reaction DESIGN

CHEMKIN-PRO

Predicting Efficiency from Chemical Production Operations

Combustion efficiency in chemical production operations is important for both production costs and environmental regulations. CHEMKIN-PRO's reactor models can be combined to simulate combustion processes in burners and predict combustion efficiency. The mixing, flow, and combustion in a burner or combustion device create a complicated scenario, but a network of reactors allows simulation of this complex situation. Here, we demonstrate using Perfectly Stirred and Plug-flow Reactor models to create a network for predicting CO and UHC emissions from a typical burner to predict combustion efficiency.

Assembling the Network

A simplified burner reactor network consists of a flame/ignition zone, a recirculation zone, and a post-flame zone (Figure 1). As the complexity of the flow field increases, additional reactors and inlets are added to properly represent the combustor.

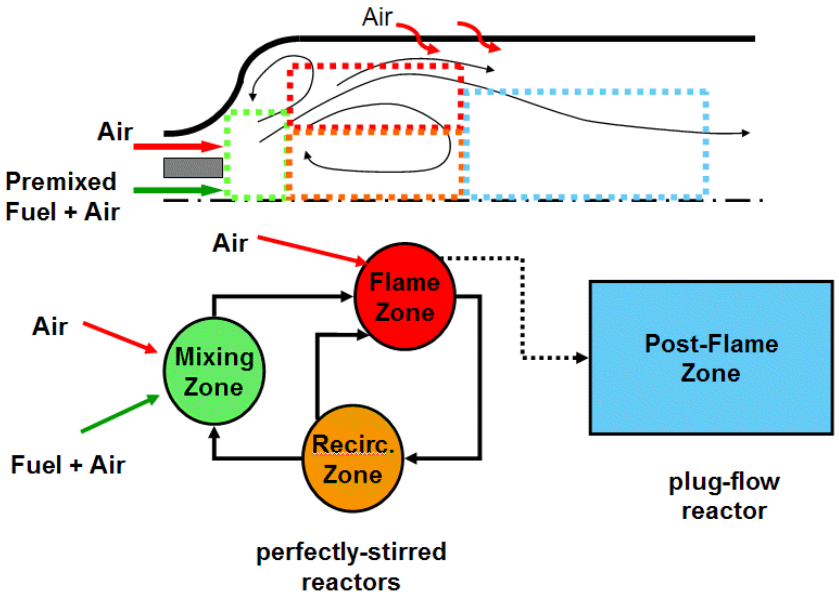

Figure 1. Schematic of the modeled burner network, a typical configuration.

The CHEMKIN-PRO reactor network shown in Figure 2 has two clusters: C1 represents the region around the flame and C2 uses a single Plug-flow Reactor (PFR) for the post-flame region between the flame and turbine inlet. Because the fuel stream is partially premixed, the first Perfectly Stirred Reactor (PSR) is the mixing zone. A flame-zone PSR is directly connected to the mixing zone and is followed by a recirculation zone for back mixing of hot combusted gas. The solutions of the through-flow from the flame zone (the last reactor of cluster 1) are automatically fed to the post-flame zone (the second cluster) as indicated by the pink line in Figure 2.

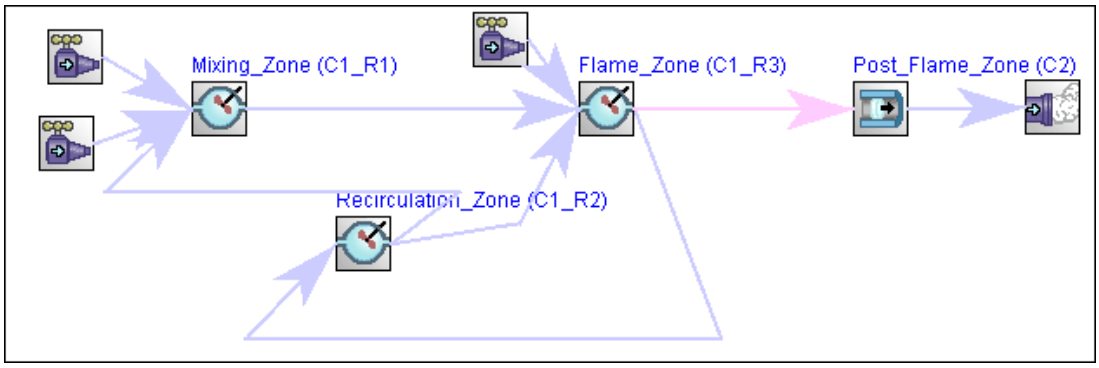

Figure 2. CHEMKIN-PRO diagram of the modeled burner network in Figure 1.

Seeing the Cause and Effect

The solutions from the reactor network are shown in Figure 3 and Figure 4. The temperature solutions in Figure 3 indicate that the gas mixture ignites in the third reactor (flame zone) and the temperature continues to increase in the second reactor (recirculation zone) where part of the recycled CO is consumed. Gas temperature increases slightly in the post-flame region (the second cluster) as remaining CO is converted to CO_2 in the hot flue gas (see Figure 4).

The NO profiles are shown in Figure 4. As we expected, the NO level continues to rise in the post-flame region, mainly due to the thermal NO formation.

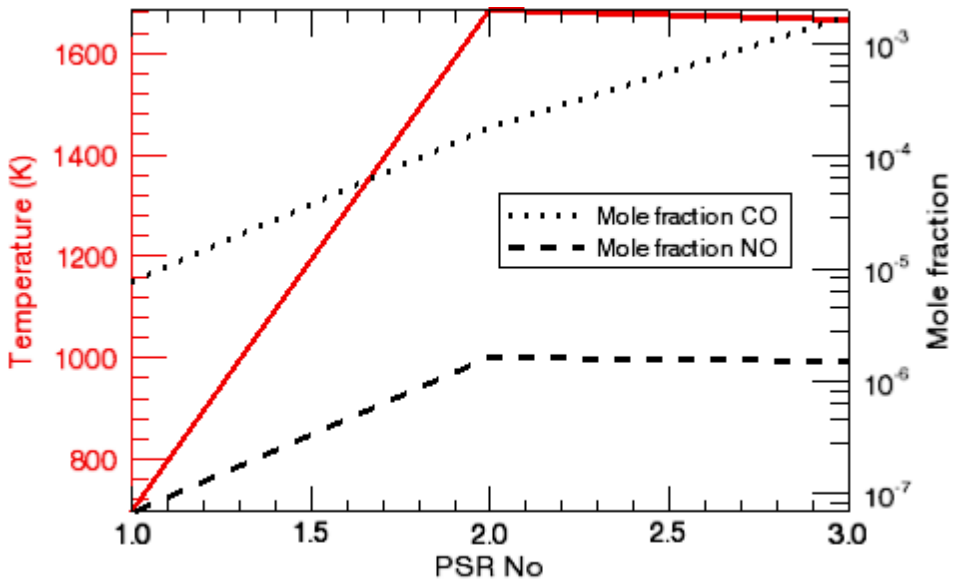

Figure 3. Temperature comparisons among PSRs in the CHEMKIN-PRO reactor simulation.

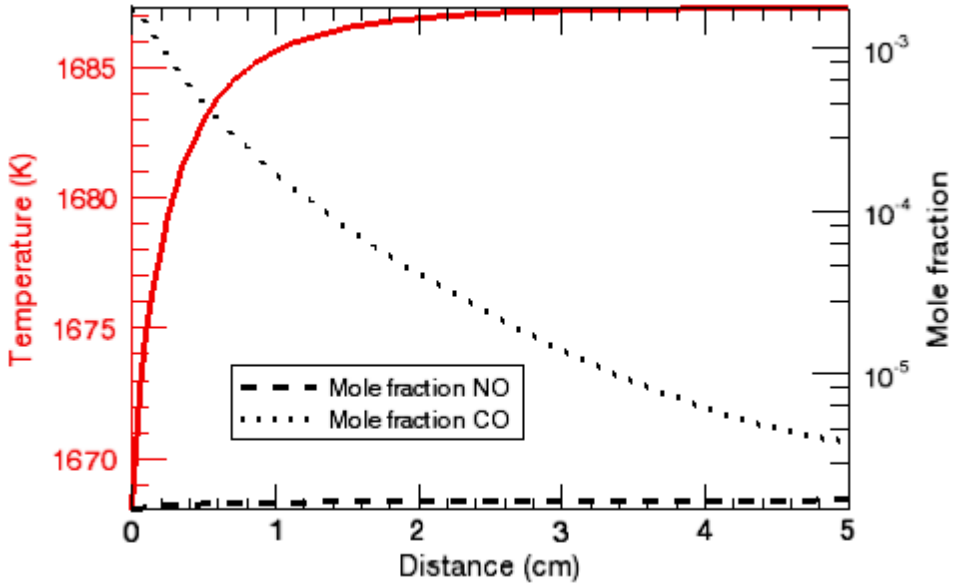

Figure 4. NO levels rise in post-flame region in the CHEMKIN-PRO reactor simulation.