Jet Flame Analysis with an Equivalent Reactor Network

CAPP-GT-3 (v2.0) August 30, 2010

Summary

This application note describes the mechanics of constructing a PSR (perfectly stirred reactor) Equivalent Reactor Network (ERN) to represent a non-premixed jet flame using CHEMKIN.

Introduction

CFD simulations for chemically reactive flow systems often either ignore or greatly reduce the treatment of chemical kinetics. However, for predictions of pollutant emissions, the assumption of local chemical equilibrium is not appropriate and a detailed reaction mechanism is needed. For example, the characteristic chemical time scale of NO is much larger than that of a typical fuel component or product species and is comparable to the characteristic time scale, or residence time, of the flow system. Consequently, the local NO concentration level is far from its equilibrium value and depends on both the local chemical state and the history of the gas mixture.

For simple flow fields, the exit concentration of a species can be obtained by simply integrating its production rate along streamlines (or streamtubes). In such cases, a detailed reaction mechanism can be used to determine production rates at each location, based on the local chemical state. However, this approach is not suitable for complex flow fields as strong mixing or recirculation make tracking streamlines difficult. Building an ERN from "cold" CFD solutions is a plausible approach under this situation, as it can use the detailed reaction mechanism while preserving some key fluid dynamic features that are important to emission predictions, such as the residence time. General guidelines on deriving reactor networks from CFD solutions can be found, for example, in papers by Bhargava et al.[1] and Faravelli et al.[2]

Application Setup

For this application, we consider a flame formed when a jet of fuel is injected into hot air, forming a jet flame with air entrainment. This non-premixed flame can be modeled with an ERN comprised of perfectly stirred reactors connected with mass flows and inlets representing the air and fuel sources. The residence times of these reactors, as well as the connectivity and mass flow rates among them, could be obtained from the velocity solutions of a CFD simulation, for example. A PSR network representing the diffusion jet flame is given in Figure 1.

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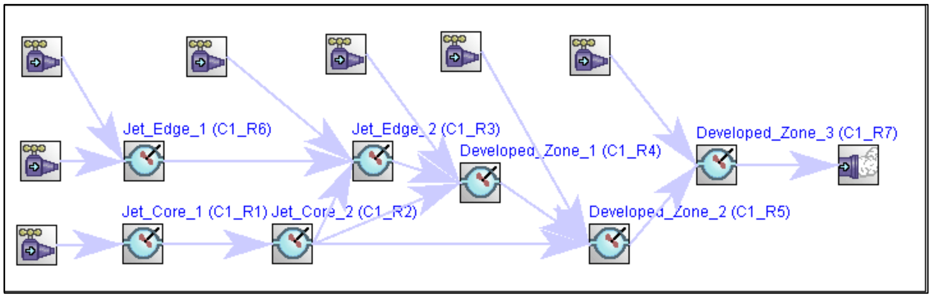
[1] Bhargava, A., *J. of Engineering for Gas Turbines and Power* **122**: 405-411 (2000).
[2] Faravelli et al., *Computers and Chemical Engineering* **25**:613-618 (2001).

Figure 1. Jet Flame Network—Diagram View



CHEMKIN's Recycling panel allows you specify the fraction of exit mass flow from one reactor that flows into another reactor, whether the receiving reactor is "upstream" or "downstream" of the source reactor. The recycling fraction must be a non-negative number and the sum of recycling fractions from a reactor must equal to one, to conserve mass.

The predicted temperature distribution as a function of reactor number is shown in Figure 2. Here we note that reactor C1_R6 represents the outer edge of the fuel jet and physically is located right next to the fuel jet nozzle in an upstream region. On the other hand, reactors C1_R5 and C1_R7 are the flame zone and the post-flame region, respectively, and are both located downstream from reactor C1_R6. When we look at the solution plots as a function of the reactor number, we should therefore not be concerned with the sudden changes corresponding to reactor C1_R6, since this reactor is not physically connected to C1_R5 and C1_R7.

The adiabatic flame temperature of the stoichiometric CH_4-air mixture is also given in Figure 2 for reference. We can see that reactors C1_R3, C1_R4, C1_R5, and C1_R7 have temperatures close to the adiabatic flame temperature, which would be expected for the flame zone and post-flame region. The reactor temperature dropping when coming from reactor C1_R5 to reactor C1_R7 is appropriate since C1_R7 is in the post-flame region. We can further analyze the flame behavior by checking the solutions of other variables. The jet flame is slightly lifted from the fuel jet nozzle because the outer edge of the fuel jet (reactor C1_R6) stays at a relatively low temperature.

Figure 2. Jet Flame Network Temperature Distribution

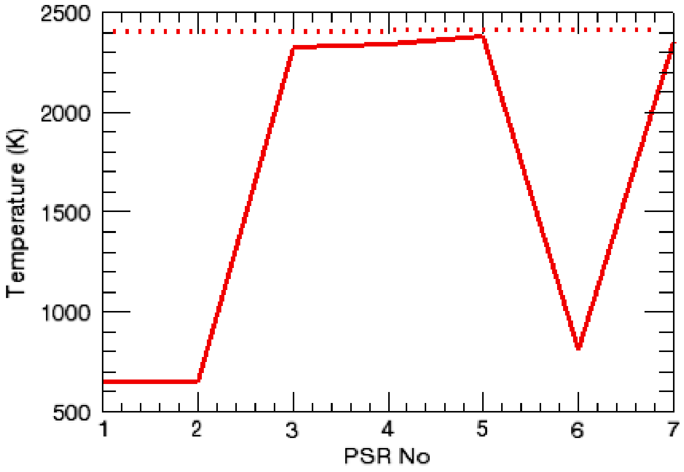
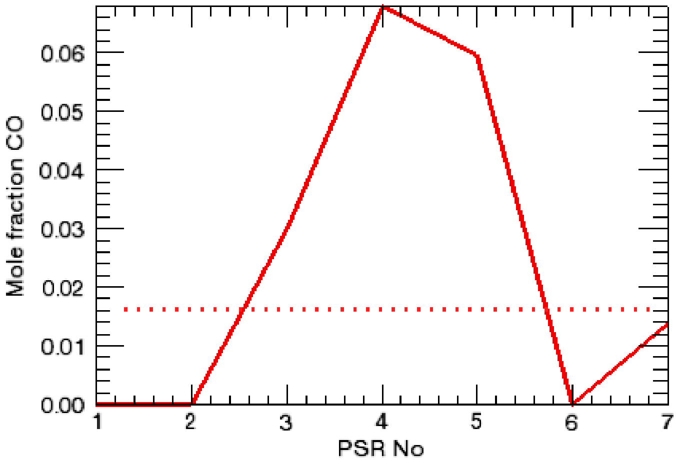


Figure 3 gives the CO mole fraction distribution among the reactors. The CO mole fraction at the adiabatic flame condition is provided to show where the combustion zone ends. The CO profile shows a spike starting from reactor C1_R3 to reactor C1_R7. We ignore reactor #6 because it does not connect either to reactor C1_R5 or reactor C1_R7. This CO spike resembles the one we observe in a typical flame zone and indicates that the flame zone ends before reaching reactor C1_R7. The predicted CO mole fraction in reactor C1_R7 is also lower than its adiabatic flame value, which is expected for the post-flame region.

Figure 3. Jet Flame Network—CO Distribution



One of the advantages of using an ERN is the ability to predict NO formation without running a full CFD calculation with detailed chemistry. The NO profile in Figure 4 shows that NO starts to form in the flame zone (reactors C1_R3, C1_R4, and C1_R5) and continues to rise in the hot post-flame region (reactor C1_R7). We can find out which NO formation mechanism is responsible for the NO increase in the high temperature region. In the absence of fuel nitrogen, NO in our jet flame can be formed via prompt NO and thermal NO mechanisms[3]. Since the prompt NO mechanism is characterized by the existence of radicals such as CH and HCN, we can plot the profiles of these radicals to find out the region where thermal NO is the dominant NO formation mechanism. From the profiles in Figure 5, we can see that all prompt-NO–related radicals disappear in the post-flame region (reactor C1_R7), so we can conclude that thermal NO is the main NO formation mechanism in the hot post-flame region. The reactor model also shows that, unlike gas temperature and CO mole fraction, the "exit" NO mole fraction is far below its equilibrium value. This is in accord with the fact that the characteristic chemical time scale of NO is greater than the fluid mechanical time scale of our jet-flame system.

Figure 4. Jet Flame Network—NO Distribution

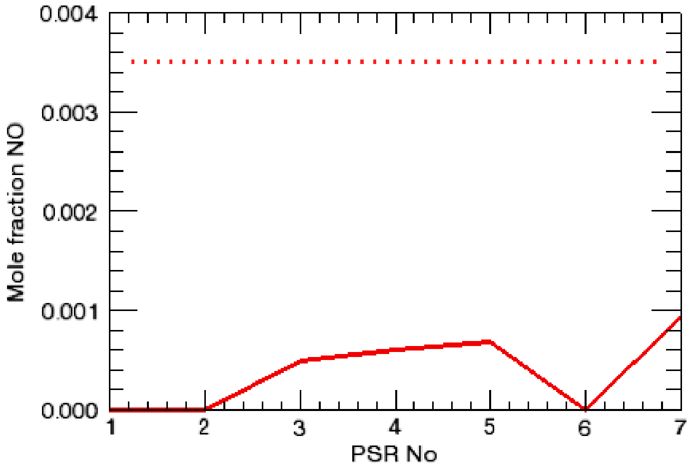
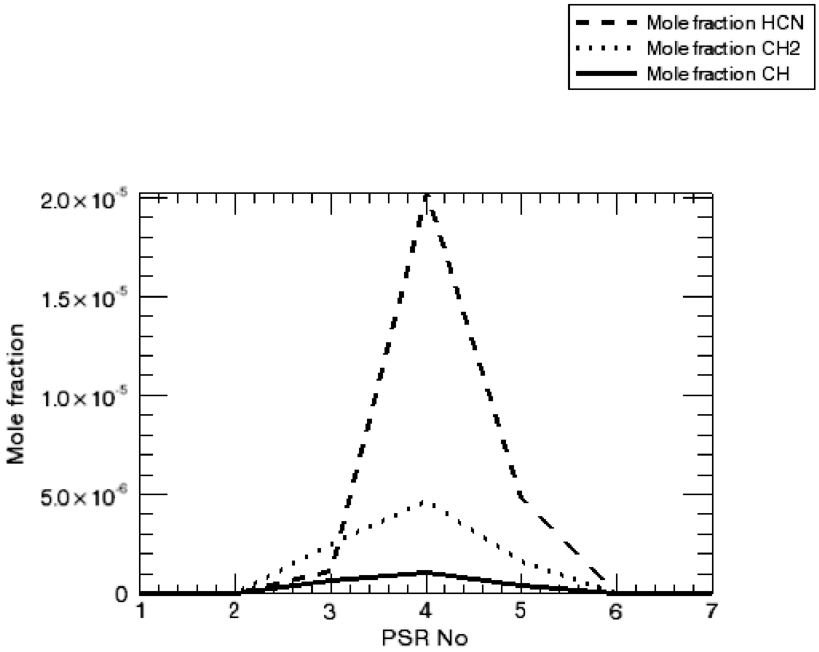


Figure 5. Jet Flame Network—Mole Fractions



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[3] Miller and Bowman, *Prog. Energy Combust. Sci.*, **15**:287-338 (1989).

About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN and CHEMKIN-PRO, the *de facto* standards for modeling gas-phase and surface chemistry, providing engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design also offers the CHEMKIN-CFD software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the production plant. Reaction Design serves more than 350 customers in the commercial, government and academic markets.

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