reaction DESIGN

CHEMKIN-PRO
Particle Tracking in Internal Combustion Engines

Emissions regulations continue to become more stringent concerning acceptable levels of NO_x, unburned hydrocarbons (UHC), and CO, as well as particulate matter (PM). For particulate matter, focus on controlling particle sizes (as well as total mass) is one outcome of recent studies that show the detrimental impact of nanometer-scale particles to human health. To model particle size distributions, a high-fidelity model is needed that is capable of capturing both the chemical processes such as nucleation and particle interactions with the surrounding gas as well as physical processes such as particle-particle collisions that lead to aggregation. Internal combustion engine designers use CHEMKIN-PRO to investigate the impacts of fuel composition variations and operating conditions on particulate matter emissions.

The Particle Tracking options in CHEMKIN-PRO allow users to specify the different chemical processes via a surface chemistry input file, and the physical processes via the reactor model data. Using the Particle Tracking capability, the effects of different operating conditions (temperature, pressure, equivalence ratio, etc.) can be studied to determine their effect on average particle size, particle number density, and total mass/volume of particles, for example.

Setting Up in CHEMKIN-PRO

The Particle Tracking Feature in CHEMKIN-PRO uses either the Method of Moments model for average particle size and number density or the Sectional Method for size distribution. The Method of Moments model can provide overall properties of a particle system, e.g., particle number density, total particle volume fraction, total particle surface area density, and average particle size. Using the Method of Moments model, the effects of operating conditions, varying fuel compositions, etc., can be efficiently studied to determine the characteristics of a particle system. For this example, consider a Jet Stirred Reactor (JSR) / Plug Flow Reactor (PFR) system that provides a good platform for kinetic studies of soot formation and growth. In the model, the JSR represents a pre-heat and flame zone of a premixed flame and the PFR is used to simulate the post-flame region. A schematic of the configuration is shown in Figure 1.

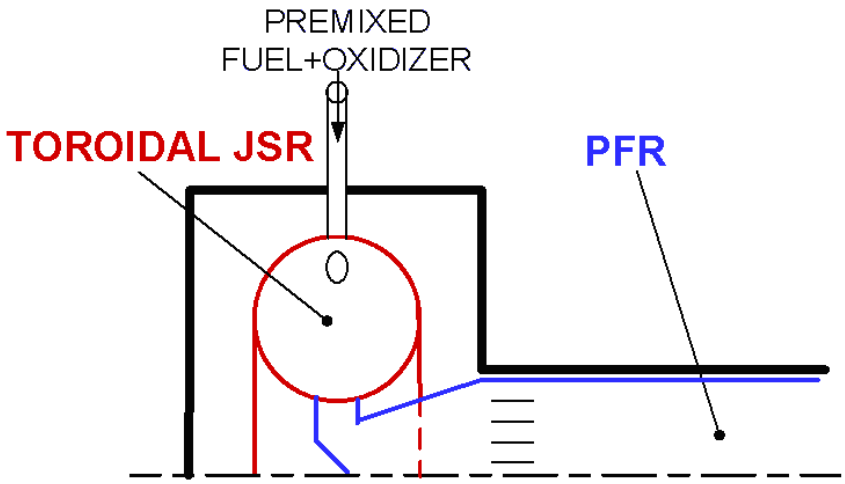

Figure 1. Schematic of JSR/PFR System.

In the example, the Particle Tracking Feature is used to simulate a $C_2H_4/O_2/N_2$ mixture. The CHEMKIN-PRO reactor network is shown in Figure 2. It consists of a PSR and two PFR's in series. The first PSR is used to represent the flame zone, while the first PFR represents the transition from the PSR to the post-flame PFR region where the measurements are performed. The primary purpose of the transition PFR is to allow the PSR exhaust to cool from 1630 K to the experimentally measured temperature of 1620 K.

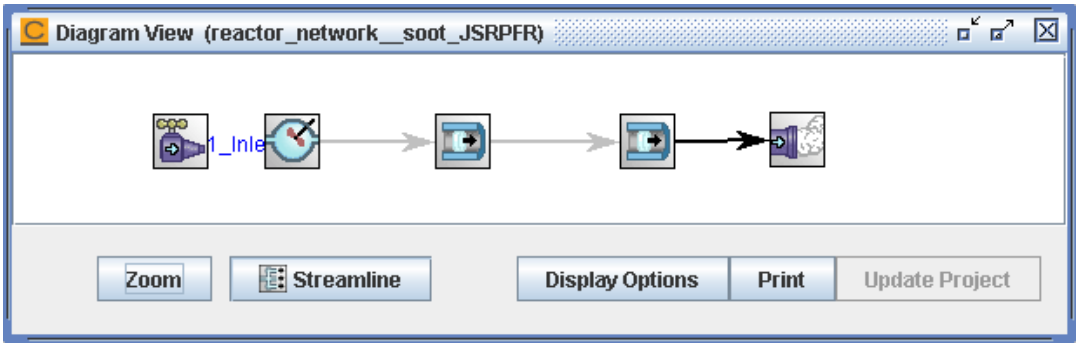

Figure 2. Schematic of CHEMKIN-PRO Reactor Network.

To activate the Particle Tracking Feature in CHEMKIN-PRO, the "Dispersed" keyword is included in the surface chemistry input file to indicate that the material is dispersed in the gas, rather than being bound to a solid wall. This keyword will activate the Particle Tracking option in CHEMKIN-PRO. The inputs to the Particle Tracking Feature are available on the Dispersed Phase tab in the Reactor Physical Properties input dialog and will be available for all reactors in the network.

Results

To test different growth mechanisms of soot, two simulations are performed: one with growth in the forms of both H-abstraction-C_2H_2-addition (HACA) and PAH condensation and the other one with HACA growth reactions only. The simulation results (Figure 3) indicate that the HACA-only does not properly capture the slow soot mass growth in the post-flame region. On the other hand, the HACA + PAH mechanism shows much better agreement with the experimental data.

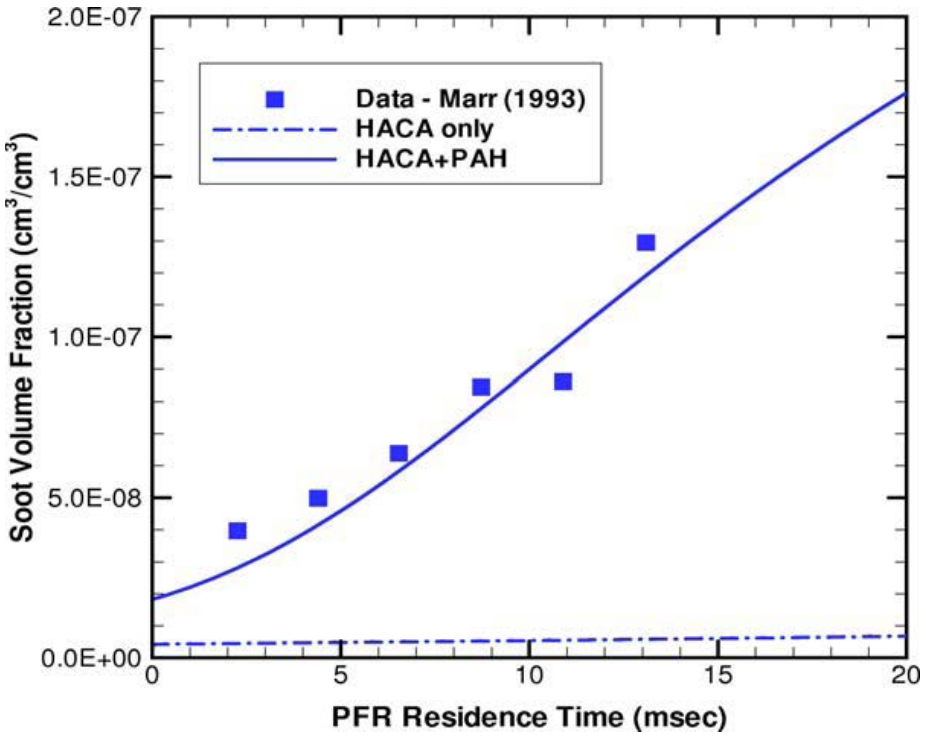

Figure 3. Comparisons of soot mass concentration profiles inside the PFR for the 1630K, phi = 2.2 case of $C_2H_4/O_2/N_2$.