68 Large-eddy simulation of a supercritical CO2 combustion field in a realistic combustor

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Abstract(Click to expand)

As global demand for energy increases while environmental regulations tighten, novel power generation cycles are being developed to meet market needs. In order to meet this demand, 8Rivers Capital Limited Liability Company has been engaged in the development of an environmentally conscious thermal power generation system based on a Supercritical CO2 gas turbine cycle (Allam cycle). Toshiba ESS has been developing a turbine and a combustor for the Allam cycle. The cycle requires oxy-fuel-CO2 combustion at approximately 30MPa and 1150° C turbine inlet temperature. Designing a durable hardware capable of thousands of hours of operation with efficient combustion as well as production of clean CO2 exhaust is a challenging task which also requires an approach using numerical simulations. However, there are few reports of combustion simulation in such ultra-high pressure. In this study, large-eddy simulation (LES) is applied to a Toshiba's supercritical CO2 combustor. In order to take the supercritical conditions into account, the Soave-Redlich-Kwong equation of state is applied, and the Chung model is used for transport properties. A dynamically thickened flame model is employed as a turbulent combustion model, and the (5 species, 2 reactions model) is used for the reaction mechanism. Due to extreme operation conditions inside the combustor, it is crucial to keep the combustion liner at adequate temperature. To predict the wall heat load on the combustion liner, a coupled fluid-structure conjugate heat transfer method is applied. The computation is carried out using an unstructured LES solver FrontFlow/Red modified by Kyoto University, CRIEPI, and NuFD (FFR-Comb). The computational mesh for the combustor consists of 129 million vertexes and 204 million cells. The computation took approximately one week using 10,000 cores of the "K computer" at RIKEN Advanced Institute for Computational Science.It was observed that a stable flame is formed and the liner wall temperature is strongly affected both by cooling CO2 stream which flows over the outer and inner surface of liner wall and the flame temperature. The metal temperature results have also been examined form the simulation results.

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INTRODUCTION

It is imperative that the global community implements a path to achieve significant reductions in current greenhouse gas emissions, principally CO2.NET Power LLC, a company owned by Exelon Generation, McDermott International, 8 Rivers Capital and Oxy Low Carbon Ventures has constructed a 50MWth demonstration power plant which is based on Allam cycle (Figure 1) and it is capable of complete CO_2 capture at high pressure and purity for sequestration or reuse. The plant produces power at low cost and high efficiency with reduced plant footprint due to its high pressure and simple design.. **The responsibility of Toshiba ESS is the development of the turbine and combustor for the 50MWth demonstration power plant (Figure 2). Toshiba ESS have now completed the supercritical CO2 combustion test and are progressing further testing of the NET Power demonstration facility.** Natural gas and pure oxygen separated from air combined with recycled CO_2 is provided to combustor as inlet flows (Figure 3). The products of combustion (CO_2 and water vapour) enters the turbine, which turns a generator to generate electrical power. The turbine exhaust gas is cooled by the regenerative heat exchanger and transfers its heat to the high-pressure CO_2 gas after the excess CO_2 removal stage. The cooled gas is then passed to a water separator where condensed water is removed. The remaining CO_2 is pumped up to a high pressure where the excess CO_2 generated by combustion of the gas fuel can be collected directly with no additional separation unit. The remaining CO_2 is recirculated back to the process to form a semi-closed loop cycle. The cycle requires oxy-fuel-CO2 combustion at approximately 30MPa and 1423K turbine inlet temperatures.

Allam Cycle

Problem
In order to meet the world's carbon targets, we must develop cost-effective technology to eliminate CO2 emissions from carbon-based fuels.

Key Innovation
Using high pressure CO2 as the system working fluid.

Solution
An entirely new power cycle that generates emissions-free electricity from carbon-based fuels for lower costs than traditional, emitting technologies.

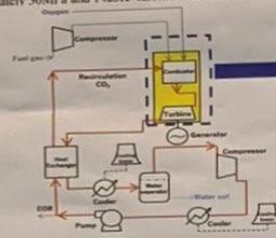


Fig.1 : Allam Cycle

Fig.2 : Toshiba's sCO2 Combustor and Turbine

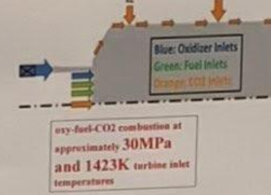


Fig.3 : Combustor inlet flow

NUMERICAL METHOD

Governing Equations

Continuity: $\frac{\partial \bar{\rho}}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{u})=0$

Navier-Stokes: $\frac{\partial \bar{\rho}\tilde{u}}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{u}\tilde{u})=-\nabla\bar{p}+\nabla\cdot\bar{\sigma}+\nabla\cdot\tau$

Enthalpy: $\frac{\partial \bar{\rho}\tilde{h}}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{u}\tilde{h})=\nabla\cdot\left[\bar{\rho}\left(EFD_h+(1-\Omega)D_t\right)\tilde{h}\right]+\frac{D\bar{p}}{Dt}+\tau:\nabla\tilde{u}$

Species: $\frac{\partial \bar{\rho}\tilde{Y}_k}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{u}\tilde{Y}_k)=\nabla\cdot\left[\bar{\rho}\left(EFD_k+(1-\Omega)D_t\right)\tilde{Y}_k\right]+\frac{E}{F}\dot{S}_{comb,k}$

Where flame sensor and flame thickening factor are

$\Omega=\tanh\left(\alpha\frac{s}{s_{max}}\right)$, $F=c(F_{max}-1)\Omega+1$

$\bar{\ }$: filtered mean value; $\tilde{\ }$: Favre averaged value; ρ: density; P: pressure; h: enthalpy; Y_k: mass fraction of species k; u: the velocity vector; τ: stress tensor including SGS stress; D_h: thermal diffusivity; D_k: mass diffusivity; $\dot{S}_{comb,k}$: reaction rate of species k; Ω: flame sensor; E: efficiency function; F: the flame thickening factor

EOS and Reaction model

Equation of state:

$$P=\frac{R_{mol}T}{V-b}-\frac{a(T)}{V(V+b)}$$

Soave-Redlich-Kwong (SRK) model

where the constants, a, b are

$a=\Omega_a\frac{R^2T_c^2}{P_c}\alpha(T)=a_c\alpha(T)$ $\quad\Omega_a=\frac{1}{9(2^{1/3}-1)}$

$b=\Omega_b\frac{RT_c}{P_c}$ $\quad\Omega_b=\frac{2^{1/3}-1}{3}$

$\alpha(T)=\left[1+f\left\{1-\left(\frac{T}{T_c}\right)^{1/2}\right\}\right]^2$

$f=0.480+1.574\omega-0.176\omega^2$

Westbrook 2 step reaction (2 spices)	
1	$CH_4+3/2O_2\rightarrow CO+2H_2O$
2	$CO+1/2O_2\rightarrow CO_2$

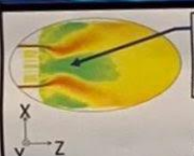
P: gas pressure[Pa]; V: specific volume[m3/kg]; T: temperature[K]; R: gas constant [J/mol K]; a: attractive force constant between molecules; b: volume correction constant; T_c: Critical temperature[K]; P_c: Critical Pressure[Pa]

LES Setting

Turbulent model	Standard Smagorinsky SGS
Fluid model	compressible
Real gas model	Soave-Redlich-Kwong EOS Chung's transport property
Combustion model	Dynamically Thickened Flame
Reaction mechanism	Westbrook 2 step reaction
Convection term discretization scheme	Velocity: 2nd order central 90% +1st order upwind 10% Temperature/ Species: 2nd order upwind
Time integration method	Euler implicit
Time step size [s]	1.0E-6

The computational mesh for the combustor consists of 125 million vertexes and 203 million cells. The computation took approximately one week using 10,000 cores of the "K computer" at RIKEN Advanced Institute for Computational Science.

RESULT AND DISCUSSION



● **There is a negative flow velocity at the vicinity of the injector which represents reverse flow.**
● **It is expected that this region affects flame holding.**
● **As flow goes downstream, the reverse catchment area disappears.**

-160.0 -80.0 0.0 80.0 160.0 (m/s)
-200.0 -120.0 -40.0 40.0 120.0 200.0

Fig.4 : Time-Averaged Velocity of Z axis Distribution

● Around the middle of the combustor, the temperature decrease is observed due to the mixing with the dilution CO2 injected into the combustor in that region.

● **The gas temperature near the combustor liner wall is kept relatively low due to the film cooling by recirculation CO2 injected from the cooling slots.**

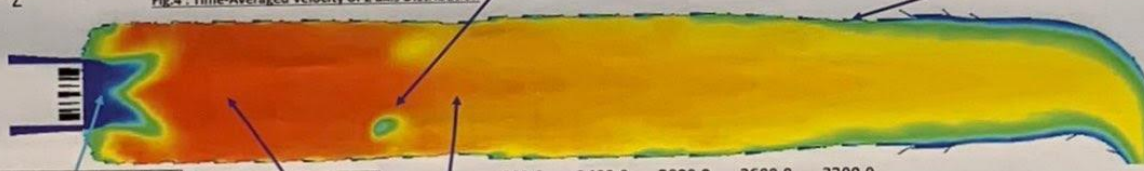


Fig.6 : Time-Averaged Gas Temperature Distribution

● The temperature at the vicinity of the injector is relatively low as the reaction did not start because of improper mixing of CH4 and O2, the mixing gradually comes in effect and a change in temperature is observed.

● The majority of the reaction and the rapid temperature is observed at the shear zone of swirling oxidizer jet where the remaining fuel is mixed with the oxidizer.
● CH4 and O2 are completely consumed as soon as they are mixed together.

● Temperature further comes down due to CO2 dilution and the concentration of CO2 gradually increases

● H2O concentration decreases as the gas goes downstream due to the addition of CO2.

Fig.7 : Time-Averaged Volume fraction CH4 Distribution

Fig.8 : Time-Averaged Volume fraction of O2 Distribution

Fig.9 : Time-Averaged Volume fraction of CO2 Distribution

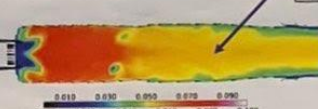


Fig.10 : Time-Averaged Volume fraction H2O Distribution

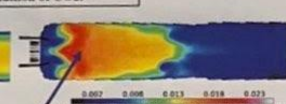


Fig.11 : Time-Averaged Volume fraction of CO Distribution

CO is primarily formed at the region where higher temperature is observed

In the vicinity of the injector, the CO2 concentration is relatively low (Fig. 9) because of CH4 and O2 mixing (Fig. 7 and Fig. 8). However, just outside the vicinity of the injector and the oxidizing agent shows that the CO2 concentration is close to 100%, and the CO2 concentration is the highest in this region (Fig. 9). The CO2 concentration is still relatively low even around central axial area downstream of the recirculation zone, and this part coincides with the region where the H2O concentration is large as seen in Figure 7.

CONCLUSION

In this study, a large-eddy simulation (LES) of a combusting field for a 50 MWt supercritical CO2 combustor was performed. **Most of the fuel and oxygen reacted in a region slightly away from the injector. The CO2 formation and the temperature profile makes significance and gives appropriate results such as temperature profile and emission zone to validate the design. The exhaust gas has low concentration of "CO" and "O2", providing appropriate condition for the Allam cycle.** Toshiba ESS has also conducted an actual combustion test to validate the combustion chamber design and emission under the operating conditions of Allam cycle and thus for the future work will compare the simulation results with the actual experiment test results and based on that study will appropriately check the accuracy of the simulation results in order to optimize the chemical kinetic model that can provide accurate combustion results in least amount of time and will provide a direction to the advancement of combustion and simulation science at extreme high pressure combustion under CO2 environment.

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