reaction DESIGN

FORTÉ
Predicting Soot Formation and Volume Fraction

Soot, or Particulate Matter (PM), emissions from internal combustion engines represent a major challenge to engine manufacturers as new regulations worldwide are requiring greater than 90% reductions. Compounding this problem is the widening range of fuel options that engines must accept and increased potential for fuel composition variability. Engine simulation has the potential to reduce development cost and time; however, traditional combustion CFD tools are limited by their inability to make use of accurate fuel chemistry models and produce reliable results within an acceptable Time-to-Solution window. Some innovative engine and fuel designers are taking advantage of FORTÉ's ability to handle accurate soot chemistry mechanisms to improve soot simulation accuracy. This Solution Brief describes the application of accurate chemical models and software simulation capabilities for predicting soot in engines.

Setting it Up

The most common soot modeling technique in conventional CFD is to use severely reduced chemistry mechanisms and then to employ empirical correlations to predict soot emissions, such as with the 2-step particulate model that employs only a single soot precursor (acetylene). Using a model that attempts to predict soot particle formation without any intermediate steps is a great simplification that has proven to be inaccurate. In reality, acetylene is only one of many precursors that contribute to carbon growth and the formation of the single-ring molecule benzene (C_6H_6), which will further grow to form polycyclic aromatic hydrocarbons (PAH), such as pyrene ($C_{16}H_{10}$), which then contribute to particle nucleation as well as to particle growth. There are also multiple pathways to oxidation of a soot particle.

Modeling this cascade of chemical reactions accurately requires an accurate fuel-combustion mechanism that can capture the details of the precursor kinetics. In this example, we use a multi-component diesel fuel model with over 394 species that includes soot formation as a "pseudo-gas" species. This mechanism allows the prediction of soot volume or mass fraction from multiple precursors in FORTÉ. The results using the accurate pseudo-gas soot mechanism are compared to results using a severely reduced diesel mechanism with 35 species and the 2-Step soot model that is also included in FORTÉ.

Results

The MFC derived chemistry model used in these simulations contains over 400 chemical species and 1000 kinetic reactions. FORTÉ can solve the in-cylinder diesel-engine combustion problem with this chemistry overnight using 16 processors on a typical computer. As part of collaborations within the Model Fuels Consortium (MFC), IFP Energies Nouvelles (IFPEN) generated diagnostic measurement of soot in an optical engine that can be used to validate the soot chemistry model in FORTÉ simulations[1].

The IFPEN experimental data are shown in the left image in Figure 1 as the crank angle progresses through the cycle from top to bottom with ignition occurring at 366 degrees. The corresponding visualization of the FORTÉ-predicted soot concentrations are shown on the right side of Figure 1. This figure shows that FORTÉ, when used with the MFC chemistry model, is able to predict the location of soot formation in the cylinder, as well as the timing of the formation and oxidation of soot within one crank angle from the data.

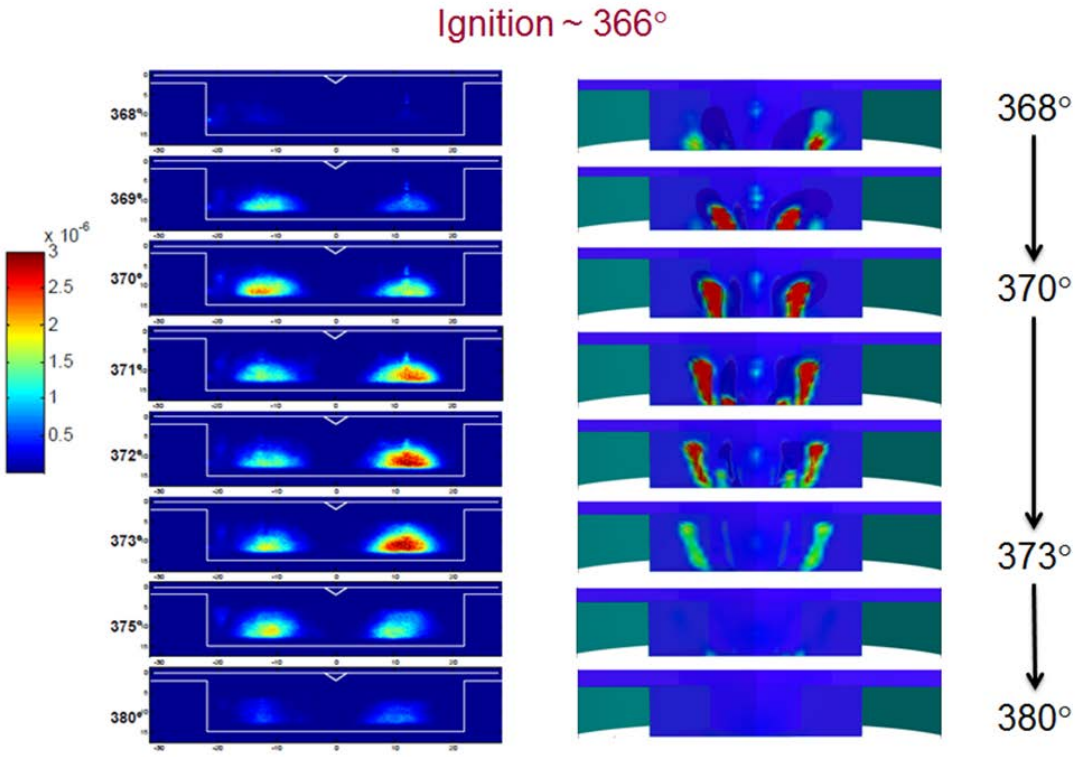

Figure 1. Calculated results for spatially averaged soot number density, and the mole fraction of pyrene, which is a nucleating species.

[1]Reaction Design, "Model Fuels Consortium II Year 3 Annual Report," San Diego, CA, 2011.

A comparison of soot with NOx results for a diesel engine with high amounts of EGR shows that the MFC derived multi-component soot chemical model produces much more accurate trends in the regions of highest soot propensity than traditional 2-step soot models with severely reduced chemistry models (Figure 2). In this figure, the soot and EINOx (g NOx/kg-fuel) are compared to the soot and EINOx values for the low EGR cases.

It is important to note that the traditional 2-step soot model approach proved to be more accurate for conditions with very low soot, yet failed to predict the soot trends at conditions where soot emissions are of greatest concern (e.g. high EGR cases). Results like these are providing engine designers what they have been missing, the ability to predict soot in cases where soot is most important.

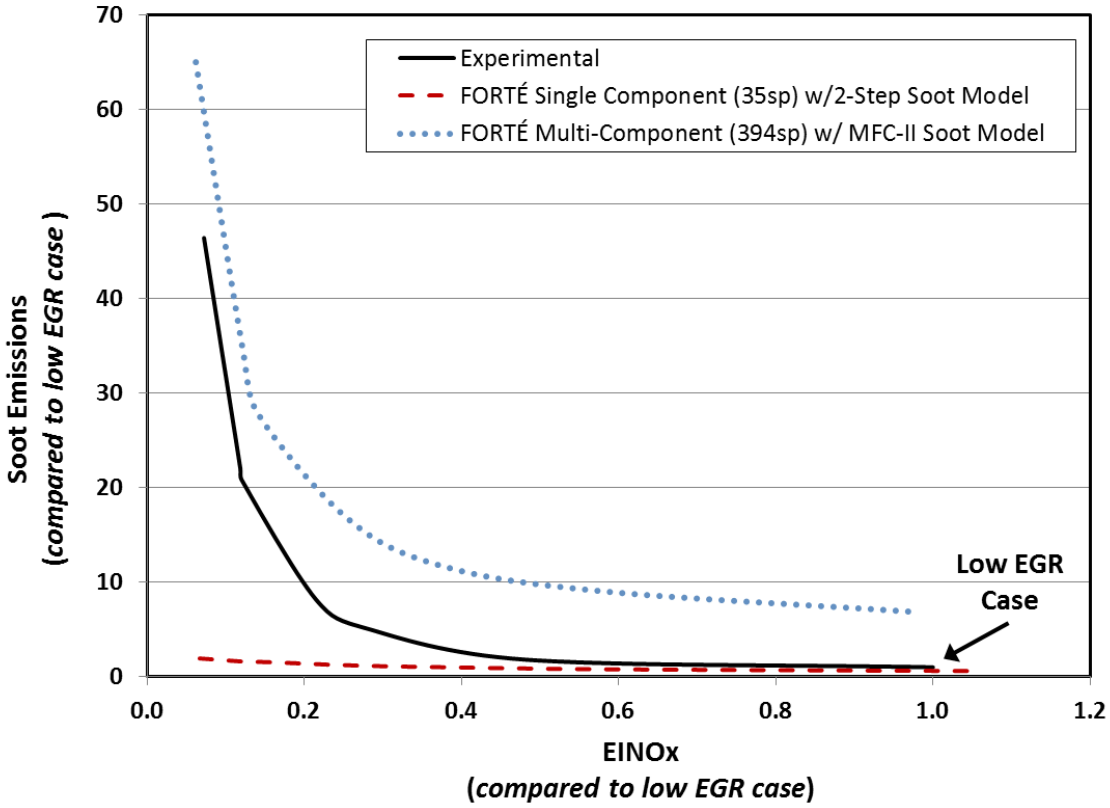

Figure 2. Comparison of FORTÉ soot and NOx results in a high EGR diesel simulation using multi-component MFC soot model and traditional 2-step soot modeling approach.