Multi-Component Spray Modeling with FORTÉ

FORTÉ-APP-Spray (v1.0) April 4, 2011

Overview

This applications note provides instructions for performing 3-D diesel-engine spray combustion simulations with advanced spray models and accurate detailed chemistry. The simulation employs a multi-component diesel-fuel surrogate mechanism with 437 species that was reduced for the conditions of interest from a comprehensive and well validated master mechanism. The results show prediction of spray penetration for low-temperature combustion conditions. The results also demonstrate some advantages of using a multi-component surrogate to capture vaporization stratification within the engine cylinder.

Spray Modeling Overview

Conventional and advanced engine designs depend upon effective use of spray to control the distribution of the liquid fuel for greatest benefit. Sprays in diesel engines control ignition, power and emissions. It is important that the spray models used in 3-D simulation for sprays have the ability to accurately predict liquid breakup, droplet formation, distribution and evaporation.

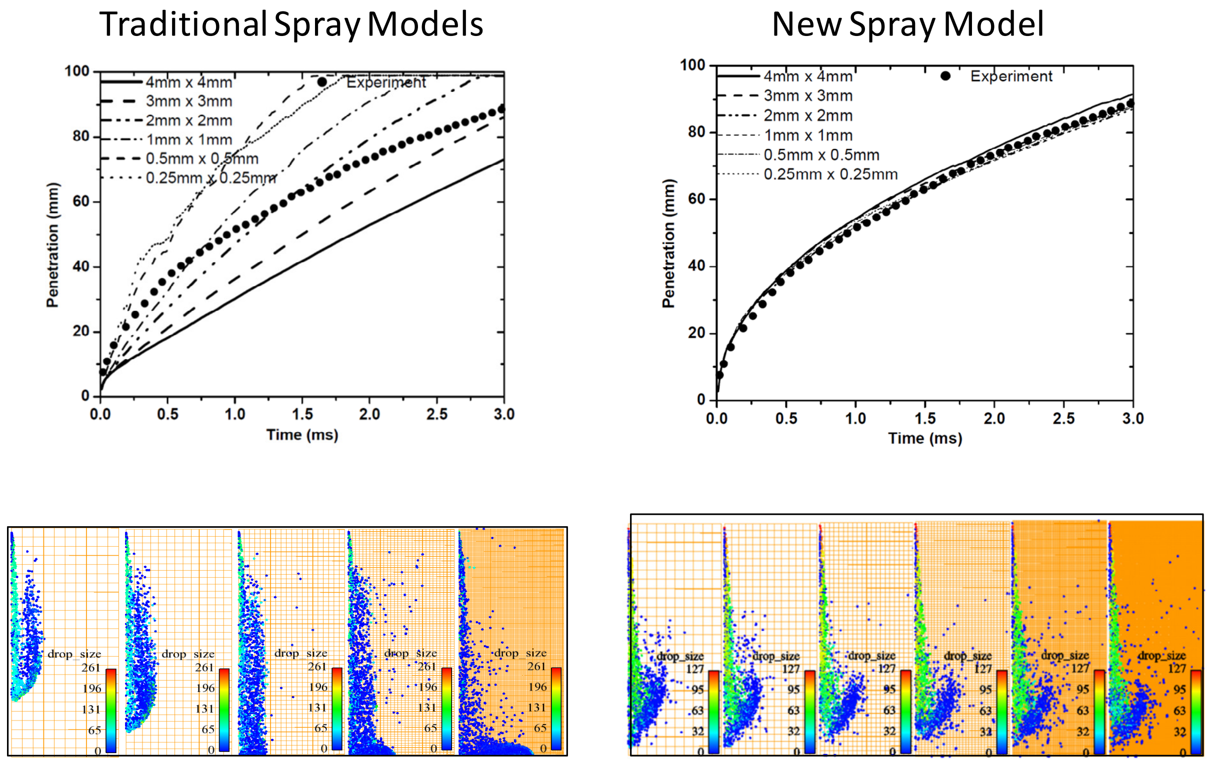
The FORTÉ Simulation Package uses an advanced KH-RT spray model that simulates liquid breakup, secondary droplet breakup, distribution and evaporation. The FORTÉ spray model has been shown to produce consistent results independent of mesh size (Imamori, et al, 2009). This can be seen on the left of

Figure 1 where traditional CFD spray models are shown to be quite mesh dependent while the KH-RT spray model in the FORTÉ simulator on the right show consistent results for a variety of different mesh sizes.

Test Case Description

The details for setting up this test case are provided in the Diesel Sector Mesh Application Note. This application note focuses on the specifics of setting up the spray case and a description of the spray results.

Figure 1: The FORTÉ KH-RT spray model provides results that are not affected by mesh size when compared with traditional CFD spray models.



The model represents a single-cylinder, direct-injection (DI), 4-stroke diesel engine based on a Cummins N-series production engine that has been extensively tested and diagnosed at Sandia National Laboratories (Singh, et al, 2006). The engine has a bore of 139.7 mm and a stroke of 152.4 mm with a cylindrical cup piston bowl, yielding a displacement of 2.34 liters for its one cylinder. The engine has a swirl ratio, which is the ratio of the flow rotation speed to the engine rotation speed, of approximately 0.5 near top dead center (TDC).

The engine is equipped with a non-production, high-pressure, electronically-controlled, common-rail fuel injector. Specifications for the fuel injector are included in Table 1. For the conditions modeled here, an eight-hole, mini-sac injector cup (tip) was employed, having an included angle of 152° (14° down-angle from the firedeck). The eight fuel orifices are equally spaced and have nominal diameter of 0.196 mm.

Table 1: Engine and Injector Specifications and operating conditions (REF)

Engine specifications	
Combustion chamber	Quiescent, direct injection
Swirl ratio	0.5
Bore × Stroke (cm)	13.97 × 15.24
Bowl width, depth (cm)	9.78, 1.55
Displacement (L)	2.34
Connecting rod length (cm)	30.48
Compression ratio	16:1
Fuel injector type	Common rail , pilot valve actuated
Number of holes	8, equally spaced
Spray pattern included angle	152°
Rail pressure, bar	1200
Nozzle orifice diameter (mm)	0.196
Nozzle orifice L/D	5
Operating Conditions	
Engine speed (rev/min)	1200
IMEP (bar)	3.9
Intake temperature (K)	365
Intake pressure (kPa)	214
Start of injection, SOI (°ATDC)	-22.5
Duration of injection, DOI (°ATDC)	7.75
O_2 volume % (air diluted by N_2)	12.7

FORTÉ Spray Model Setup

To setup the problem in the FORTÉ simulator, we begin by reading in an existing mesh file and fuel mechanism and then we will input the information required to setup and run the test case.

1. In the Editor panel, select the **IC Engine** option and check **Use Injector Spray Model**.

2. Import the sample case mesh ***Sandia.fmsh***. You can see the geometry in the viewer window and use the mouse to rotate, re-size and manipulate the view.

3. Set up the Fuel Model:

   - Import the fuel chemistry set ***Diesel_3compSurrogate_437species.cks***, which is located in the data directory of the FORTÉ install folder.

   - Define the vaporization model for the fuel surrogate, as described in the FORTÉ User Guide for this diesel-fuel mechanism, in the Fuel Spray Composition Editor panel. The intended surrogate composition is 51% n-tetradecane, 35.5 n-decane, and 15.5 1-methylnaphthalene. The corresponding species symbolic names for these species are: nc14h30, nc10h22, and amn, respectively.

- For each species added for the 3-component kinetics model, select the same corresponding fuel name for the spray vaporization model, using the pull-down menus to the left of the species. By default these are the same as the kinetics species selected.

4. Define the Nozzle properties and Fuel Injection events as illustrated in Figure 2.
   - A Solid Cone Injector is typical of diesel engines. Select this as the injector nozzle type.
   - Define the coordinate position of the nozzle hole in the cylinder, as well as the tilt relative to the cylinder axis.
   - For this case, we use a discharge coefficient to represent the nozzle-discharge properties, rather than a nozzle-flow model, which is another option in FORTÉ. User interface.
   - Define the Spray Injections. Select the Injections tab and click the **Setup Injections** button. Select **New…** from the **Profile Shape** selector to create a new custom injection profile.
   - Give the profile a name and enter the values from Table 2 into the Profile Manager. Alternatively, you can import the data from the ***InjectionProfile.csv*** file by clicking the **Import from CSV** button. After using one of these methods to set up the profile, click **Apply Changes** and close the Profile Manager shown in Figure 3. Note that this profile is unitless and will be scaled according to the total mass of fuel injected and the injection duration specified in the injection panel.
   - Set up the rest of the injection data according to Figure 4. Here note that the fuel specified is the total mass for the engine cylinder, not per sector.
   - Define the spray model settings as shown in Figure 5.

Figure 2: Injections Editor - Nozzles and Injections tabs

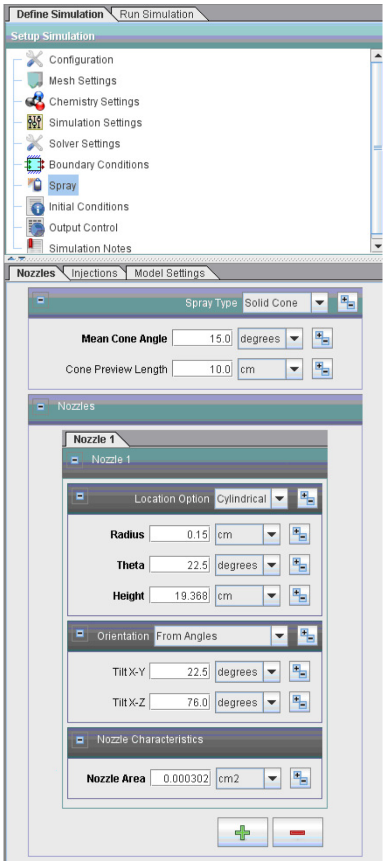


Table 2: Spray model profile data

INJECTION #	VALUE	INJECTION #	VALUE
1	0.45524	***10***	9.3663
2	1.8127	***11***	9.5303
3	2.7241	***12***	9.4750
4	5.6538	***13***	8.8534
5	7.4606	***14***	7.7184
6	7.9150	***15***	5.8252
7	8.1631	***16***	3.6407
8	9.1185	***17***	1.9108
9	9.4380	***18***	0.97991

Figure 3: Profile Manager - Applying Changes

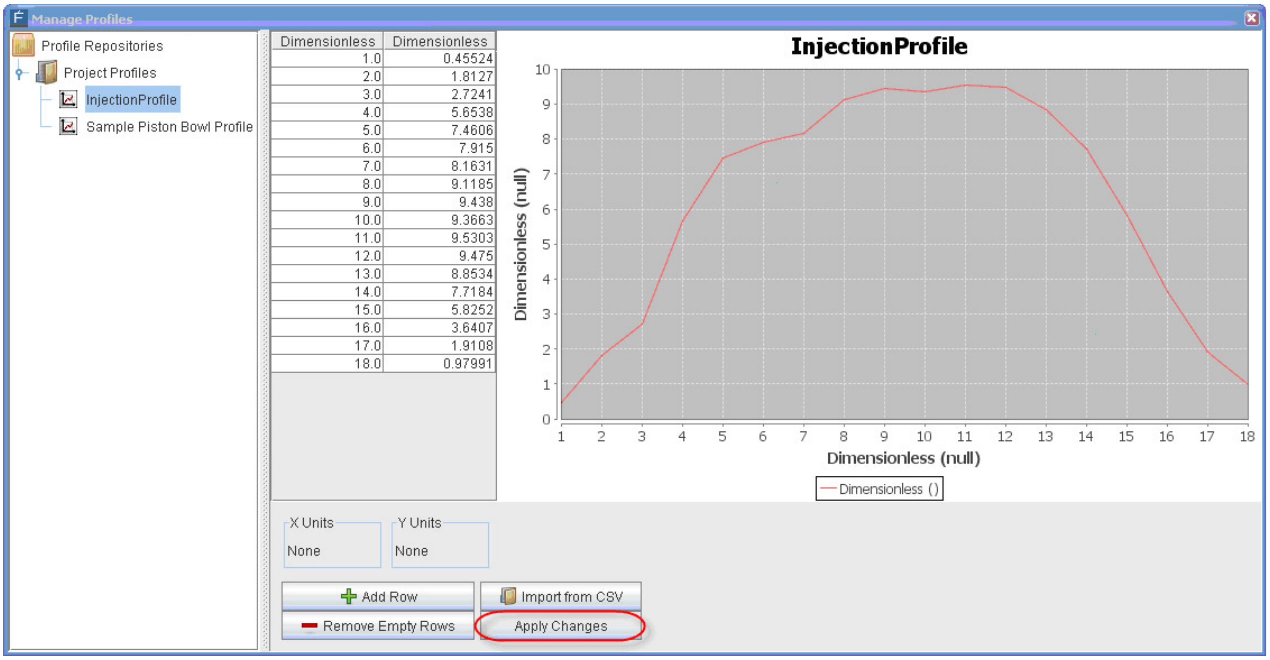


Figure 4: New profile creation

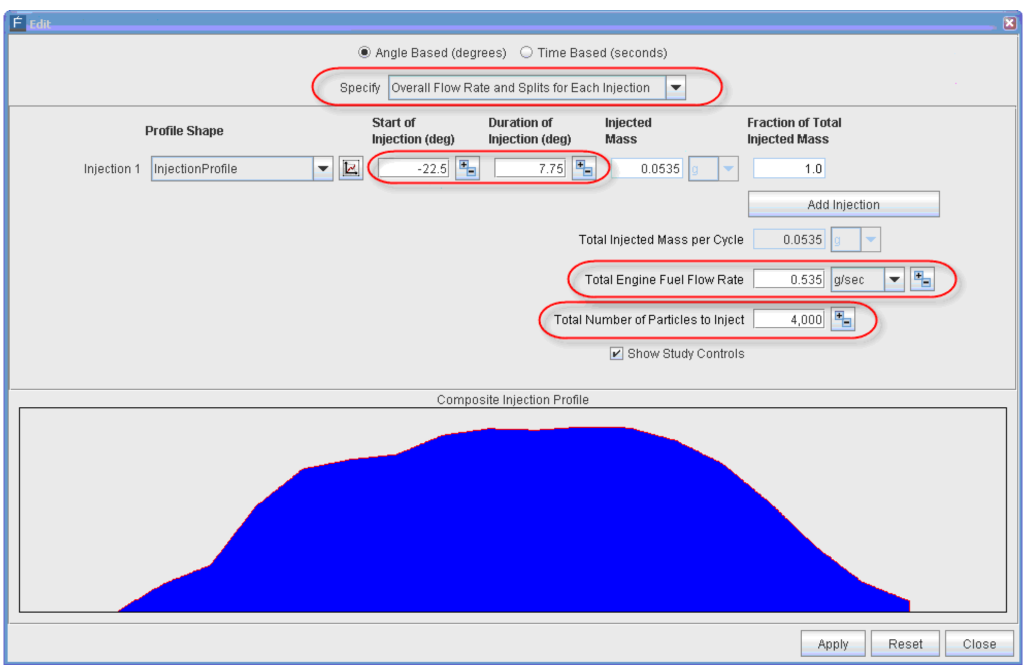
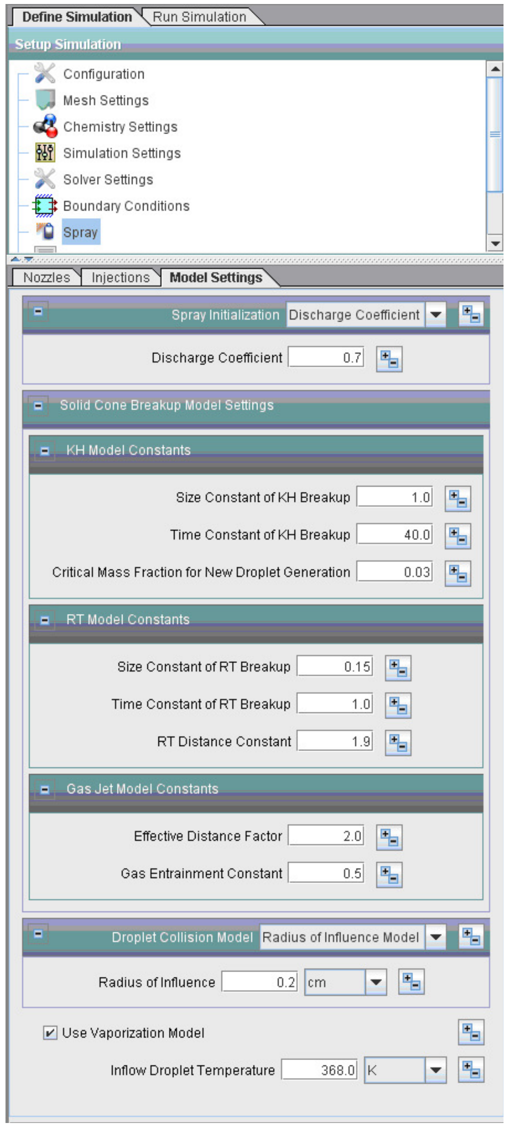


Figure 5: Spray Node - Model Settings tab



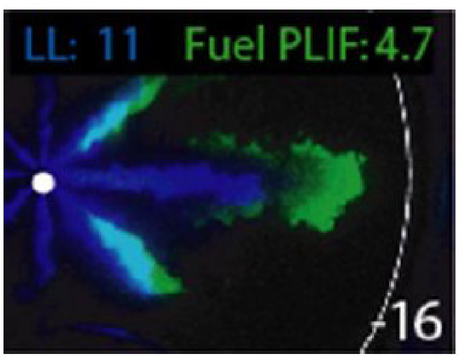
Results

The engine spray simulation results of simulated fuel vapor and temperature contours are compared to the images measured by (Singh et al. 2006). The calculation using the fuel surrogate is used for this comparison because its pressure and heat release curves best match the experiment. All the images shown below are on the cut-plane along the spray axis. First, the simulated and measured spray patterns at -16 °ATDC are compared in Figure 11. CA=-16 °ATDC is selected because this crank angle location is close to the end of injection (spray is still developing but a significant portion of liquid fuel has been vaporized), and thus this location is representative of the overall spray process. The image on the left in Figure 6 shows experimentally observed liquid fuel distribution (blue) measured using Laser-light

Mie-Scattering (LMS) technique and fuel vapor contour (green) measured using BroadBand-Planar Laser Induced Fluorescence (BB-PLIF). The simulated spray pattern is shown on the right in Figure 6, where the red particles represent groups of identical fuel droplets and the green contour shows fuel vapor (mass fraction) distribution. As seen, though the liquid fuel penetration is slightly under-predicted, the simulated fuel vapor penetration matches the experimental image pretty well, indicating that the gas phase environment is well captured by the model.

Based on the reality check, we examine the fuel species distribution at -16°ATDC. Figure 7 shows the vapor mass fraction contours of n-decane, n-tetradecane and AMN, the components of the fuel surrogate. The contours at -16°ATDC show that the vaporization rate of n-decane (the lightest component in the surrogate) is different from that of the other two fuel species, thus its fuel vapor distribution pattern is also different. Then the contours at -12°ATDC show that a large portion of n-decane has been converted to other species due to ignition at this crank angle. And this indicates that n-decane is a major contributor to the low temperature heat release. The images in Figure 7 serve as a good example that shows the use of multi-component spray and kinetics models provides better flexibility and more detailed information in engine modeling.

Figure 6: Experimentally observed LMS (blue) and BB-PLIF (green) and model predicted liquid-fuel (red)



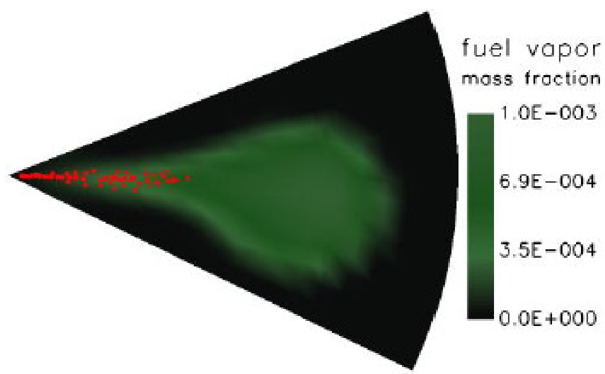
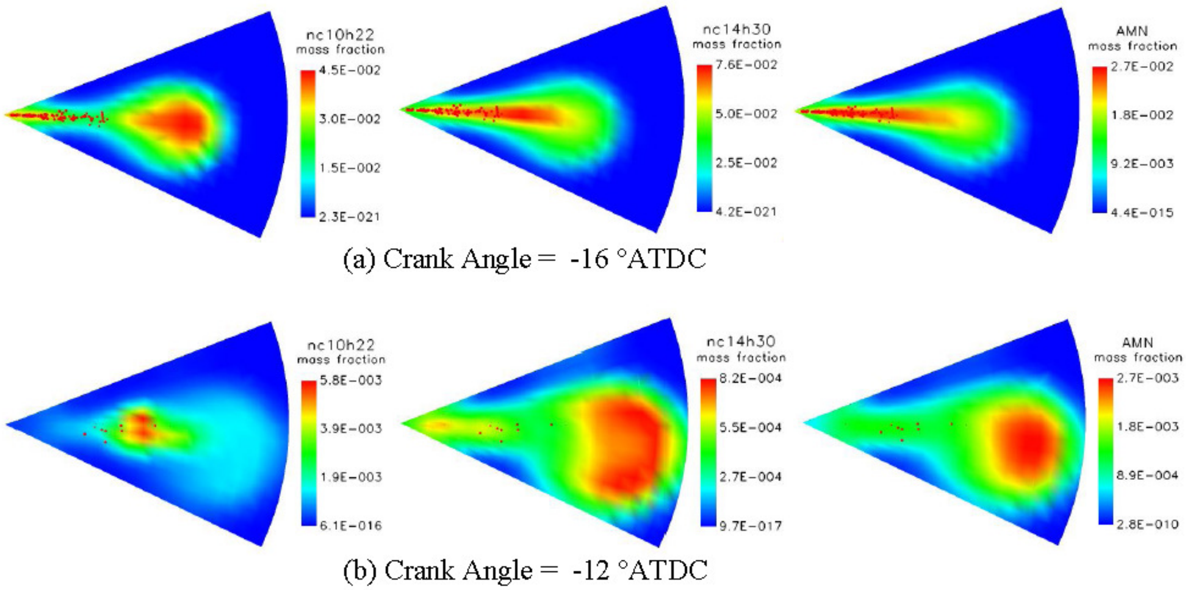


Figure 7: Simulated fuel vapor (mass fraction) contours along the spray axis at -16 and -12 °ATDC in the case



Summary

In this application note, we used the FORTÉ Simulation Package to simulate diesel spray combustion in an engine and compared those results to experimental data. The FORTÉ advanced spray model allows matching between the multi-component fuel surrogate and the spray parameters. A multi-component fuel surrogate was used and the spray parameters are set up to accurately simulate the droplet breakup and evaporation. Good comparison with experimental results for the fuel components and spray penetration are also shown.

References

Brown, P.N., G.D. Byrne, G.D., Hindmarsh, A.C., *SIAM J. Sci. Stat. Comput.* **10**, 1038–1051 (1989).

Imamori, Y., Hiraoka, K., Murakami, S., Endo, H., Rutland, C.J., and Reitz, R.D., "Effect of mesh structure in the KIVA-4 code with a less mesh dependent spray model for DI diesel engine simulations," SAE Paper 2009-01-1937, 2009.

Liang, L., Naik, C.V., Puduppakkam, K.V., Wang, C., Modak, A., Meeks, E., Ge, H.W., Reitz, R.D. and Rutland, C.J., “Efficient Simulation of Diesel Engine Combustion Using Realistic Chemical Kinetics in CFD,” SAE Paper No. 2010-01-0178, Detroit, Michigan, April 2010.

Singh, S., Reitz, R., and Musculus, M., “Comparison of the Characteristic Time (CTC), Representative Interactive Flamelet (RIF), and Direct Integration with Detailed Chemistry Combustion Models against Optical Diagnostic Data for Multi-Mode Combustion in a Heavy-Duty DI Diesel Engine,” SAE Paper No. 2006-01-055, Detroit, Michigan, April 2006.

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