reaction DESIGN

CHEMKIN-PRO
Exhaust Aftertreatment for Gas Turbine Combustors

Increasing public concerns and regulations dealing with air quality are creating the need for gas turbine combustors with lower emissions, beyond what has already been achieved with lean premixed combustors and catalytic reduction aftertreatment.

A common approach for minimizing NO_x emissions from a gas turbine combustor is to keep the gas temperature low by operating the combustor under ultra-lean conditions, but a low fuel-air ratio can cause flame stability problems. This, in turn, is deterred by implementation of a catalytic combustor. A catalytic combustor produces essentially zero NO_x and can convert very lean fuel-air mixtures at relatively low temperatures. Catalytic combustors, however, have their own issue, which CHEMKIN-PRO simulations can capture: a large pressure drop, and a slow response to changes in operating conditions. Additionally, the precious metals used as catalysts are usually very expensive, leading operating conditions to be optimized to prolong catalyst life.

CHEMKIN-PRO has the flexibility to simulate raising the catalytic combustor exit gas temperature (< 1200 K) to the desired temperature (~1475 K), such as by adding a second-stage, homogeneous combustor. In such a two-stage combustor system, we expect that almost all NO_x emission will come from the homogeneous combustor. Because the gas mixture entering the homogeneous combustor is already at an elevated temperature, the fuel-air ratio should be as lean as possible to minimize NO_x generation while still avoiding flame-stability issues. If the exit temperature of the second combustor becomes too high for the turbine rotor, a third stage could be added to cool the gas down with excess air.

Setting Up a Two-Stage Catalytic Combustor Simulation

For this problem, we need to design a virtually zero-NO_x combustor for a sub-scale test unit of our micro-turbine system. The combustor-related design specifications normally include total mass flow rate of the gas turbine system and the turbine rotor inlet temperature, TRIT.

We set up the problem using GRImech 3.0 for the gas-phase combustion and a surface reaction mechanism.[1] We use the CHEMKIN-PRO Perfectly Stirred reactor, Plug Flow reactor, and Honeycomb Monolith and Gas Mixer, with methane as the fuel.

[1]Deutschmann *et al.*, *Proceedings of Combustion Institute*, **26**:1747-1754 (1996).

Since we want to make the catalyst last longer to reduce operating costs, we need to keep the catalyst surface below its maximum operating temperature. Theoretically the maximum surface temperature in the catalytic combustor should not exceed the adiabatic flame temperature of the inlet gas mixture. In other words, we can determine the maximum equivalence ratio of the fuel-air mixture entering the catalytic combustor by comparing the adiabatic flame temperatures against the maximum catalyst operating temperature.

The adiabatic flame temperature of a given equivalence ratio can be easily obtained by using CHEMKIN's Equilibrium Reactor Model. Of course, the minimum equivalence ratio of the inlet fuel-air mixture is the one below which no light-off is observed on the catalyst surface. Accordingly, we set the equivalence ratio to 0.185.

With all the basic information defined, we are ready to build a simple reactor network model for our two-stage combustor system. We choose the Honeycomb Monolith Reactor Model to represent the first-stage catalytic combustor and a Plug Flow Reactor Model for the second-stage homogeneous combustor. Since all of the initial fuel is expected to be consumed by the catalytic combustor, we have to inject additional fuel to the second-stage homogeneous combustor. To achieve this, we need to add a gas mixer between the Honeycomb Monolith Reactor and the Plug Flow Reactor in our reactor network model. A fourth reactor, which can be either a PSR or a PFR, is added after the PFR (the homogeneous combustor) to simulate the post-flame flow in transition to the gas turbine and to allow the introduction of excess air to cool down the flue gas if needed. Figure 1 shows the “diagram” of our combustor system model that comprises four reactor clusters. We will run these clusters in sequence.

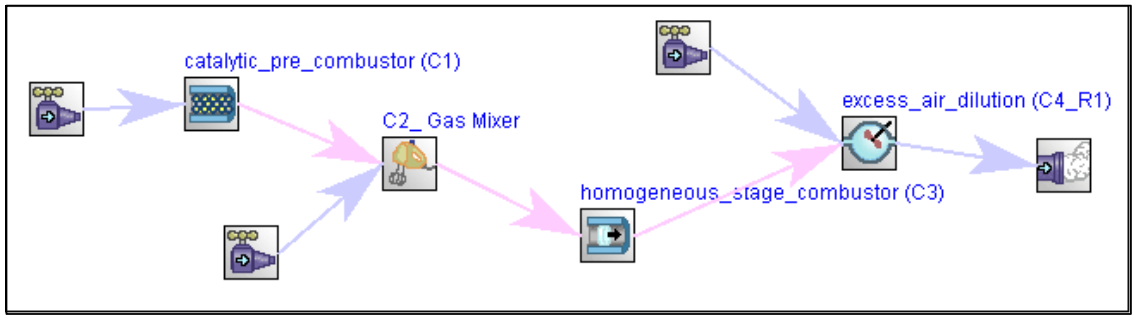

Figure 1. CHEMKIN-PRO diagram view of two-stage catalytic combustor.

Results

The CHEMKIN-PRO simulation runs as a series of reactor clusters, with each cluster acquiring information from the solution of the previous cluster. After finishing all four cluster runs, we want to see if the predicted mass flow rate and gas temperature at the exit of the last (fourth) reactor cluster match the gas turbine design point targets.

The predicted mass flow rate for each combustor is 163.4 g/sec so the total mass flow rate is 980.4 g/sec (= 6*163.4). The predicted exit gas temperature, TRIT, is 1432 K. Both values are very close to the targets. Since our goal is a zero-NO_x combustor, we want to find out NO, NO_2, and N_2O emissions from our new combustor. The solution shows the mole fractions of NO, NO_2, and N_2O are 0.22 ppm, 0.003 ppm, and 0.27 ppm, respectively. All these concentrations are below 1 ppm and are not detectable by instruments. Before we can say a job well done, we need to check on CO and UHC (unburned hydrocarbon) emissions as well. Sometimes CO and UHC concentrations increase when we try to minimize NO_x formation. Our model indicates our combustor has sub-ppm CO emission (~0.7 ppm) and essentially no UHC.

We are also interested in knowing how the gas temperature varies inside the combustor system and whether the maximum temperature inside the catalytic combustor exceeds its safe operating temperature. We can use the CHEMKIN Post-Processor to obtain profiles along the two-stage combustor for quick visual confirmation. We only need to load solutions of the first (catalytic combustor) and the third (homogeneous combustor) clusters into the CHEMKIN Post-Processor because the other two clusters yield a single solution point each. The “axial” profiles of gas temperature and the mole fractions for CO and NO are shown in the following figures.

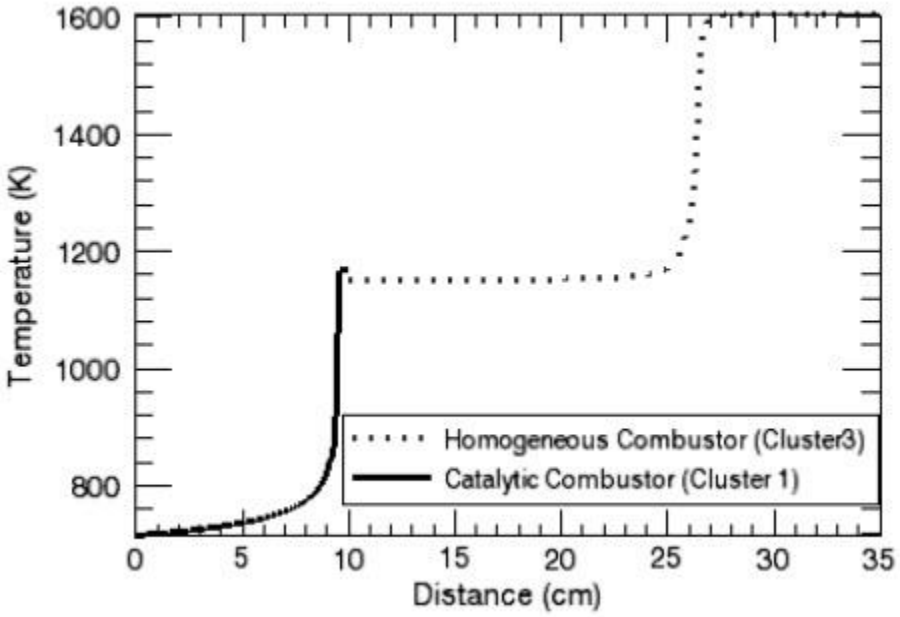

Figure 2. Temperature comparison between first and second combustors.

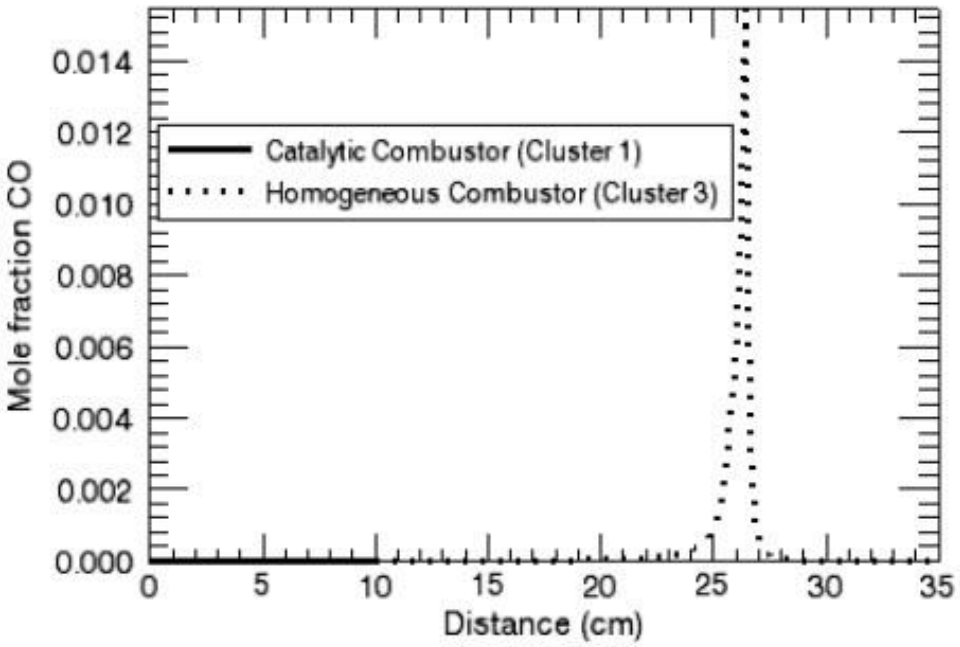

Figure 3. CO comparison between first and second combustors.

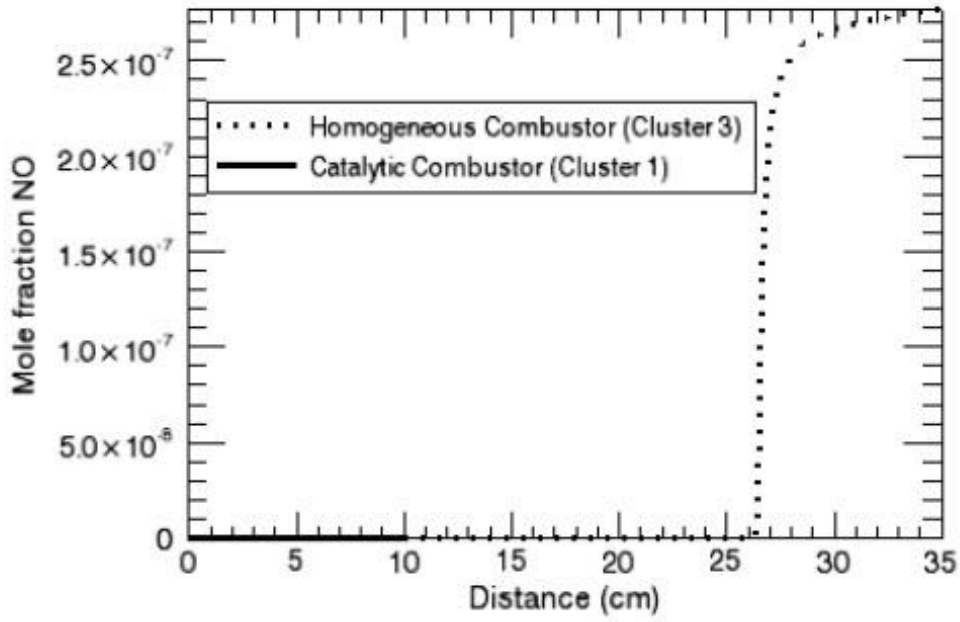

Figure 4. NO comparison between first and second combustors.

The temperature profile (Figure 2) indicates that the gas temperature is increased in two steps. The catalytic combustor has a lower operating temperature and only raises the gas temperature to about 1100 K. The homogeneous combustor, which can operate at higher temperatures, further raises the gas temperature to more than 1600 K before the excess air cools the gas mixture down to the target TRIT at about 1450 K. The CO profile (Figure 3) has a spike inside the homogeneous combustor corresponding to the gas-phase ignition and all CO generated is later consumed in the post-flame region. The model also predicts that NO_x is formed after gas-phase ignition and, unlike CO, its concentration continues to grow in the post flame region (Figure 4).