Updated 16 August 2012

a. Objectives for the session

- Collaborative comparisons of measured and modeled soot volume fraction (SVF) and other soot-related quantities
- Collaborative comparisons of experimental measurements of SVF and other quantities
- Collaborative comparisons of computed SVF and other quantities using different models
- Definition of best practices for comparisons between experimental and modeling results
- Definition of desired experimental data for model validation

b. Inter-workgroup objectives

- For parametric variations, assessing the achievability of target conditions in harmony and reaching a consensus for the priority of predefined conditions among the different workgroups for a complete set of data.
- An increased communication with other workgroups will be established for the diagnostics of phenomena playing key roles in soot processes such as concentrations of gas-phase species (e.g., OH, C_2H_2, PAHs).
- A consensus on submitted result format for standardization purposes.
- A consensus on result submission deadline.

c. Full description of target conditions

Modeling Side:

- The target configurations are Spray H (n-heptane) and Spray A (n-dodecane)
- Because teams submitting soot results also will need to simulate spray and combustion, each team should review the guidelines that have been posted for ECN2 under the Spray Development and Vaporization, Mixing and Velocity, and Ignition and Lift-Off Length topics. Each team should also review the modeling recommendations and results from the ECN1 Proceedings.
- For Spray H (n-heptane)
    - Injector/spray characteristics and ambient oxygen levels, temperatures and densities are specified on the ECN website
    - Updated soot volume fraction data have been posted on the ECN website
    - First priority are variations in ambient O_2 level and in ambient temperature
        - 8% to 21% O_2 for T = 1000 K, ρ = 14.8 kg/m^3
        - T = 750 K to 1300 K for 21% O_2, ρ = 14.8 kg/m^3
- For Spray A (n-dodecane)
    - Injector/spray characteristics and ambient oxygen levels, temperatures and densities are specified on the ECN website
    - Soot volume fraction data are being posted on the ECN website
    - First priority are variations in ambient O_2 level and in ambient temperature

Experimental Side:

- Spray A (n-dodecane) will be the priority for new experimental measurements. Problematic conditions for soot diagnostics have been identified and shared with modelers. A set of target conditions has been identified that includes variations in ambient O_2 level and/or temperature.
- Specifics on data that are available for Spray H and for Spray A were discussed during a Webex for the soot teams on 10 July 2012. For Spray A, the conditions for the soot measurements differ slightly from the conditions for the other measurements.
- The identification of future target configurations and fuels will be a subject of discussion at the workshop.

d. Quantities to be compared

- Specifics are provided below

- Physical quantities
    - First priority is SVF
    - Second priority is primary particle size
    - Other quantities of interest (for the future) include particle size distribution functions (PSDFs), characterization of agglomerates

- Averaging
    - First priority is the mean value
    - RMS values, higher-order statistics, and histograms or PDFs are of interest to characterize fluctuations and intermittency
    - Statistics may be phase-averaged over realizations at specified times after start of injection, and/or time-averaged over an appropriate time interval in the quasi-stationary flame for point-wise diagnostics

- "Raw" experimental signals should be reported, in addition to the derived quantities of interest
    - e.g., measured radiative intensity in addition to derived SFV
    - To facilitate more direct comparisons between experiment and model

e. Spatial position and timing ASI of these quantities

- Specifics were discussed during the 10 July 2012 Webex

- Timing
    - SVF related quantities should correspond to the quasi-steady flame
    - Primary particle related data of TEM analysis will correspond to the average of complete combustion
    - Primary particle size measurement at different times ASI is an interest of the soot workgroup

- Spatial positioning
    - Details are specified below
    - 1D profiles
        - Axial: along the injection axis
        - Radial: at fixed axial positions, relative to the axial location of computed peak mean SVF.
    - 2D maps
        - On a cutting plane that contains the injection axis

f. Format of submitted results

- Details are provided below

g. Deadline for submitted results

- 24 August 2012

ECN2 Soot Team
Specifications for Soot Modeling Results Submissions
16 August 2012

All results should be emailed to Dan Haworth (dch12@psu.edu) by 24 August 2012.

At a minimum, each group that submits model results should send two files: one soot model specification Excel file, and one global soot results data file for at least one model at one operating condition.

Please follow the file formatting and naming conventions below; example file names are in blue font.

Please use spaces between columns for all ASCII data files.

For details on how the Sandia (Spray H) soot volume fraction measurements were made, see item 79 under the definitions provided on the ECN website (http://www.sandia.gov/ecn/cvdata/dsearch/dataDef.php) and the link that is provided there.

Units for all quantities should be the same as those used on the ECN website: initial density (kg/m^3), initial O_2 level (vol%), initial temperature (K), SVF (ppm), and distances (mm).

Soot Model Specification

A fill-in Excel workbook file is provided. This is the same as the one used to report the model setup for ignition delay and liftoff length results for ECN2, with additions for information on the soot model, the radiation model (if any), and the time after start-of-injection or the time interval (if time averaging is used) at which model results are reported corresponding to the quasi-steady flame.

File naming conventions

- 3-character institution identifier
  - ETH: ETH Zurich
  - LTH: Lund University
  - PSU: Penn State University
  - TUE: Eindhoven University of Technology
  - UWM: University of Wisconsin-Madison
- 1-character model number
  - To be used to distinguish results from different models in data file names (see below)
    - e.g., PSU1, PSU2, PSU3, . . .
- 1-character spray-flame identifier
  - H: Spray H (n-heptane)
  - A: Spray A (n-dodecane)
- Example: Penn State Spray H model specification Excel workbook
  - PSU_H_sootmodel.xlsx
  - There should be a separate sheet in the workbook for each model for which results are submitted

Data for x-y Plots

Results should be submitted for the quasi-steady flame.

File naming convention for ASCII text files:

- 4-character institution and model identifier (as above)
- 1-character spray-flame identifier (as above)
- Operating conditions (initial ρ, O_2 and T) and spatial location (where appropriate) – see below
- Example: Penn State model 1 Spray H global results for ρ = 14.8 kg/m^3, 21% O_2, with variations in T
  - PSU1_H_14.8RHO_21O2_vT.dat

Data to submit:

1. Global results
   - Four-column ASCII text files
     - Value of parameter varied, computed liftoff length, computed axial location of maximum mean SVF (xmax), computed maximum mean SVF (SVFmax)
       - For variations in initial O_2 with fixed initial ρ and T
         - O2 (%), LOL (mm), xmax (mm), SVFmax (ppm)
         - Example: PSU1_H_14.8RHO_vO2_1000T.dat
       - For variations in initial T with fixed initial ρ and O_2
         - T (K), LOL (mm), xmax (mm), SVFmax (ppm)
         - Example: PSU1_H_14.8RHO_21O2_vT.dat

2. Profiles of mean or rms SVF along the injection axis
   - Two-column ASCII text files
     - Distance from injector tip (mm), computed mean SVF or rms SVF (ppm)
       - Example (mean SVF): PSU1_H_14.8RHO_21O2_1000T_SVFvsX.dat
       - Example (rms SVF): PSU1_H_14.8RHO_21O2_1000T_rmsSVFvsX.dat

3. Radial profiles of mean or rms SVF at specified axial locations
   - Two-column ASCII text files
     - Distance from axis (mm), computed mean SVF or rms SVF (ppm)
       - At xmax (axial location of maximum computed mean soot volume fraction)
         - Example: PSU1_H_14.8RHO_21O2_1000T_SVFvsR_XMAX.dat
       - At +/-10 mm increments in the axial direction wrt/xmax
         - Examples:
           - @ xmax+10 mm: PSU1_H_14.8RHO_21O2_1000T_SVFvsR_XMAXp10.dat
           - @ xmax+20 mm: PSU1_H_14.8RHO_21O2_1000T_SVFvsR_XMAXp20.dat
           - @ xmax-10 mm:
           - PSU1_H_14.8RHO_21O2_1000T_SVFvsR_XMAXm10.dat
           - etc . . .

Data for 2D Contour Plots

Results should be submitted for the quasi-steady flame.

For Spray H, see the mean soot volume fraction data posted on the ECN website, using the open data search utility (http://www.sandia.gov/ecn/cvdata/dsearch.php). Four files are provided there for each operating condition under the "Soot fv" column:

img – a .jpg image file with color contours of mean soot volume fraction; the measured liftoff length is indicated

fv – a .zip file containing an ASCII data file of the 2D mean soot volume fraction data

png-img – an 8-bit .png image file of 2D mean soot volume fraction data

png2fv – a text file explaining how to convert the .png image file into mean soot volume fraction

Modelers who wish to submit computed 2D mean soot volume contours should submit a separate .jpg file for each operating condition. The image should cover the same spatial extent and the same range of mean soot volume fractions as in the corresponding experimental .jpg file. The computed liftoff length should be indicated clearly in the image.

Example: PSU1_H_14.8RHO_21O2_1000T_2DSVF.jpg