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## Optimized Air Staged Injection for the Oxidation of Low Calorific Value Gases

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This paper describes a simplified numerical model used for the prediction of an optimized air staged plug-flow combustor for low calorific value gas mixtures. The parameter used for optimization,  $Z$ , is the summed flow rates of fuel components leaving the combustor. An optimized combustor is one of a given length and input mass flux that minimizes  $Z$ . Since a mathematical proof describing the importance of global interactions remains lacking, the model employs both a "local optimization" procedure and a "global optimization" procedure. By exercising and comparing both procedures, the model shows that "local optimization" is sufficient to provide an optimized solution. The sensitivity of  $Z$  to deviations in the air injection profile and inlet temperature is also examined.

## 1. Introduction

The oxidation of low calorific value gas mixtures is required for a variety of applications including coal gasification, bio- and landfill- gasification, and fuel cells. Many combustion related studies have already been performed on the first three applications, whereas the later has received little attention, if any. Unique to the fuel cell application is a relatively low fuel energy density in the anode exhaust (AX) gas stream--approximately 30 to 40 BTU per standard cubic foot. This residual fuel energy needs to be oxidized to achieve acceptable emissions and thermal efficiency. To date, catalytic combustors are usually selected to complete the oxidation of this gas stream. Such systems are expensive and add to the initial cost of the fuel cell "balance of plant", as well as subsequent operational costs. By improving our understanding of the AX gas oxidation processes, cheaper and easier to operate combustion systems can be achieved. In addition, current conceptual system designs integrate fuel cells with gas turbine engine, Williams et al. (1995). These systems, with projected record thermal efficiencies as high as 74%, will require the oxidation of the AX gas prior to entering the gas turbine system. Hence, understanding the combustion behavior of these low energy fuel mixtures will aid the future development of these systems as well.

While all fuel cell power generation applications require some form of oxidizer downstream of the anode, this work is directed toward the molten carbonate fuel cell application. When this fuel cell is powered by natural gas, the residual energy is in the form of approximately 8% hydrogen and 5% carbon monoxide, with the balance being 48% carbon dioxide and 39% water vapor. This gas mixture has a heating value near 30 BTU per standard cubic foot.

## 2. The Reaction Model

Because the optimization procedure itself is computationally intensive, a simplified reaction model is used for the oxidation of the residual hydrogen and carbon monoxide. Specifically, we have:

$$\frac{d[H_2]}{dt} = -A_{H_2} [O_2]^{1/2} [H_2] T^{n_{H_2}} \exp\left(-\frac{E_{H_2}}{RT}\right) \quad E.1$$

$$\frac{d[CO]}{dt} = -A_{CO} [O_2]^{1/2} [CO] T^{n_{CO}} \exp\left(-\frac{E_{CO}}{RT}\right) \quad E.2$$

where  $E_{H_2}=4.2e5$  joule/mole,  $A_{H_2}=6.9e12$ ,  $n_{H_2}=4.0$ ,  $E_{CO}=3.7e5$  joule/mole,  $A_{CO}=1.4e13$ , and  $n_{CO}=2.6$ . These reaction rate parameters were determined based on a Chemkin simulation of the oxidation of a typical molten carbonate fuel cell AX gas stream with air at an equivalence ratio of one. The Chemkin simulation employed the reaction set from

Miller and Bowman (1989). Based on the rate data calculated over the oxidation process, a non-linear least squares fit to the data was made. Hence, the above simplified reaction models for hydrogen and carbon monoxide should be representative of the fuel cell oxidation process being investigated. Its applicability to other applications would need to be determined separately.

### 3. The Combustor Model

In this work it is assumed that the oxidation of this low energy fuel proceeds by a sequence of plug flow reactors, see Figure 1. Any number of such combustor sections can be analyzed, but the current study uses only 5. At the inlet to each combustor section some quantity of air is injected and rapidly mixes with the incoming reactant mixture from the previous combustor section. The mixture then undergoes plug flow reaction using the reaction equations E.1 and E.2 until the mixture leaves the combustor section. The optimization parameter,  $Z$ , used in the current study is the summed molecular flow rates of hydrogen and carbon monoxide leaving the last combustor section. It is assumed that the "best" combustor design will have an air injection profile along the combustor that minimizes this parameter. As is evident from E.1 and E.2, there is a trade off in supplying  $O_2$  via air as the instantaneous reaction rate is optimized. Increasing the air flow rate improves the  $O_2$  concentration, but it also lowers the temperature. Hence, a search for the optimal air injection to each section needs to be made. Since the assessment of  $Z$  for each considered profile requires a downstream integration across all combustor sections, it is readily apparent that the effect of a particular combustor section on all down stream combustor sections must be considered; i.e., global downstream directed influences need to be analyzed during the assessment of  $Z$ . Since at this time there is no mathematical proof available that shows how the search domain might be constrained (and, hence, how to efficiently avoid certain profiles) a consideration of all possible profiles is required. Given the aforementioned requirements and limits on understanding, simple logic suggests that a random examination of all possible air injection profiles be performed to ensure a truly optimized solution. In the following section, a limited form of such a "global" search routine is described. In addition, a "local" optimization routine is described. The results of this later routine are compared to the global model in Section 5.

### 4. The Optimization Models

The "local" optimization procedure is the easiest to understand, and is described first. This procedure assumes that the optimal air injection profile for the overall combustion system can be found by determining the air injection at each individual section that produces the lowest total flow rate of fuel components exiting *that* section. Hence, this procedure moves sequentially downstream through the combustion system, starting at the inlet, and locally determines the optimal air injection flow rate. Because this procedure only passes through all combustion systems once, it is very efficient and offers fast solutions. The assumption that the optimal air injection profile for the *overall system* can be obtained by such a local optimization procedure is examined in the following section.

The "global" procedure assumes the possibility that the optimal air injection at combustor 'i' may require non-optimized (in the local sense) air injection at combustors upstream of 'i'. This global procedure uses a directed search method that begins with a flat air injection profile based on a prescribed value for the total injected air. The total injected air is assumed to be a fixed constraint. The search proceeds by separately considering each combustor section. During the analysis of each section, the amount of air injected at the section is increased a small amount from its prior determined (current optimal) value. Because of the constraint on the total injected air, the amount of air injected in all other combustor sections is decreased a small amount from their prior determined optimal profile values. The decrease can happen uniformly over all other combustor sections, or can occur completely over just one combustor section at a time; however, no section can have negative air injection values. Both techniques are tried separately and the entire combustion system is analyzed for the exiting flow conditions. If an improvement to the optimization parameter,  $Z$ , is discovered, then the new profile is saved from which further adjustments are also attempted to determine other improved air injection profiles. The procedure is terminated once the adjustments no longer show any improved profile.

## 5. Results

Figure 2 shows the results predicted by the "global" model for a 10 m long, 64 mm diameter atmospheric combustor supplied with an AX gas having a temperature of 880 K, flow rate of 13.7 moles/s and the aforementioned gas composition. The air for oxidation is supplied at room temperature and pressure. In Figure 2, the air injection results are shown normalized by the total injected air. As can be seen, the optimal profile requires an initial, small injection at Injector 1. Injectors 2 and 3 show significantly less air injection, followed by increasing injection at Injectors 4 and 5. Throughout the process, the temperature slowly rises, and the concentrations of H<sub>2</sub> and CO decrease. Nearly complete oxidation of H<sub>2</sub> and CO results for this configuration by the end of the combustor.

Figure 3 shows the results predicted by the "local" model for the same configuration and total air injection as used in the global model. The results come very close to those shown in Figure 2. After further computation, it was determined that for the configuration studied, the differences appear to be due to the level of resolution considered during the search for the global model's solution (however, even using the current resolution, the time to achieve a solution can take approximately 24 hours on a 30 MHz PC.)

Although no mathematical proof could be found that would show the local procedure to be sufficient to predict the optimal profile, these results currently suggest that using the local procedure is all that is required--the many other profiles examined during the global procedure need not be considered. If such a results can be shown to be generally true, relatively fast optimal solutions using the local procedure could reliably be obtained. Further analytic work in this area would be helpful.

Finally, Figures 4 & 5 show the sensitivity of the Z parameter to inlet temperature and air injection, respectively. As can be seen, even small decreases in temperature can significantly change the performance of this combustion system. Such results reflect the flame-out conditions common to most combustion systems. It is apparent, that to reliably perform the oxidation over the 10 m length combustor, the inlet temperature needs to be maintained above 880 K. If lower inlet temperatures are used, a longer combustor will be required. Regarding the sensitivity of variations in air injection, it is seen that there are relatively week effects on the rich side. For lean conditions, the sensitivity is high for all ports at the point where changes occur; however, for changes less than 4% only injectors 1 and 4 show significant effects.

## 7. Conclusions

Results from this work show that to (best) oxidize the anode gas from the molten carbonate fuel cell considered, a combustor 10 m long will be required. The optimal air injection profile requires a small addition of air at the inlet, followed by a short "cooking time", followed by a relatively large injection of air to complete the oxidation. By comparing the results from a local optimization procedure with a global optimization procedure, this work suggests that a local optimization procedure is all that is required to achieve optimized solutions. If such a situation can be proved to be of general validity for all combustion problems, then a significant reduction in the time required to obtain optimal solutions can be achieved. To reliably perform the oxidation in the 10 m long combustor, inlet temperatures above 880 K need to be maintained, and the injection of air at Injectors 1 and 4 needs to be closely controlled.

## REFERENCES

Miller, J.A. and C.T. Bowman, 1989, "Mechanism and Modeling of Nitrogen Chemistry in Combustion," Progress in Energy and Combustion Science, Vol. 15, No. 4.

Williams, M.C., P.L. Micheli, and E.L. Parsons, Jr., 1995, "Engineering a 70-Percent Efficient, Indirect-Fired Fuel-Cell Bottomed Turbine Cycle," Proceedings of the Fuel Cells '95 Review Meeting, August 1995, ed. T.J. George, DOE/METC-95/1020.

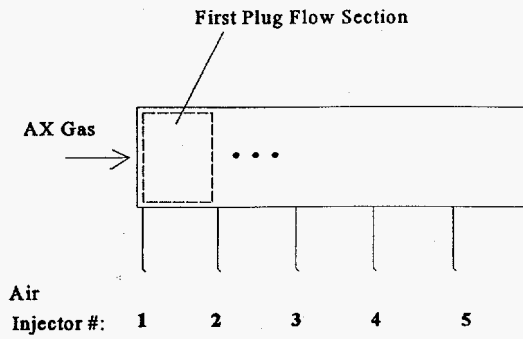


Figure 1. Air Staged Combustor

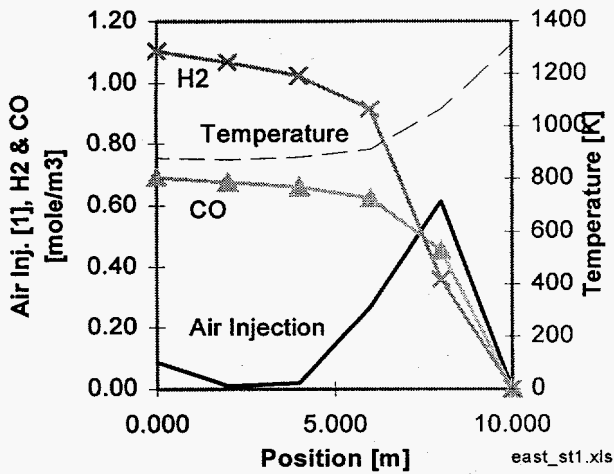


Figure 2. Global optimization results.

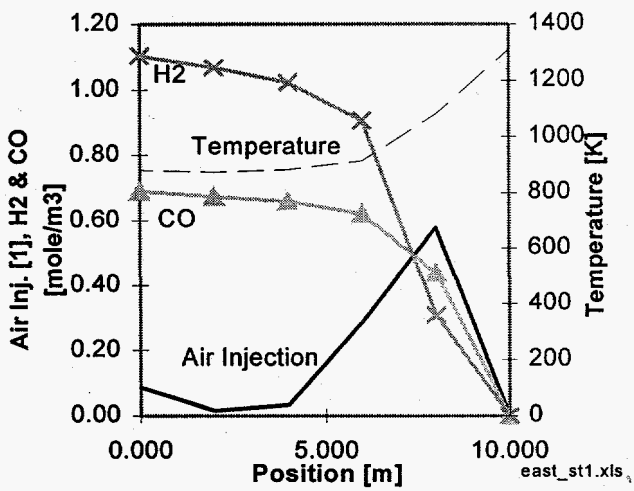


Figure 3. Local optimization results.

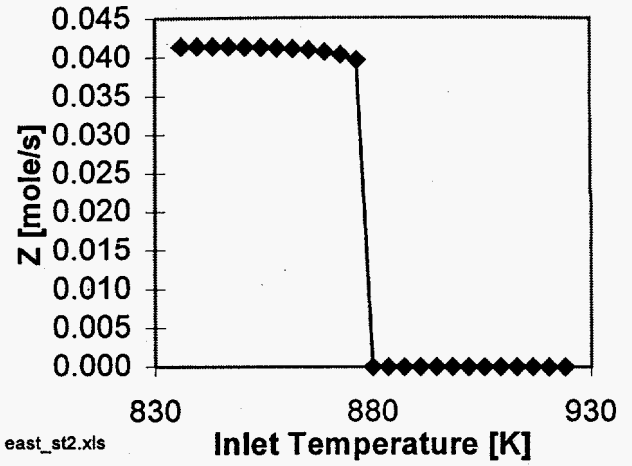


Figure 4. Inlet temperature sensitivity.

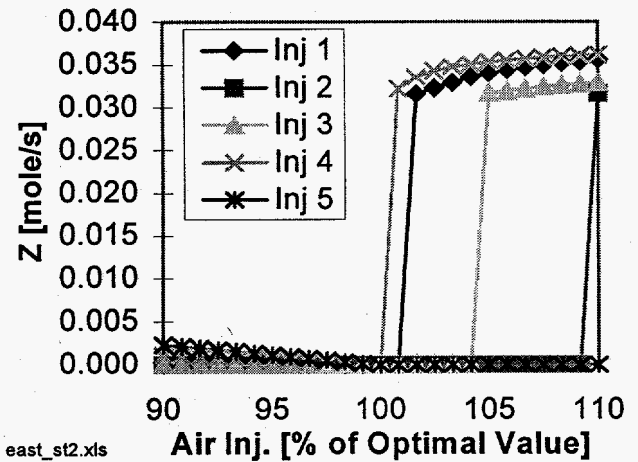


Figure 5. Air injection sensitivity.