DIESEL COMBUSTION AND EMISSIONS MODELING

Yong Sun, Song-Charng Kong and Rolf D. Reitz

NUMERICAL MODELS

- Detailed reaction mechanisms for n-Heptane were used to simulate the diesel fuel chemistry. The CHEMKIN chemistry solver was integrated into KIVA-3V for solving the chemistry

- Reduced NO Mechanism
  - $N + NO \rightarrow N_2 + O$
  - $N + O_2 \rightarrow NO + O$
  - $N_2O + O \rightarrow 2NO$
  - $N_2O + OH \rightarrow N_2 + HO_2$
  - $N_2O + m \rightarrow N_2 + O + m$
  - $HO_2 + NO \rightarrow NO_2 + OH$
  - $NO + O + m \rightarrow NO_2 + m$
  - $NO_2 + O \rightarrow NO + O_2$
  - $NO_2 + H \rightarrow NO + OH$

- Phenomenological Soot Model
  - $\frac{dM'_s}{dt} = \frac{dM_n}{dt} - \frac{dM_{ss}}{dt}$
  - $\frac{dM_{ss}}{dt} = A_m \frac{M_{ss}}{RT} \exp\left(\frac{E_m}{RT}\right)$

- Axial distribution (UCF) was used as the soot inception for soot formation. Soot oxidation rate is determined by the Nagle-Buckland-Cantrell model

TEMPERATURE AND SOOT CONTOURS

ENGINE RESULTS

SOOTING AND NON-SOOTING LIMIT

COMPETITIONS BETWEEN PLL images and predicted soot mass fraction contours indicate that:

- Predominant prediction of PLL images and predicted soot mass fraction contours with variation of ambient temperature (results from central plane of the fuel jet at 5.25 mm A/F)

University of Wisconsin Engine Research Center