reaction DESIGN

FORTÉ
Predicting Soot Particle Diameter

Soot, or Particulate Matter (PM), formation remains an ongoing issue for internal combustion engines that need to use a wider range of fuels and pass stringent emissions standards. Tracking soot evolution in engines using CFD simulations can provide valuable insights for engine design. However, conventional CFD codes are not able to take advantage of recent advances in soot formation chemistry and have proven unreliable for soot size predictions.

FORTÉ allows the use of accurate fuel models with soot chemistry using a particle tracking capability based on the Method of Moments. This soot prediction method allows calculation of spatially resolved soot volume fraction, number density and average particle diameter. Engine designers are using FORTÉ to investigate the effects of gasoline and diesel fuels on soot evolution in engines. This Solution Brief highlights the use of the soot particle tracking feature of FORTÉ in a diesel engine simulation.

Setting It Up

Single-component fuel mechanisms are not sufficient to capture fuel effects in diesel, gasoline or alternative fuels; multicomponent fuel surrogates are necessary. In this example, we use a multicomponent surrogate to accurately represent diesel fuel including the surrogate's multicomponent spray-vaporization properties.[1] We employ a detailed gas-phase chemistry mechanism that includes soot precursors as large as pyrene, and soot-surface chemistry that models interaction of soot particles with the gas-phase species. The particle-tracking model considers the statistical particle-size distribution on a cell-by-cell basis at each time step and includes the effects of particle coagulation. For the example presented here, the multi-component fuel mechanism consists of 450 species. For the engine modeling work presented in the cited paper, we focused on a direct-injection diesel engine. A sector mesh has been used for the modeling work.

1"Soot Particle Tracking with FORTÉ CFD Using Method of Moments and a Detailed Soot Chemistry Mechanism," Karthik V. Puduppakkam, Abhijit U. Modak, Chitralkumar V. Naik, Long Liang, Cheng Wang and Ellen Meeks, International Multidimensional Engine Modeling User's Group Meeting, April 15, 2013, Detroit, Michigan.

Results

It is informative to look at both spatially resolved and spatially averaged plots for soot predictions. Figure 1 indicates the calculated spatially averaged values of soot number density along with the mole fraction of a main soot nucleating species (pyrene) used in the model. The average number density peaks at around 10 CAD. The value at the peak is about 2×10^{12} particles/cm^3 and it subsequently decreases substantially with time. At 50 CAD, it is lower by a factor of 200x compared to its value at the peak.

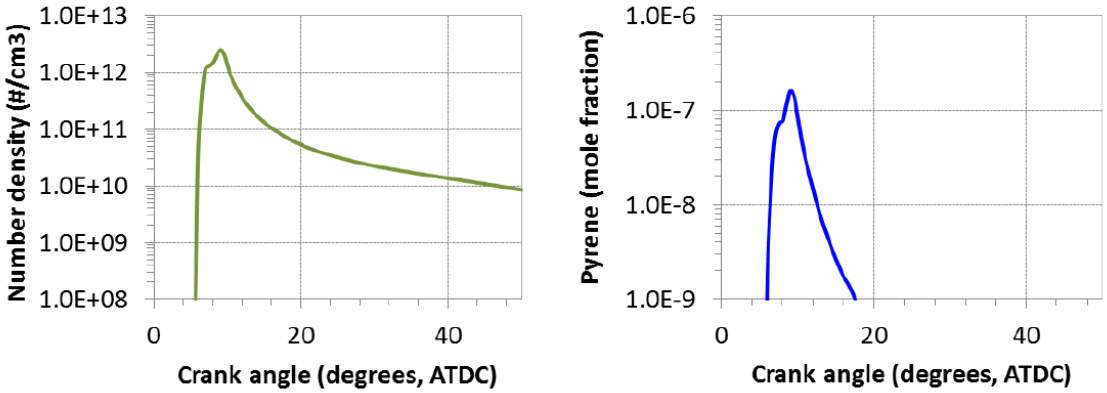

Figure 1. Calculated results for spatially averaged soot number density, and the mole fraction of pyrene, which is a nucleating species.

Three factors contribute to number density: particle nucleation produces more soot particles and hence increases the number density; particle coagulation decreases the number density; and finally, if particle oxidation leads to complete consumption of some particles, then it decreases the number density.

Based on the results shown in Figure 1, it can be deduced that soot nucleation is very active and dominates over other soot processes in the neighborhood of 10 CAD. This is confirmed by plotting a pyrene mole fraction plot (also Figure 1), as this is a main nucleating species in the soot mechanism used; pyrene concentration and the number density both peak at around the same time (~10 CAD).

Figure 2 shows the iso-contour of soot volume fraction for a value of 0.5 ppm for crank angles of 10-35 CAD. Figure 3 shows the spatially resolved plots of average soot particle diameter taken on cut-planes at 10-35 CAD.

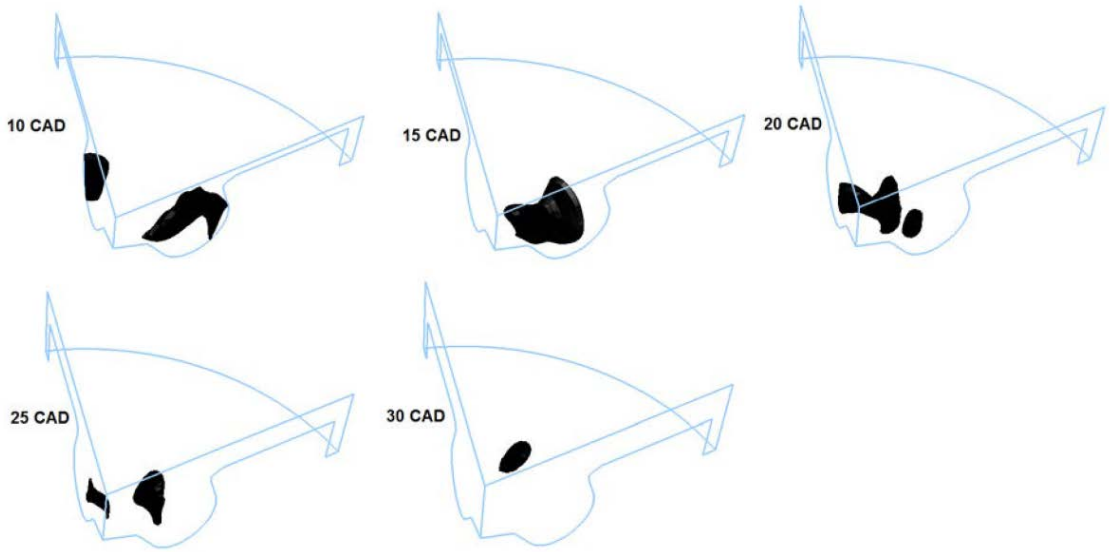

Figure 2. Spatially resolved soot volume fraction iso-contour for a value of 0.5 ppm.

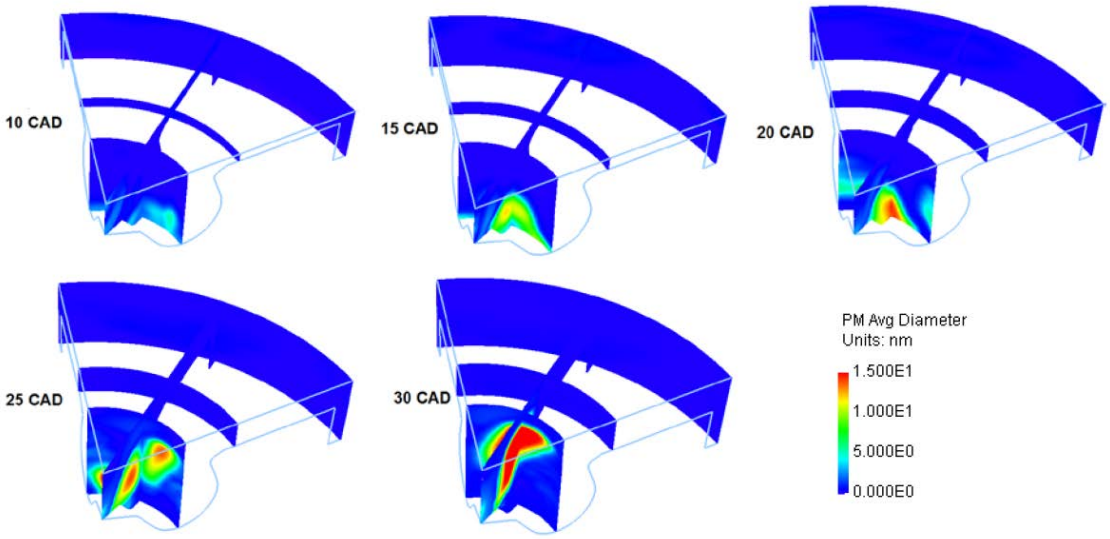

Figure 3. Spatially resolved soot average particle diameter.