cycle and uses sCO_2 as the working fluid, therefore, CO_2 produced by the direct-fired, oxy-methane combustion can be recirculated within the same cycle loop and the excess supercritical CO_2 from the cycle can be used for other commercial purposes [2]. However, current state-of-art peak operating pressures for sCO_2 combustion is approximately 300 atm [2] and the level of CO_2 dilution in the combustor is more than 95% percent by mass. Here, the presence of sCO_2 at 300 atm shows a different dilution effect on combustion phenomenon than N_2 (air-diluted combustion) due to significant differences in their thermo-chemical properties. Therefore, the mixing and reaction phenomenon, ignition and blowout phenomenon are expected to be considerably different in sCO_2 combustion than an air-diluted combustor. At these extreme pressure and dilution conditions, experiments and testing are expensive, time consuming, and dangerous. Also, during the initial development of a combustor, even finalizing the design based on 3-D simulations is a tedious task because a wide range of operating conditions or strategies needs to be tested. Therefore, initial domain of operating conditions or strategies can be minimized by accurate 0-D and 1-D simulations. Further, the detailed 3-D simulations and experiments can be carried based on the directions of the 0-D and 1-D analysis. As per the available literature, guidelines for designing and modeling sCO_2 combustors are minimal [3-12] and still there is a need for testing a large number of combinations of initial operating conditions and design strategies before successfully constructing an efficient sCO_2 combustor.

The perfectly-stirred reactor (PSR) modeling was extensively used in the 1950s to guide the development of gas turbine combustors and ramjets [13-15]. Also, complete gas turbine combustor performance analysis was carried out by coupling plug-flow reactor (PFR) and PSR models [16-18]. This method is used in [19, 20] to provide crucial design considerations for sCO_2 combustor development. In these works, only a single PSR and PFR combination is used as shown in Fig.1, because the main objective of those works is not to simulate a particular combustor but to reduce the initial domain of operating strategies. Therefore, the results shown in those papers are qualitative in nature. These works use the real gas version of CHEMKIN, i.e., CHEMKIN-RG [21] and coupled with CHEMKIN PSR and PFR codes [22, 23].

Also, some important requirements for sCO_2 combustors are as follows: 1) lower residence time/ smaller volume, 2) protection from impurities developed in the closed loop of the cycle, and 3) complete burning of fuel within the combustion chamber.

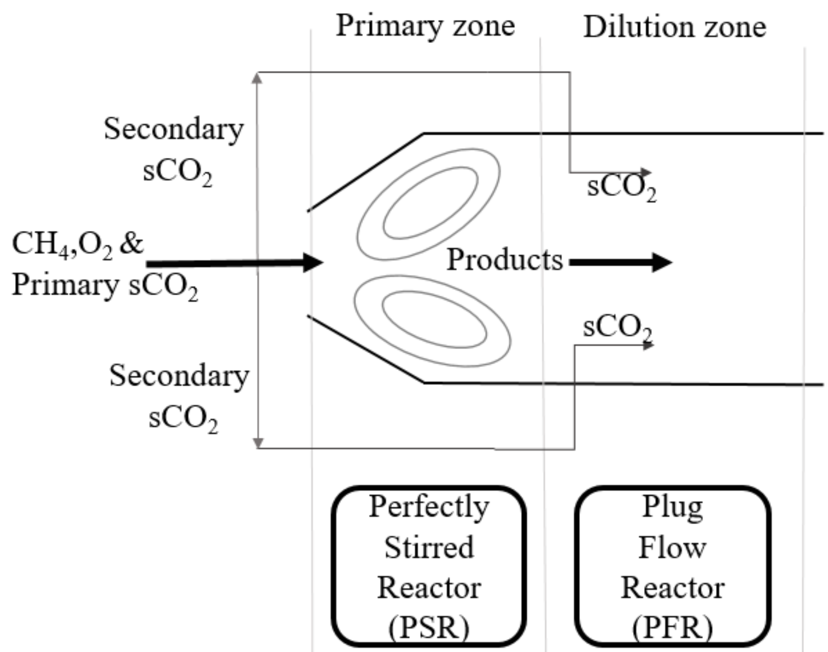


Figure 1: Modeling of sCO_2 combustor by PSR and PFR [19, 20]

The first requirement as mentioned earlier is essential from the design point of view because, the previous studies show that the sCO_2 turbine is fifty-times smaller than an equal power steam turbine, hence the combustor volume should be scaled down to an optimal level for proper alignment with the turbine. A combustion chamber primary zone volume can be reduced by having only pure oxy-methane combustion in the primary zone and by purging recycled CO_2 into the dilution zone. However, the study [19] shows that, operating the combustor without any CO_2 dilution in the primary zone is very dangerous at 300 bar pressure. On the other extreme, supplying 100% of re-cycled CO_2 into the primary zone is also not feasible because the amount of residence time required to oxidize 99.99% of the fuel is very large. Hence, the size requirement of the combustor will be large. An optimum CO_2 split between primary and dilution zones in sCO_2 combustors is 50-50% for reasonable size of the combustor and complete oxidation of CO.

The earlier works [19, 20] qualitatively show the possibility of high CO and O_2 traces for a smaller residence time combustor and recommends a novel idea of incorporating a pre-reaction chamber ahead of the combustion chamber in the sCO_2 Allam cycle as shown in the Fig. 2. This pre-reaction chamber is shown to reduce the sCO_2 combustion chamber required residence time for complete burning of fuel, however it should be noted that, a detailed cycle analysis is further needed for understanding the feasibility of using a pre-reaction chamber in Allam cycle.

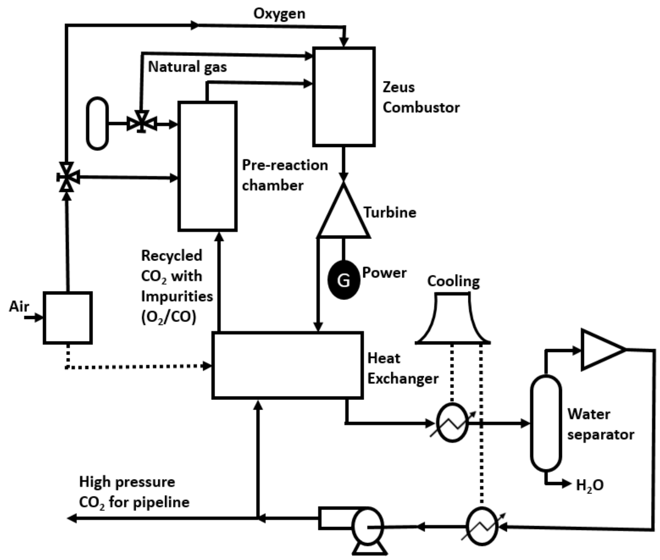


Figure 2: Allam cycle with pre-reaction chamber [20]

Also, another challenge in the sCO_2 combustor design is that the traces of CO, O_2 and H_2O may buildup over a period of closed loop operation and it may influence the combustion performance. The work of [24] showed that, impurities could significantly influence sCO_2 cycle performance. Hence, in this current work the effect of O_2 and H_2O in re-cycled CO_2 stream of Allam cycle on combustor performance is studied by using Large-eddy-simulations (LES). The LES simulations are performed by a commercial CFD tool called Converge®

MODELING

A recent sCO_2 combustor model [25] of Southwest Research Institute (SwRI), which is under development is used in these simulations as shown Fig.3 with a slight change in the dilution zone geometry. The inlet flow conditions to the combustor are reproduced from [26] and shown in Fig. 4. A detailed description of this combustor can be found in the work of [26].

Here, the oxidizer jet consists of O_2 and CO_2 and it mixes with pure a CH_4 jet inside a swirl injector in a crossflow configuration. The swirl angle of the injector is 40^o and the reacting jet which is coming out of the swirl injector mixes with fifty-percent of purging CO_2 in the primary zone. The remaining 50% of the CO_2 is distributed across the inlets of the dilution zone. Here, it should be noted that the design of the dilution zone shown in this work is different from the work of [26].

The detailed simulation parameters are listed in Table 1. Here, Large-eddy simulations are performed with the Viscous-One equation model which is developed by [27]. The Converge® CFD uses adaptive mesh refining (AMR) strategy hence the base cell size and AMR are used in order to have approximately six million cells in the combustor. Also, Soave-Redlich-Kwong equation of state is used in these simulations. Here, an Aramco 2.0 derived 23-species mechanism [28] is used and all the species transport equations are solved by using SAGE detailed chemistry in which all species conservation equations are solved. Further, the viscosity and thermal conductivity are modeled by assuming that the working fluid is pure CO_2 and these transport property profiles are obtained from NIST-REFPROP. An important point to be noted here is that, the reactor residence time for this combustor is large i.e., approximately thirty milliseconds, hence the simulation is continued until six flow-through times (180 milliseconds). A statistically stationary solution is observed after 90 milliseconds, but the data presented in this work are obtained at a sufficiently large simulation time (after 140 milliseconds) for better confidence.

Three cases as shown in Table 2 are simulated to investigate the effect of impurity in the re-cycled sCO_2 stream on the combustor performance. It must be noted that, the influence of CO impurity is not studied in this work because as a design requirement the CO must be burnt within the combustion chamber, hence no CO is considered in the re-cycled CO_2 stream. It should also be noted that the total flow rate is kept constant in each case.

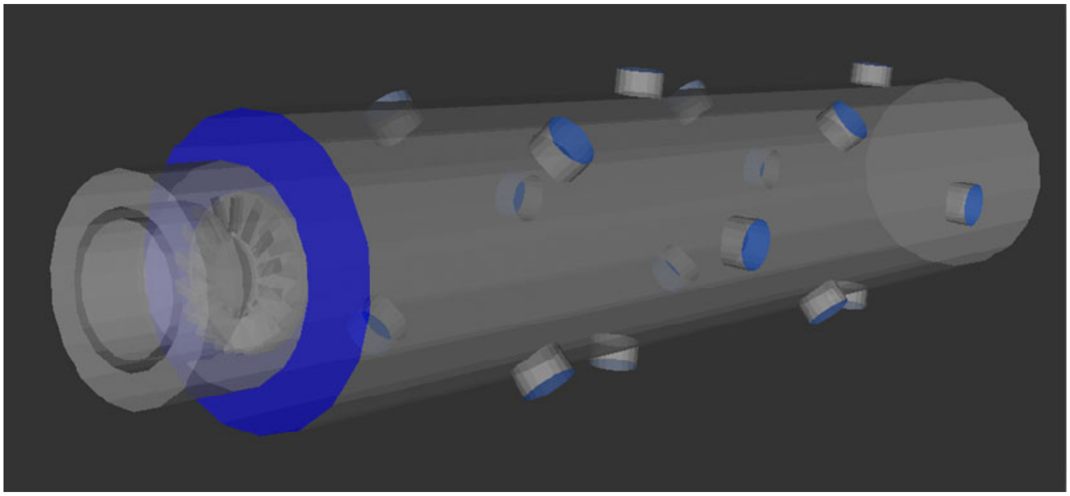


Figure 3: A three-dimensional view of recent SwRI sCO_2 combustor [25, 26]. (blue colored boundaries indicate the inlets of re-cycled CO_2 stream for dilution)

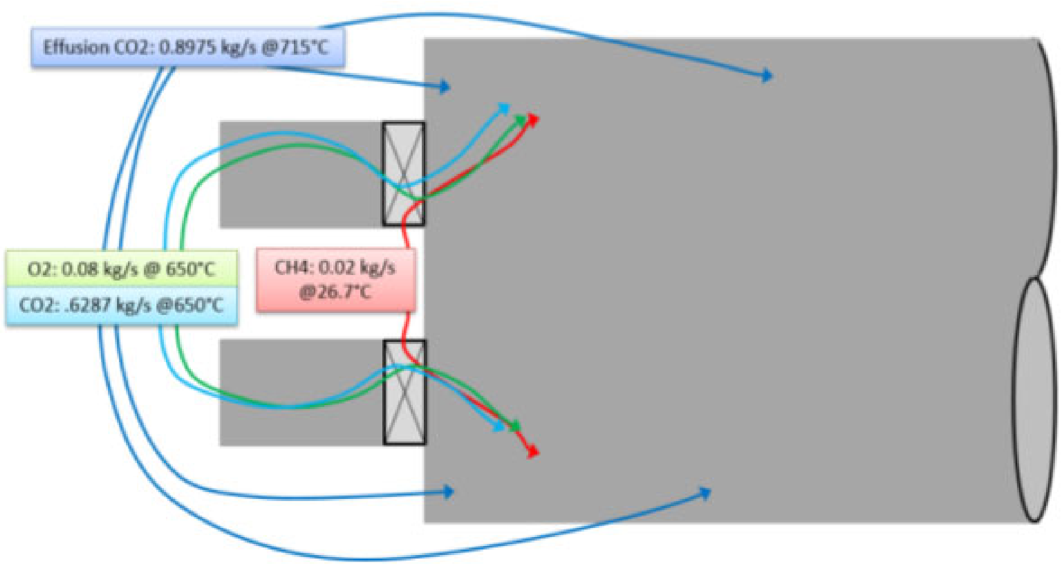


Figure 4: Inlet flow conditions to the combustion chamber; reproduced from [26]

Table 1: Simulation parameters used in this study

S. No	Modeling	Parameter /model chosen
1)	Turbulence modeling	Large-eddy simulation → Viscous One Equation. This model uses sub-grid kinetic energy in modeling the turbulent viscosity [27].
2)	Wall heat transfer modeling	O'Rourke and Amsden [29]
3)	Combustion modeling	SAGE detailed chemistry (all species transport equations are solved).
4)	Number of cells	Approximately six million cells (Adaptive mesh refinement is used)
5)	Equation of state	Soave-Redlich-Kwong equation of state based on [6]
6)	Viscosity and Thermal conductivity	Pure CO_2 properties between 800 -1600 K from REFPROP [30] are used.
7)	Chemical kinetic mechanism	A 23-species mechanism derived from Aramco 2.0 [28]
8)	Simulation time	6 follow-through times

RESULTS AND DISCUSSION

As discussed in the introduction purifying the exhaust products of the combustion to obtain 100% pure re-cycled CO_2 stream is expensive. In fact, the separation of the final traces of impurities would be costlier. Therefore, the operation cost of exhaust separation can be reduced if the combustor is designed to perform under some optimum levels of impurities. The major impurities in the exhaust stream could be CO, O_2 and H_2O. In the Allam cycle, H_2O can be separated by condensing the exhaust products, but the separation of CO and O_2 from the products is difficult. Therefore, it is recommended to design the combustion chamber in order to have either CO or O_2 [20] at the exit. As observed from the work [19], for smaller reactor residence time combustors, most of the fuel can remain in the form of unburnt CO. Also, CO does not react in the dilution zone due to the unavailability of O_2 (If re-cycled CO_2 is pure). Therefore, an optimal lean operation is necessary for sCO_2 the combustor to burn all of the CO. Now, in such cases of lean operation the major exhaust products would be CO_2, O_2 and H_2O. Therefore, three cases as shown in Table 2 are considered in the current work to understand the influence of impurities. Also, as mentioned in the modeling section, the total flow rate of the re-cycled stream is kept constant in all three cases. Here, Case-1 contains pure re-cycled CO_2 without any impurities, Case-2 has 5000 ppm of O_2 and Case-3 has 5000 ppm of H_2O in the re-cycled CO_2 stream.

Table 3 shows a comparison of time averaged temperature profiles from the LES simulation for the three cases considered. Here, there is a difference in the near burner temperature distribution in the radial direction. Radial width of temperature is smaller for Case-1 compared to Cases-2 and 3. This change is basically due to changes in the reaction zone. In Cases-2 and 3, the O_2 and H_2O present in CO_2 stream is reacting with the combustion products and increases in the reaction zone are observed.

Further, Table 4 shows the time averaged mass fraction of CO for the three cases considered. Here, it is evident that the CO in the primary zone is higher in Cases 2 and 3 compared to Case-1. Also, a high CO concentration region can be observed symmetrical to the axis in all the cases. These high CO concentration zones are formed just after the first set of radial dilution holes as seen in Fig. 5. Here, the low temperature CO_2 which is coming from the dilution holes is quenching the reaction zone products temperature and delaying the CO oxidation. It should be noted that, CO concentration just after first set of dilution holes is higher in Case-3 of Table 4 and lower for Case-2. It is because H_2O present in the CO2 is retarding the CO oxidation in Case-3 and accelerating CO oxidation in Case-2.

Table 2: Various cases considered in this study

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

Table 5 shows the spatial mean values of CO, O_2, CH_4 and temperature at the exit of the combustor. Here, the inlet CH_4 flow rate is the same for all three cases and we can see that all three cases show that the CH_4 is fully oxidized before the exit. However, the CO levels are significantly different. The CO is highest for Case-3 and lowest for Case-2. Which signifies the need of better CO oxidation strategies when we cannot separate H_2O in the water separation unit of the Allam cycle. Also, it is interesting to note that the exit temperature of Case-3 is increased slightly even though there is a plenty of CO remains at the exit. Further Case-2 shows that almost 2000 ppm of O_2 is left at the combustor exit when there is O_2 impurity in the re-cycled CO_2 stream and this case has the least CO and highest temperature. Therefore, these show that the lean operation is the best strategy to achieve a better thermal efficiency. As per current state-of-art, operating air-separation units is costlier in the Allam cycle and hence the lean operation is less acceptable. Therefore, further cycle analysis is required in this direction.

Table 3: The comparison of combustor mid-section temperature contours

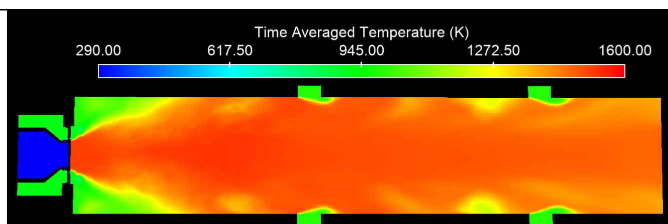
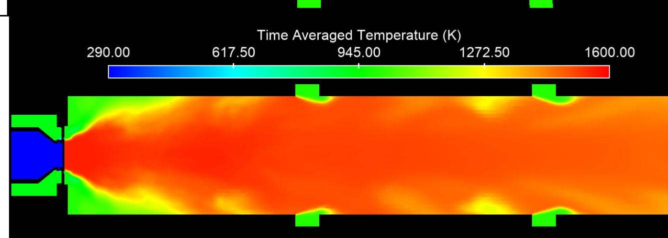
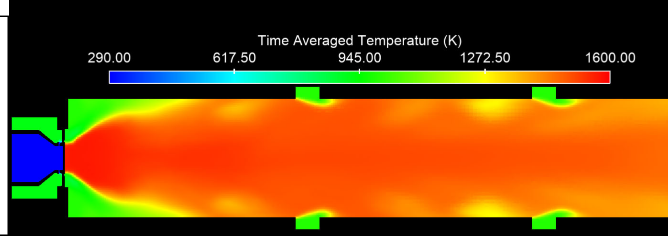
Case	Contours of Temperature
1	
2	
3	

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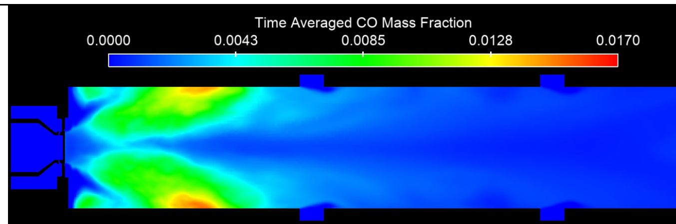
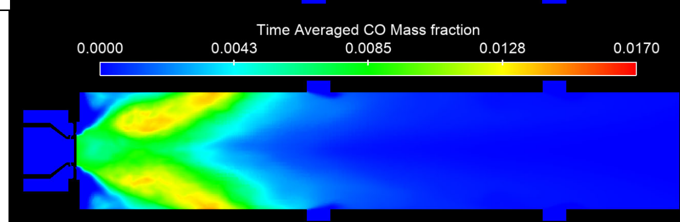
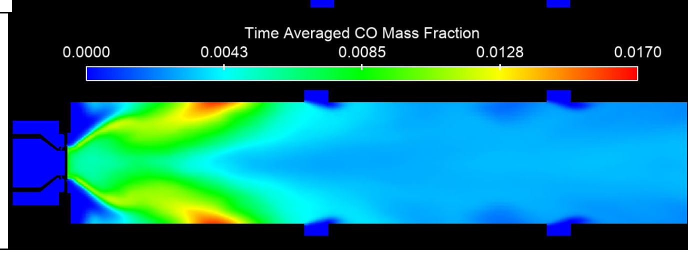
Table 4: The comparison of combustor mid-section CO contours

Case	Contours of CO Mass Fraction
1	
2	
3	

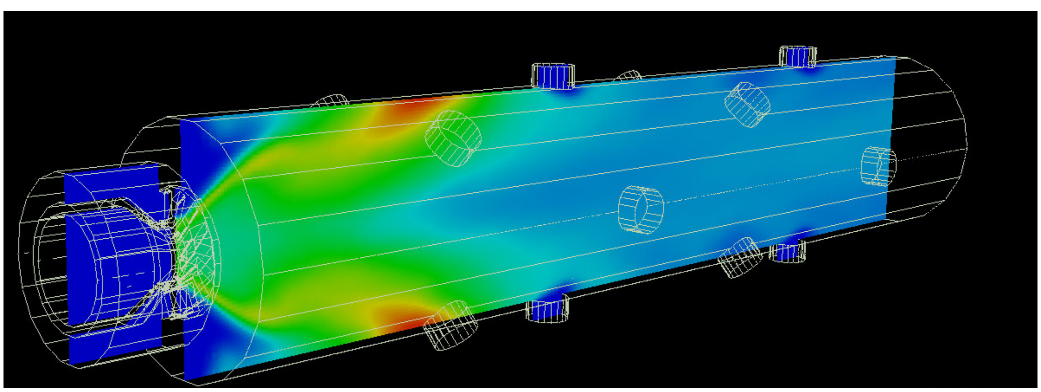


Figure 5: A 3D view of CO mass fraction distribution on the cross-section plane.

Table 5: The spatial, time averaged mean values CO, O_2, CH_4 and temperature at the exit plane of the combustor

	CO (ppm)	O2 (ppm)	CH4 (ppm)	Temperature (K)
Case1	1194	351	0	1402.3
Case2	185	2000	0	1415.9
Case3	1782	248	0	1408.4

CONCLUSIONS

In the current work, recent zero and one-dimensional design investigations for sCO_2 combustion are reviewed and large-eddy simulations are performed using the Converge® CFD tool to investigate the effect of impurities such as O_2 and H_2O in the re-cycled CO_2 stream on the combustor performance. The conclusions are as follows:

1) Presence of H_2O in the re-cycled CO_2 stream retards CO oxidation, hence higher CO concentrations can be expected at the exit of the sCO_2 combustor.

2) Presence of O_2 in the re-cycled CO_2 stream improves CO oxidation**,** hence CO can be burnt completely within the combustion chamber.

3) O_2 impurities also improve the thermal efficiency in the sCO_2 combustor.

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