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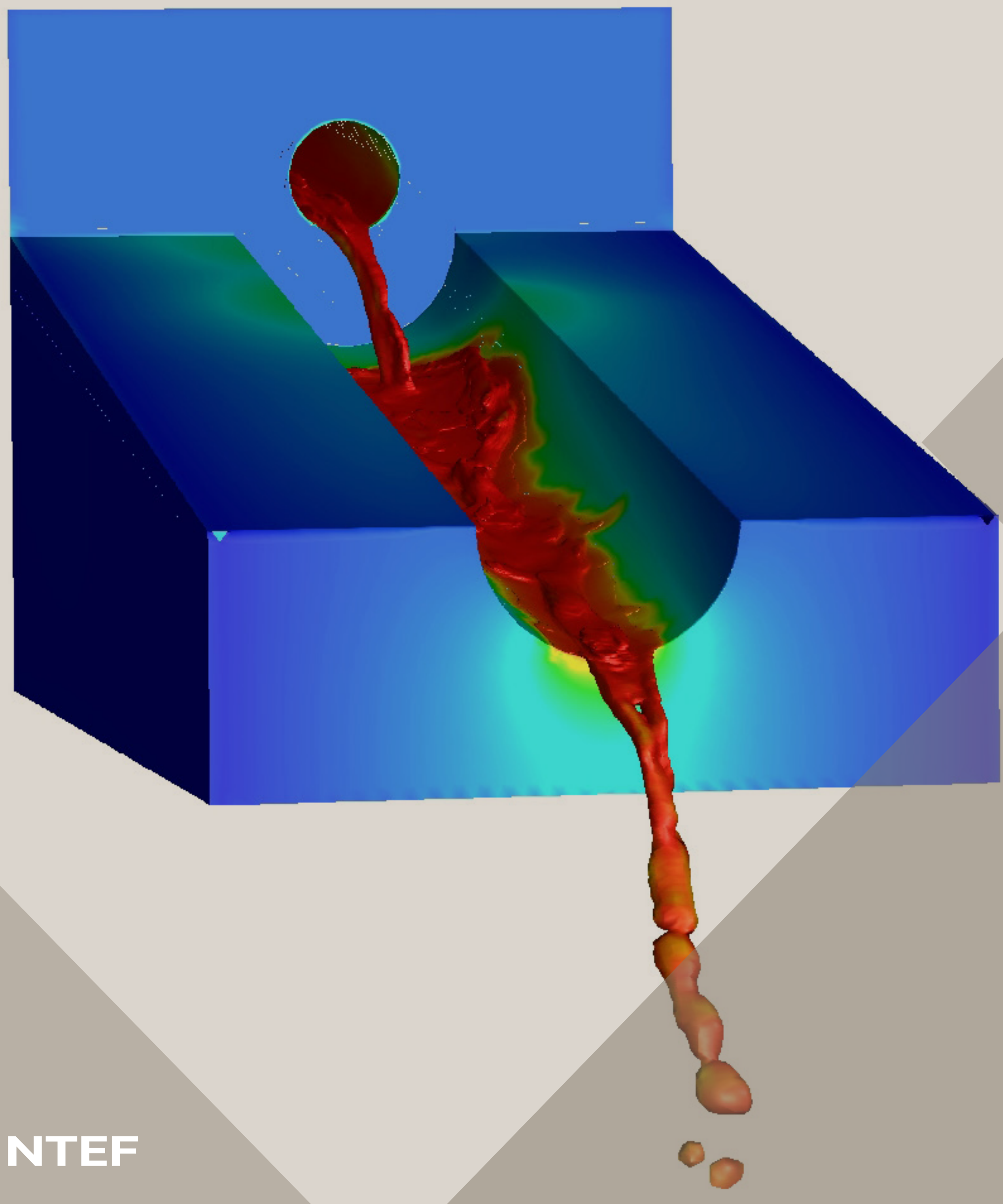

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SINTEF Academic Press
Address: Børrestuveien 3
PO Box 124 Blindern
N-0314 OSLO
Tel: +47 40 00 51 00

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CFD SIMULATIONS OF AN ADDITIONAL H_2 COMBUSTOR FOR IMPROVING EFFICIENCY IN CHEMICAL LOOPING COMBUSTION POWER PLANTS

Tijmen Scharff[1], Schalk Cloete[2,*], Jan Hendrik Cloete[2], Rob Bastiaans[1]

[1] Eindhoven University of Technology, 5600 MB Eindhoven, THE NETHERLANDS

[2] SINTEF Industry, 7465 Trondheim, NORWAY

* E-mail: schalk.cloete@sintef.no

ABSTRACT

Chemical looping combustion (CLC) is a promising technology for hydrocarbon fuel combustion with integrated CO_2 capture. The CLC process imposes almost no direct energy penalty for separating CO_2, but a large indirect energy penalty is encountered when CLC reactors are integrated into a combined cycle power plant due to the maximum reactor operating temperature that is far below the inlet temperature of modern gas turbines. Previous works have shown that additional fuel combustion after the CLC reactors can almost eliminate this energy penalty, although more expensive hydrogen fuel must be used to avoid CO_2 emissions. This study conducts CFD simulations of an added combustor fired with hydrogen, focusing mainly on mechanisms to reduce NOx formation. Three mechanisms are explored: 1) a greater number of fuel injectors, 2) increased turbulence, 3) and lower O_2 content of the air stream due to flue gas recirculation. Option 2 proved the most effective at reducing NOx, followed by Option 3. When combined, these mechanisms could result in NOx emissions below 50 ppm using a very compact combustor. In conclusion, low-NOx operation of the added combustor appears to be feasible and it is recommended for inclusion in future studies of CLC combined cycle power plants.

Keywords: Combustor, Chemical looping combustion, CFD, Gas turbine, Power production

INTRODUCTION

Urgency is building behind the global effort to combat climate change, with targets of 1.5-2 °C of warming now more broadly accepted [1]. Low-carbon technologies such as chemical looping combustion (CLC) [2] will be needed to reach such targets in a cost-effective manner.

CLC combusts hydrocarbon fuels with the aid of an oxygen carrier material to inherently avoid the mixing of nitrogen from air and CO_2 from fuel combustion. Two fluidized reactors are used for this purpose, with the oxygen carrier powder circulating between them. In the air reactor, the oxygen carrier is oxidized by air in a highly exothermic reaction. The outlet flow of this reactor consists of hot depleted air that can be used to drive a downstream power cycle. Oxidized oxygen carrier from the air reactor is then transferred to the fuel reactor where it is reduced by a hydrocarbon fuel gas (natural gas or syngas), producing an exhaust containing only CO_2 and H_2O. After simple condensation of the H_2O, the CO_2 stream is ready for storage or utilization. The reduced oxygen carrier is then circulated back to the air reactor to complete the cycle.

Gaseous fuel CLC must be coupled with a combined power cycle to achieve competitive electric efficiencies. Modern natural gas combined cycle (NGCC) power plants achieve very high efficiencies (~64%), mainly due to advances in gas turbine technology to facilitate high turbine inlet temperatures (>1600 °C). The primary challenge facing CLC in this respect is that the maximum CLC operating temperature will be around 1200 °C, limited by the stability of the oxygen carrier, as well as material constraints related to the reactors and downstream particle filters. With a turbine inlet temperature of only 1200 °C, the efficiency of a CLC combined cycle power plant is lower than that of a conventional NGCC plant with post-combustion CO_2 capture, rendering the CLC technology uncompetitive [3].

To overcome this fundamental limitation, a combustor can be deployed downstream of the CLC reactors to increase the temperature of the depleted air stream to the level that can be tolerated by modern gas turbines. This method has been shown to virtually eliminate the energy penalty of CO_2 capture in both NGCC [3] and integrated gasification combined cycle [4] power plants. The drawback of this solution is the release of additional CO_2, if natural gas is used for extra firing, or higher fuel costs, if hydrogen is used. Despite this drawback, however, added firing greatly reduces the CO_2 avoidance cost of CLC combined cycles, also outperforming NGCC with post-combustion CO_2 capture [3].

Given these promising results related to the added firing configuration, this paper sets out to study the combustion behaviour in the added combustor after the CLC reactors. A distinguishing feature of this combustor is that the hot depleted air stream is far above the fuel autoignition temperature. This means that lean premixed combustion for low NOx emissions is impossible. When hydrogen fuel is used, however, lean premixed combustion is problematic in any case [5], mainly due to the extremely high flame speed of hydrogen and the risk of flashback. Instead, the fuel must be injected directly into the hot air stream where it will spontaneously combust. Technically, lean premixed combustion performance can also be approached in this case in the limit of perfect mixing

(e.g., infinite turbulence or an infinite number of small fuel injectors). Alternatively, flame temperatures and the associated thermal NOx formation can be reduced by diluting the hydrogen fuel with steam or reducing the air oxygen content by recirculating some of the flue gas. Previous work has indicated that the former imposes a small energy penalty, whereas the energy penalty is negligible in the latter case [6].
For these reasons, the present work will investigate the NOx mitigation potential of increasing the number of fuel injectors, increasing the amount of turbulence, and reducing the O_2 content of the air via flue gas recirculation. The modelled combustor is based on the H-class gas turbine modelled in a prior study [3] where hydrogen added firing was used to increase the depleted air temperature from 1160 °C after the CLC reactors to 1648 °C at the combustor outlet.
Given the lack of experimental data for this type of combustor, the present model has not been thoroughly validated. Thus, it should be viewed as a first qualitative numerical investigation of this novel combustor concept, illustrating the potential of different mechanisms to achieve low-NOx combustion. This initial study can pave the way for a more elaborate future project including dedicated experiments and more detailed modelling.

MODEL DESCRIPTION

The simulation campaign was completed in ANSYS Fluent v19.3 using a one-sixth pie-slice of a simple cylindrical combustor geometry – 0.4 m in diameter and 1 m in length. As shown in Figure 1, the geometry features multiple fuel injectors injecting hydrogen into a large stream of hot air from the CLC reactors. The geometry is sized based on an H-class gas turbine with 18 combustors and a flow velocity inside the combustors of ~80 m/s.

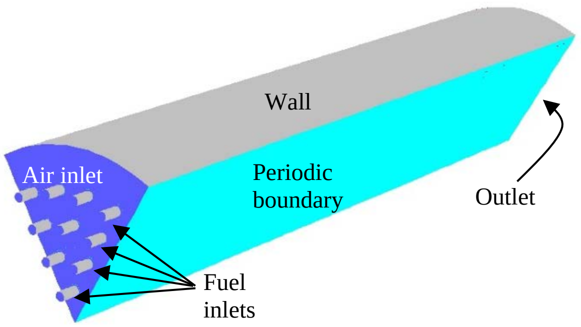

Figure 1: The simulated geometry.

Mesh

Meshes, consisting primarily of hexagonal cells with a cell length of 0.6 cm, were created in ANSYS Meshing. Smaller cells are used in the vicinity of the nozzles to ensure a minimum of 6 cells across each nozzle, but the cell length of 1 cm is maintained in the axial direction.
To increase numerical accuracy without making the solution computationally unaffordable, one level of adaptive refinement was performed according to temperature gradients, in order to only refine on the edges of the flames where the highest gradients in temperature and species concentrations must be resolved. In cases with a long flame, this refinement doubled the number of cells in the domain up to approximately 500 000. In cases with shorter flames, a much smaller volume was adapted, leading to meshes with as low as 280 000 cells. Refining the mesh caused virtually no change in the temperature and conversion profiles in the combustor, but it did change the predicted NOx emissions by about 6%. This moderate solution change on refinement was deemed acceptable for the present study where the primary aim is to compare cases to each other for studying the relative attractiveness of various NOx reduction mechanisms. Hence, a single level of adaptive refinement to the mesh is used in all the cases presented in this study.

Model setup

Steady state simulations were completed using standard combustion modelling settings in Ansys Fluent [7]. The combustion of hydrogen in air was modelled using a single-step, global reaction mechanism, and the reaction rate was described using the eddy dissipation concept (EDC) [8]. In the EDC, it is assumed that the reaction occurs within small turbulent structures, accounting for the mass transfer limitation to small eddies due to limited turbulent mixing. The default Fluent values were used for the reaction kinetics of hydrogen combustion, based on a reaction that is first order with respect to hydrogen and oxygen, and an Arrhenius temperature dependency. Turbulence was modelled according to the realizable k-ε model [9] and radiation according to the P1 model [10].
NOx formation was modelled using standard functionalities in Ansys Fluent [11]. Considering that hydrogen without any hydrocarbons is used as fuel, only thermal NOx formation was included, based on the extended Zeldovich mechanism and using rate expressions from the evaluation of Hanson and Salimian [12]. The equilibrium approach is followed for O radicals and the partial-equilibrium approach for OH radicals.
Turbulence interaction during NOx formation is modelled in Ansys Fluent using a probability density function (PDF) approach to account for the effect of the variance in temperature and species concentrations on the mean reaction rates. In this study, a beta function is used for the probability distribution and the algebraic form of the variance transport equation is used for both temperature and species. This approach requires a maximum limit for the temperature used in the integration of the PDF to be set, in this case as the local temperature multiplied by a factor, T_{max}. It was found in the present study that, although the default value of $T_{max} = 1.1$ was used, the amount of NOx formation predicted was highly sensitive to this parameter. Due to this uncertainty, future combined simulation and experimental work will be required for solutions of high quantitative accuracy.

Boundary conditions

Inlet conditions were chosen to match our prior techno-economic assessment study [3], assuming that the flows are divided equally between 18 combustors feeding the H-class gas turbine. The outlet pressure was set to 22 bar. As shown in Table 1, three different turbulent intensities and O_2 mole fractions were explored. For simplicity, uniform velocity profiles were specified at all inlets. This assumption should be refined in future studies. In addition, inlet turbulence is another important assumption that merits further investigation. In the present study, this uncertainty is investigated via a sensitivity analysis on three turbulent intensities.

Table 1: Summary of boundary conditions.

	Air inlet	Fuel inlet
Flow rate (kg/s)	6.653	0.0389
Turbulent intensity (%)	4, 6, 8	4
Turbulent length scale (m)	0.4	0.01
Temperature (°C)	1160	289
Species mol %	15.6, 12.6, 9.6 O_2; balance N_2	100 H_2

RESULTS

Results will be presented in four sections. The first three sections present the effects of the number of injectors, the inlet turbulent intensity, and the degree of flue gas recirculation, whereas the final section investigates the effect of changing the turbulent intensity and the flue gas recirculation simultaneously. All four sections share a common base case with 60 fuel injectors, 4% turbulent intensity, and no flue gas recirculation (15.6% O_2)

Effect of the number of injectors

Three cylindrical combustor geometries with equally spaced injectors numbering 18, 36 and 60, were simulated with 4% turbulent intensity and no flue gas recirculation. The effect on the cross-sectionally averaged NO concentration and fuel conversion profiles is illustrated in Figure 2.

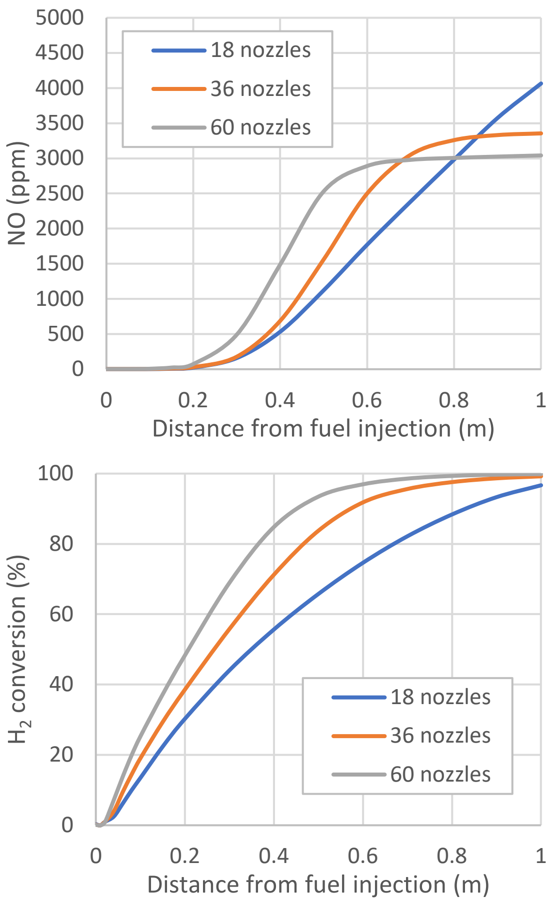

Figure 2: Cross-sectionally averaged profiles of NO concentration and fuel conversion along the length of the combustor for different numbers of nozzles.

Increasing the number of injectors causes a mild reduction in the amount of NO present at the combustor outlet, but it is clear that an impractically large number of injectors will be required to reduce NO below 100 ppm as required in many regions around the world. The figure also shows that a larger number of nozzles has a large positive impact on the rate of fuel conversion. In the case with only 18 injectors, a significant amount of fuel remains unconverted at the combustor outlet, whereas virtually complete conversion is achieved in the other two cases. This is the result of better contact between the air and the fuel when the fuel is injected more uniformly through many injectors.

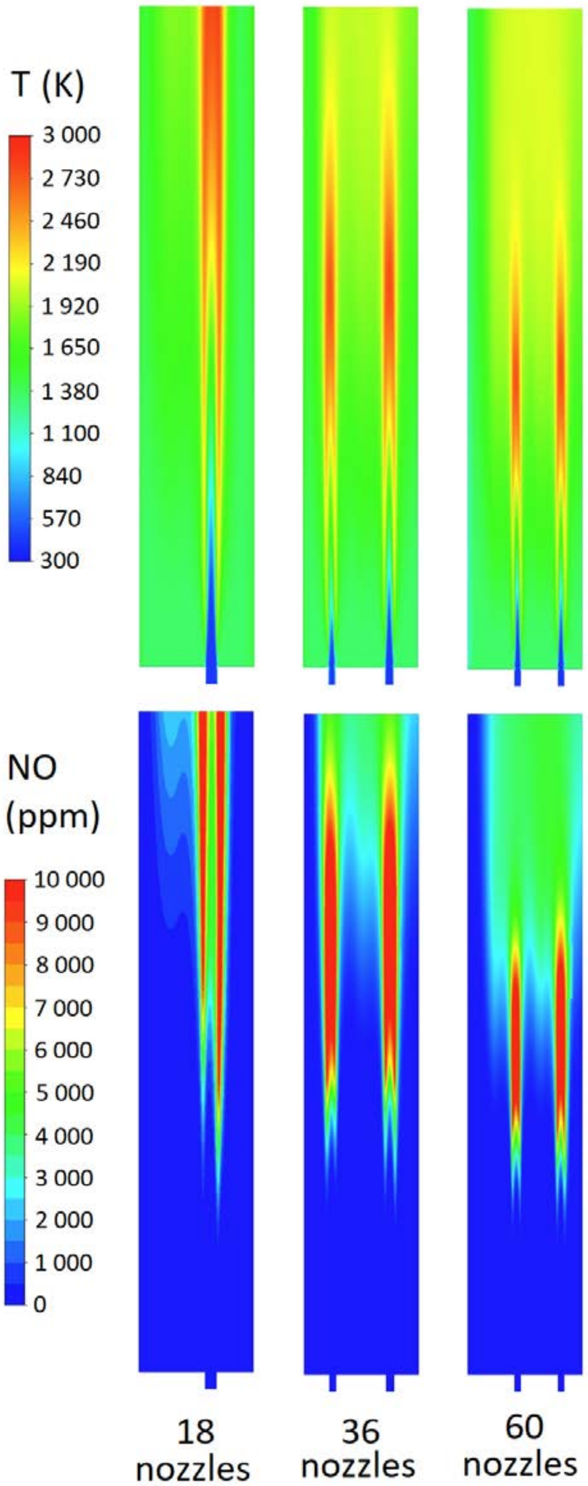

Figure 3: Temperature and NO concentration contour plots on the central plane in the three different geometries.

The high NOx formation is the result of very high flame temperatures (>2700 K) that are observed in this case (Figure 3). Clearly, the injection of pure H_2 into a greatly pre-heated oxidant stream with excess O_2 will require additional measures to reduce the flame temperature and suppress the formation of thermal NOx. Figure 3 also shows how the flame length increases when fewer injections are used. This slower fuel conversion is due to the increased mass transfer limitation created by the larger surface to volume ratios of the larger fuel jets injected in cases with fewer injectors.

Effect of inlet turbulent intensity

Three air inlet stream turbulent intensity values of 4%, 6%, and 8% were investigated in the case with 60 injectors and no flue gas recirculation. The lower bound is representative of a case with no added measures for increasing turbulence, whereas the upper bound represents additional measures to enhance mixing, such as swirl blades.

The inclusion of greater turbulence at the inlet of the combustor had a large positive influence on NOx reduction and significantly increased the rate of fuel conversion. Greater mixing in the combustor allows high flame temperatures to dissipate more rapidly and increases fuel-O_2 contact. The case with 8% turbulent intensity showed only 134 ppm of NO at the combustor outlet, which is close to meeting emissions limits.

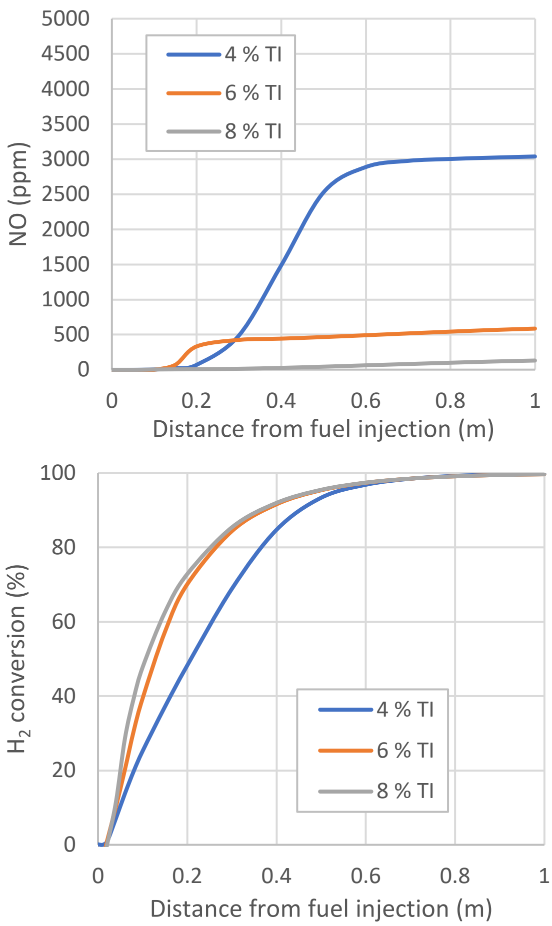

Figure 4: Cross-sectionally averaged profiles of NO concentration and fuel conversion along the length of the combustor for different turbulent intensities (TI).

The large dispersive influence of increased inlet turbulence is clearly illustrated in Figure 5. In the case with 8% turbulent intensity, the temperature field becomes essentially uniform before the half-way point along the combustor length. Most importantly, the maximum flame temperature is greatly reduced by the diffusive effect of turbulence. These results also show that the combustor length could be shortened substantially for the cases with high turbulence, minimizing the combustor cost.

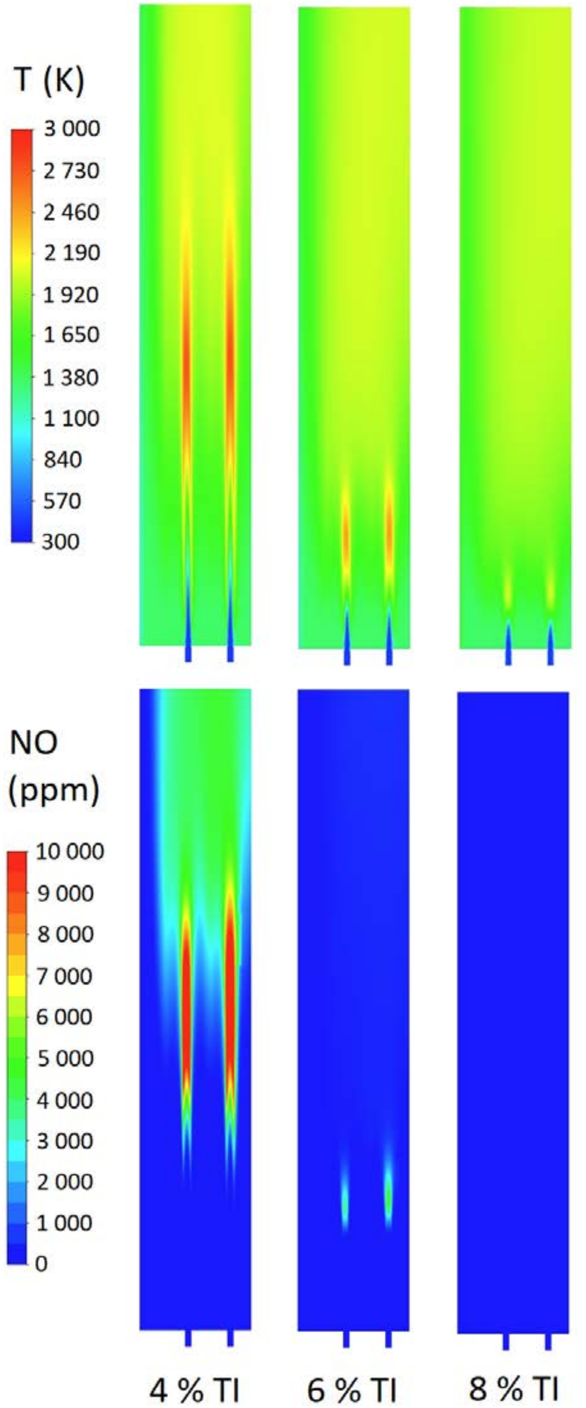

Figure 5: Temperature and NO concentration contour plots on the central plane for the three different inlet turbulent intensities.

These results also indicate the large effect that uncertainties related to inlet boundary conditions can have. For example, the assumption of a uniform inlet velocity profile could significantly impact results. In future work, more upstream details should be included in the geometry to ensure a reasonable flow profile at the start of the combustion zone.

Effect of flue gas recirculation

Flue gas recirculation was represented by reducing the amount of O_2 in the inlet air stream. Hence, three O_2 mole fractions of 15.6%, 12.6% and 9.6% were investigated in the case with 60 injectors and 4% turbulent intensity. The combustion process reduces the O_2 mole fraction by about 4.6 %-points, implying that the lowest case investigated still supplies considerable excess oxygen to the combustor, resulting in an outlet O_2 mole fraction of 5%.

Figure 6 shows that flue gas recirculation strongly reduces NOx formation by creating a shortage of O_2 in the highest temperature regions of the flame. Even so, the rate of fuel conversion is only reduced marginally, suggesting that greater flue gas recirculation should be practically achievable, potentially reducing NOx below 100 ppm, even without any measures to increase mixing.

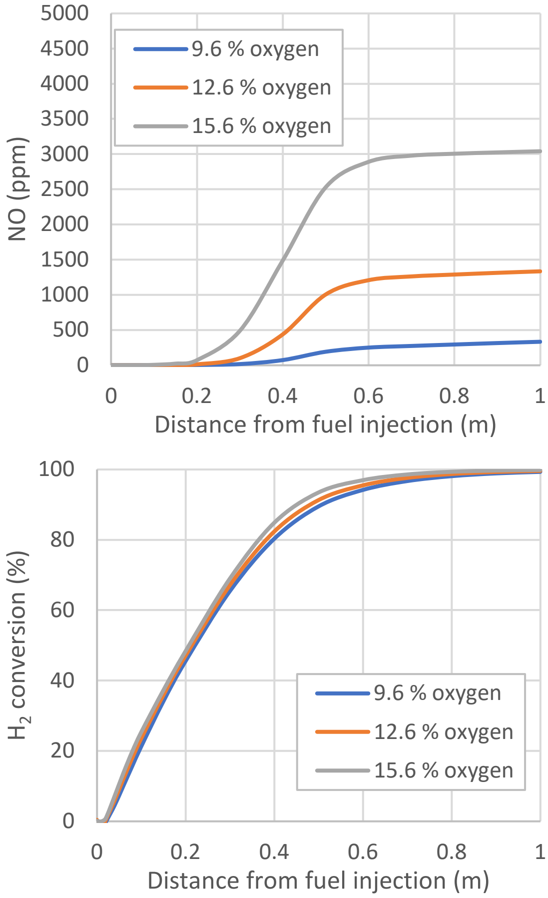

Figure 6: Cross-sectionally averaged profiles of NO concentration and fuel conversion along the length of the combustor for different O_2 mole fractions from flue gas recirculation.

Figure 7 illustrates the effect of reduced O_2 mole fractions more clearly. An increasing shortage of O_2 is observed in the highest temperature regions when the O_2 inlet concentration is reduced. This both avoids additional exothermic reactions in the hottest regions to reduce flame temperatures and causes a greater shortage of O_2 required for NO formation.

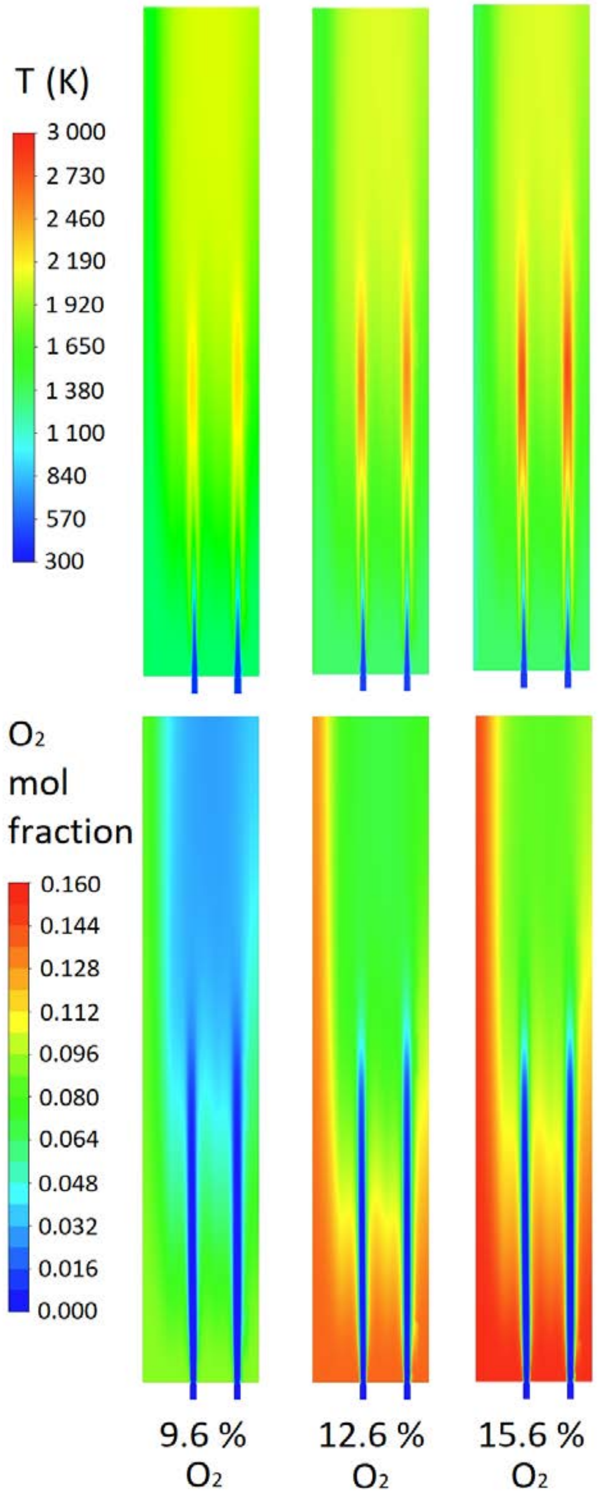

Figure 7: Temperature and O_2 mole fraction contour plots on the central plane for the three different O_2 inlet mole fractions.

Combining turbulence and flue gas recirculation

The optimal design of this combustor will most likely feature a combination of the three NOx reduction mechanisms investigated here. To investigate the potential of such a strategy, the two most influential factors (turbulent intensity and flue gas recirculation) were increased simultaneously in the case with 60 nozzles.

As illustrated in Figure 8, adding flue gas recirculation to the cases with more inlet turbulence further reduces NOx formation without significantly reducing the rate of fuel conversion. Outlet NO is reduced as low as 87 ppm in the case with the most turbulence and lowest O_2 content. However, it is likely that the linear increase in NOx observed in this case will continue between the outlet of the combustor and the inlet of the turbine, leading to an increase relative to the 87 ppm value reported above. The pathway between the combustor outlet and turbine inlet should therefore be as short as possible.

On the other hand, this result may be pessimistic, given that almost all the NOx is formed after more than 90% of the fuel has been converted and the mixture of air and remaining fuel is almost uniform. As mentioned in the model description section, the T_{max} factor of 1.1, describing the sub-scale temperature distribution, is an important uncertainty in this simulation. It is likely that the sub-scale temperature is virtually uniform in the well-mixed latter regions of the combustor with high turbulence, suggesting that the T_{max} factor should be closer to unity. For perspective, a case was run with Tmax = 1, halving the outlet NO concentration to only 46 ppm. Alternatively, the last 0.4 m of the combustor can be removed, leaving the final 1% of fuel conversion to happen in the turbine. In this case, the NOx emissions halve again to 43 ppm for T_{max} = 1.1 and 20 ppm for T_{max} = 1. Such low emissions will ensure compliance with future regulations.

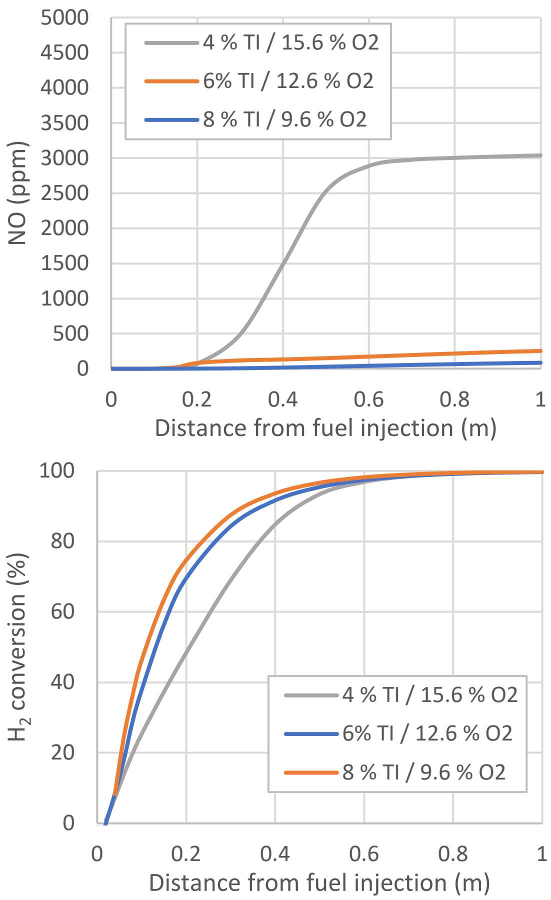

Figure 8: Cross-sectionally averaged profiles of NO concentration and fuel conversion along the length of the combustor for a combined increase in inlet turbulence and flue gas recirculation.

DISCUSSION

All three NOx-reduction mechanisms explored above have some drawbacks. There will be a limit to the number of fuel injectors that can be practically accommodated in the combustor. Turbulence generators like swirl blades impose additional pressure drop and, with a CLC outlet temperature of 1160 °C, might need some blade cooling. Flue gas recirculation will impose some added complexity to divert part of the flue gas back to the main compressor. More detailed combustor design studies will be required to find the optimal combination of these measures for ensuring practical and economical NOx mitigation.

Another interesting possibility that can be explored in future work is further simplification of the combustor. As shown in the results with higher turbulence above, 90% of the reaction happens spontaneously in as little as 30 cm after the fuel is injected with no need for separate combustion zones or premixing. This means that the fuel could be injected close to the gas turbine blades in a simplified combustion zone. Such an arrangement also opens the possibility for simplified multistage combustion and expansion where such a simple combustion zone can be inserted shortly before different stages of the turbine for increasing the inlet temperature of downstream turbine stages to increase turbine power output and overall cycle efficiency.

Future work should also investigate part-load operation of the added combustor. In this case, the ability of the CLC reactors to maintain a constant temperature of the depleted air being fed to the combustor could be advantageous. Since the turbine inlet temperature reduces under part-load operation, the amount of added H_2 combustion required after the CLC reactors will reduce under part-load operation, improving economics and potentially reducing NOx. The sensible heat storage capacity in the CLC oxygen carrier will also be beneficial for start-up after a short shutdown period.

CONCLUSION

This study investigated the feasibility of an added combustor for raising the CLC reactor outlet temperature to the level of modern gas turbines for highly efficient power production with integrated CO_2 capture. The focus was mainly on NOx reduction.

Out of the three NOx mitigation measures investigated, increased turbulence showed the largest effect. It also increased the rate of fuel conversion in the combustor. Using flue gas recirculation for reducing the O_2 content in the depleted air stream fed to the combustor also caused large reductions in NOx emissions with only minimal reductions in the fuel conversion rate. Increasing the number of fuel injection nozzles only had a mild NOx mitigation effect, but substantially increased the rate of fuel conversion by improving air-fuel contact. Combining these measures could achieve NOx emissions well below 100 ppm. However, more detailed studies (including dedicated experimental validation work) are required to draw quantitative conclusions, given uncertainties in the model, particularly regarding the highly sensitive NOx-turbulence interaction model.

In conclusion, this study showed that the concept of adding a H_2-fired combustor after CLC reactors holds promise and merits further investigation. Future work should aim to capitalize on the simplicity that can be achieved by this concept where fuel can simply be injected into the hot air stream to rapidly achieve complete and clean combustion.

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