



# Using the Partially Stirred Reactor to Assess Turbulence-Kinetics Interactions in a Combustor

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## Summary

This application note describes how the partially stirred reactor model in CHEMKIN can be used to explore the effects of imperfect mixing on the exit flow condition from a premixed gas turbine combustor.

## Introduction

When chemical kinetics are the limiting factor of the reacting system under investigation, a perfectly stirred reactor (PSR) model can be a very useful tool for predicting the chemical, thermodynamic and flow state of the system of interest. In such systems, near-perfect mixing of reactants and products is usually accomplished with mixers or multiple-jet injections. However, a gas-turbine combustor normally does not have these mixing mechanisms and has to rely on fluid motion or large-scale eddies and turbulence, to provide the mixing. Local turbulence is particularly important as it promotes micro-scale mixing among the gas species.

If the turbulence is too weak to provide fast mixing among the gas species, the micro-mixing process will interfere with the chemical kinetics. In some cases, when the reactants (non-premixed cases) or the reactants and the products (premixed cases) fail to mix microscopically before they are blown out of the combustor, no combustion zone can be established inside the combustor. CHEMKIN-PRO'S partially stirred reactor (PaSR) model can be used to assess the extent of turbulence-kinetics interaction in a gas-turbine combustor or to provide information on how turbulence intensity will affect combustion.

## Application Setup

For this example, we consider a premixed methane/air combustor and use the PaSR model to determine how different levels of turbulent mixing would affect the combustion process.

Molecular mixing is important to this problem despite the fact that the fuel and air are premixed before entering the combustor. For premixed problems, fast mixing between the fresh reactants and the burned products is required to anchor the combustion zone inside the combustor. To provide a good starting point for the back mixing, we need to initialize the PaSR with the burned state. This is similar to starting a gas-turbine combustor with a pilot flame. We can use the equilibrium model or a steady-state PSR model to obtain the burned state of the premixed fuel-air mixture. Effects of the initial condition on the solutions will be minimal once the simulation time passes the residence time of the combustor.

There are several model parameters that are unique to the PaSR model. First, we need to specify how the PaSR will treat chemical reactions. In the current case, we want to use finite rates defined by the reaction mechanism. Secondly, we have to select a Monte Carlo mixing model and define parameters for the mixing model. The choice of mixing model depends on how we envision the mixing process to occur in the combustor. In this case, we choose the modified Curl's model because we think turbulence eddies in our combustor have a relatively large size variation. The mixing time (0.0001 sec) is actually the mechanical time scale of the turbulence, or the large-eddy turnover time. A "factor for mixing models" entry provides the scaling factor between the mechanical and scalar time scales and is usually set to 2. We also need to specify the maximum time step size for the Monte Carlo simulation. The time step size should be no greater than the mixing time scale. Finally, we define the size of our PaSR simulation, in terms of statistical events or "particles" that we will track. The solution time profiles will be smoother if we use more particles in the simulation. However, the run time and memory requirement also increase with the number of statistical events in the ensemble.

In addition to providing the time profiles of the mean and root-mean-squared (rms) values of scalar variables, the PaSR model can generate probability density functions (pdf) of scalars in separate output data files. The pdf profile shows the instantaneous distribution of a scalar at the end of the simulation time. The shape of a pdf profile is a result of the turbulence-chemistry interaction. The pdf will become a delta function (a spike) if the PaSR behaves similarly to a PSR. We can also use the pdf's to find out the distribution of states inside the combustor. Here we would like to examine the pdf of gas temperature at the end time for the simulation.

We also want to compare solutions from two cases with different mixing time scales so we can find out how turbulence intensity would affect our premixed combustor. The first case is a relatively strong mixing case with a mixing time of 0.1 msec. The weak mixing case will have a mixing time of 1 msec. To switch to the weak mixing case, we increase the mixing time to 0.001 sec.

## Summary

The mean and rms gas temperatures are shown in Figure 1 and Figure 2 for mixing times of 0.1 msec and 1 msec. The mean temperature profile of the strong mixing case (mixing time = 0.1 msec) indicates that a combustion zone is established inside the combustor and the outlet temperature is around 1800 K. On the other hand, the mean outlet temperature of the weak mixing case continues to drop because poor mixing between the fresh gas and the burned products fails to stabilize a combustion zone. The rms temperature profile of the weak turbulence case has a higher peak value than that of the strong mixing case. This large temperature variation indicates that part of the gas mixture inside the combustor does not burn in the weak mixing case. As most of the initial burned products get pushed out of the combustor, the statistics contain more and more non-burned events and the temperature variation starts to decrease consistently. Statistics of the strong mixing case are mainly made up of burning states so that the temperature variation is relatively small and stable. Similar trends are also shown by the mean CO mole fraction profiles in Figure 3.

Figure 1. PaSR Methane/Air—Temperature Comparison

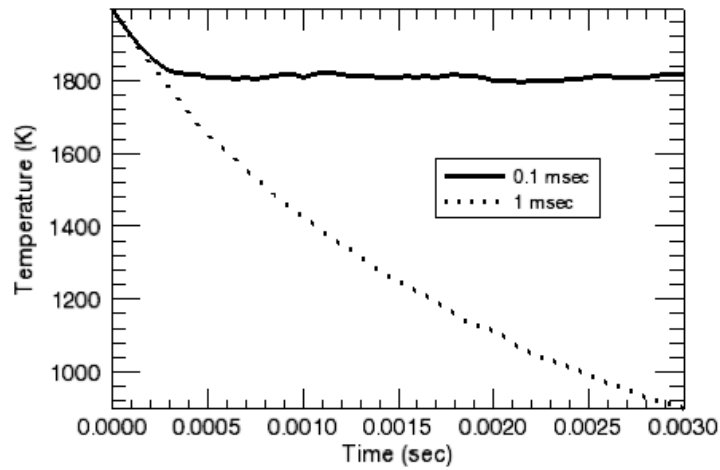


Figure 2. PaSR Methane/Air—Temperature Variance Comparison

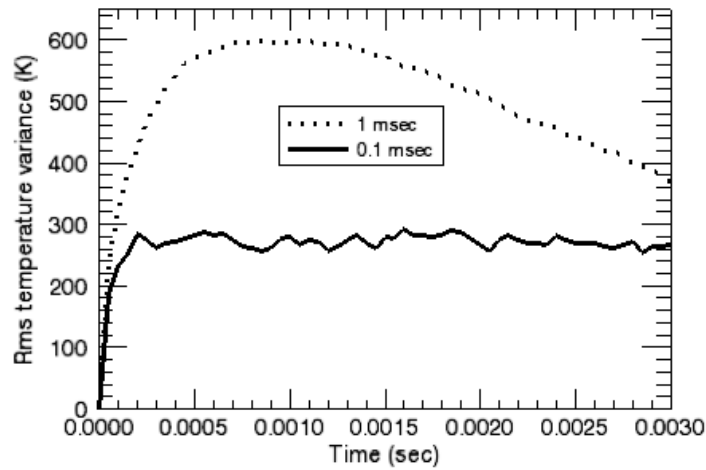
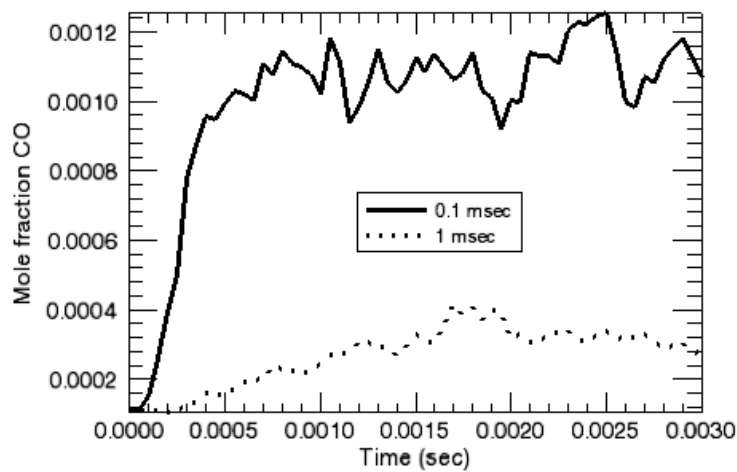
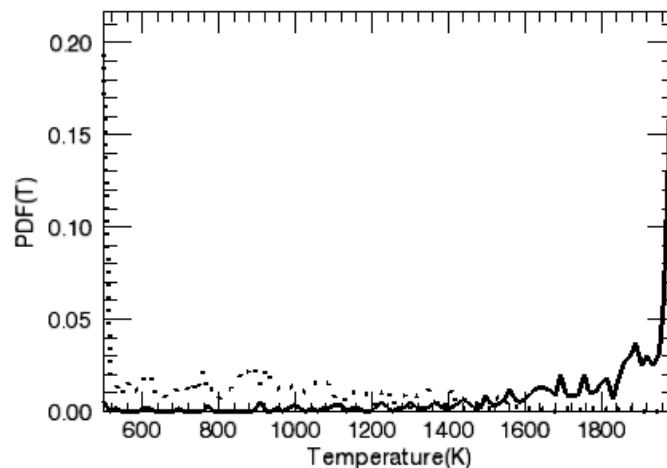


Figure 3. PaSR Methane/Air—CO Comparison



As shown in Figure 4, the pdf of the strong mixing case peaks around 2000 K with a small “tail” over temperatures slightly lower than the peak value. We can conclude that a stable combustion zone is established in the strong mixing combustor. The weak mixing case, however, has two peaks in its temperature pdf profile. A smaller peak is located near 2000 K, suggesting there is still some initially burned gas mixture left in the combustor. The large peak of the temperature pdf indicates the combustor most likely has a temperature of 500 K, which is the temperature of the inlet gas mixture. Although there might be limited chemical reactions, the slow mixing process cannot sustain a combustion zone inside the combustor.

Figure 4. PaSR Methane/Air—PDF(T) Comparison



## 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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