**ECN4 TOPIC 6 – EMISSIONS**

**SUBMISSION GUIDELINES**

**Version 141001**

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# INTRODUCTION

ECN 3 included a soot dataset for Spray A and its parametric variants from only one institution. As has been done for ignition delay time, lift-off length, vapor penetration, and other measurements, it is important for the purposes of the ECN to collect measurements of the same combustion indicator/property from several institutions. As such, we admonish all participating institutions who have soot diagnostic capabilities to measure the soot volume fraction (SVF) during the quasi-steady period for Spray A and its parametric variants in ambient temperature. Beyond the collection of quasi-steady soot data, another primary focus of the emissions topic will be on transient soot and PAH characterization and multiple injections using high-speed extinction imaging diagnostics, soot LII, and PAH PLIF. With regard to unburned hydrocarbons (UHC), formaldehyde in the near injector region has been observed using 355-nm PLIF imaging. Under some conditions, the formaldehyde is consumed by a propagating ignition event (see Skeen et al. Proc. Comb. Inst. 2014). At ambient temperatures below 900 K (22.8 kg/m3, 15% O2), a near injector ignition event is not observed suggesting that unburned hydrocarbons may be present. Nitric oxides (NOx) may also be present in the combusting spray under certain conditions, but can be difficult to quantify with optical diagnostics at engine relevant pressures. Gas sampling with offline analysis by time-of-flight mass spectrometry will be performed to characterize UHC and NOx under the Spray A conditions. The presence and fate of these species represents a difficult target for simulation efforts. Thus, simulation submissions to the “Emissions” topic for the Spray A (AR) condition should include an evaluation of UHC and NOx.

# OBJECTIVES

## Experimental objectives

The experimental objectives should be prioritized in the following order.

1. Measurements of SVF under Spray A (n-dodecane) conditions from multiple institutions with injector 370 and a 5 ms injection duration.
2. Measurements of SVF under ambient temperature variants (850 K, 1000 K, 1100 K, 1200 K) of Spray A (n-dodecane) from multiple institutions with injector 370 and a 5 ms injection duration.
3. Time-sequenced images of single shot LII and/or LIF before, during, and after soot onset and through the oxidation/burnout period after EOI (1.5 ms single and 0.5/0.5 dwell/0.5 ms and/or 0.3/0.5 dwell/1.2 ms multiple injections)
4. High-speed soot extinction imaging of the entire single or multiple injection spray event
5. Species characterization in the soot precursor region by probe sampling and offline mass spectrometry for NOx and PAH
6. Species characterization in the near nozzle region after EOI to investigate UHC by probe sampling and offline mass spectrometry (Spray A, 900 K, 800 K)

## Modelling objectives

ECN 3 modeling contributions showed inconsistency in predicting ignition delay times and lift-off lengths. For ECN 4, efforts must be directed at first obtaining good agreement with experiment in ignition delay and lift of length in conjunction with deliverables for Topic 5. Once this is satisfied, further evaluation of soot transients, multiple injections, NOx, and UHC after EOI can proceed. Some effort to establish an ECN standard soot mechanism is also desirable and all modeling should include some level of NOx chemistry. For consistency with Topic 5 Modeling efforts, modelers should use injector 675 characteristics. The modeling objectives should be prioritized in the following order.

1. Minimize inconsistencies between modeled and experimental vapor penetration and mixture fraction field. Minimize inconsistencies between modeled and experimental ignition delay times and lift-off lengths.
2. Provide SVF under Spray A (n-dodecane) conditions 5 ms injection duration.
3. Provide SVF for Spray A under ambient temperature variants (850 K, 1000 K, 1100 K, 1200 K) of Spray A (n-dodecane) 5 ms injection duration.
4. Time-sequence of SVF before, during, and after soot onset and through the oxidation/burnout period after EOI (1.5 ms single and 0.5/0.5 dwell/0.5 ms multiple injections)
5. Time-sequence of SVF through the entire single (1.5 ms) or multiple (0.5/0.5 dwell/0.5 ms and 0.3/0.5 dwell/1.2 ms) injection spray event
6. NOx and PAH levels through entire spray event
7. UHC levels after EOI Spray A density and O2 concentration (800 K), single and multiple injections.

## Analysis objectives

Comparisons between experimental and modeled results for Topic 6 will be straightforward and will rely heavily on analysis efforts in Topic 5. Beyond the combustion indicators investigated in Topic 5, Topic 6 analysis will consider differences in chemical mechanisms describing soot, NOx, and UHC.

# TARGET CONDITIONS

## SPRAY A (baseline + parametric variations)

Target injector for experiments will be 370 because the largest experimental soot database exists for this injector. The target modeling injector will be 675 for consistency with Topic 5. The discharge coefficients for 370 and 675 are nearly identical and consistency among models is deemed more important than consistency between model and experiment. Consistent with Topic 5, injection duration coding will be:

* SHORT = 1.5 ms actual injection duration. This is the standard Spray A injection duration.
* LONG = 5.0 ms actual injection duration. This will be the reference for the analysis of flame evolution, so that steady flame conditions are achieved.
* SHORT2 = 0.5 ms actual injection duration. This will be used as a reference for multiple injection studies.
* MULT1 = 0.5/0.5 dwell/0.5 ms
* MULT2 = 0.3/0.5 dwell/1.2 ms

Consistent with Topic 5, the following coding will be used to indicate the ambient conditions:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ACRONYM | O2 [%] | Ta [K] | Dens [kg/m3] | Pinj [MPa] | Inj Duration |
| AI | 0 | 900 | 22.8 | 150 | LONG |
| AR | **15** | **900** | **22.8** | **150** | **SHORT/LONG/SHORT2/MULT1/MULT2** |
| T5 | 15 | 1200 | 22.8 | 150 | LONG |
| T4 | 15 | 1100 | 22.8 | 150 | LONG |
| T3 | 15 | 1000 | 22.8 | 150 | LONG |
| T2\* | 15 | 850 | 22.8 | 150 | LONG |
| T2 | 15 | 800 | 22.8 | 150 | LONG/SHORT2/MULT1/MULT2 |

Table 1 – Nomenclature for submission of Spray A parametric variations

## SPRAY A – multiple injections

Multiple injections will be investigated according of the recommendations on Spray A parametric variation:

* 0.5 ms pulse/0.5 ms dwell/0.5 ms pulse
* 0.3 ms pulse/0.5 ms dwell/1.2 ms pulse

<http://www.sandia.gov/ecn/cvdata/targetCondition/SprayAParametric.php>

# PARTICULAR RECOMMENDATIONS FOR CALCULATIONS

When performing calculation, the following indications have to be followed:

* INJECTION RATE: Mass flow rate at the nozzle exit from virtual ROI tool from CMT and measured nozzle coefficients (<http://www.cmt.upv.es/ECN03.aspx>).
* CHEMICAL MECHANISM: Recommendations by ECN4 Topic 4 will be followed, but in the mean time, two chemical mechanisms are recommended:
  + Narayanaswamy et al.: a 255 species mechanism (K. Narayanaswamy, P. Pepiot, H. Pitsch, (2013), Combust. Flame (2013), http://dx.doi.org/10.1016/j.combustflame.2013.10.012).
  + Luo et al.: 111 species skeletal mechanism, which was defined as follows:
    - The starting detailed mechanism was Sarathy et al. (S.M. Sarathy, C.K. Westbrook, M. Mehl, W.J. Pitz, C. Togbe, P. Dagaut, H. Wang, M.A. Oehlschlaeger, U. Niemann, K. Seshadri, and others, Combust. Flame 158 (12) (2011) 233-2357).
    - This was reduced to a skeletal mechanism as outlined in Luo et al. (S. Som, D.E. Longman, Z. Luo, M. Plomer, T. Lu, (2011), Three Dimensional Simulations of Diesel Sprays Using n-Dodecane as a Surrogate, Fall Technical Meeting of the Eastern States Section of the Combustion Institute Hosted by the University of Connecticut, Storrs, CT Oct 9-12, 2011).
    - To the skeletal mechanism, OH\* was added (Y. Pei, E.R. Hawkes, S. Kook, G.M. Goldin, T. Lu, (2014), Modelling n-dodecane spray and combustion with the transported probability density function method, Combust.Flame, submitted). Precursor species for CH were also added per Sarathy et al. (S.M. Sarathy, C.K. Westbrook, M. Mehl, W.J. Pitz, C. Togbe, P. Dagaut, H. Wang, M.A. Oehlschlaeger, U. Niemann, K. Seshadri, and others, Combust. Flame 158 (12) (2011) 233-2357).
* TURBULENCE-COMBUSTION INTERACTION (TCI): Each contribution can use a particular TCI model.

## Comparability of mixture fields for spray A

Submissions should follow the guidelines provided for Topic 5, which are included below for reference.

To enable a comparability among TCI and/or chemistry approaches, participants will have to submit the following information for the inert spray A configuration (AI condition from Table 1 with LONG injetion) at an intermediate deadline:

* Spray Tip penetration and maximum liquid length according to the instructions within section 8.1.
* 2D maps of the following variables

|  |  |
| --- | --- |
| Data | ACRONYM |
| Axial velocity (m) | U |
| Radial velocity (m) | V |
| Mixture fraction | Z |
| Temperature (K) | T |
| Density (kg/m3) | RHO |
| Mixture fraction variance | Zvar |
| Turbulence kinetic energy (m2/s2) | K |
| Turbulence kinetic energy dissipation rate (m2/s3) | EPS |

Table 3 – 2D-resolved data required from comparison of spray mixture distribution from modelling

The following conventions should be met:

* 2D (axial-radial) Favre-averaged fields (ensemble averaged if Favre average impossible)
* Spatial discretization: Variables should be interpolated onto a uniform Cartesian mesh with the following discretization
  + Radial: 0 to 20mm; 0.04mm spacing (501 points)
  + Axial: 0 to 100mm; 0.2mm spacing (501 points)
* Time discretization: from 100μs to 7000μs After Start of Injection, each 100μs.

After the comparison is performed, those groups with large departures from the mixing field will have to review their spray models.

# DEADLINES

The following deadlines have been established for Topic 5 and should be followed for Topic 6 submissions:

* Modelling results for Spray A inert spray comparison: March 1st 2015.
* Experimental and modelling results for reacting conditions: June 15th 2015.

# PARTICIPANT LIST

|  |  |  |
| --- | --- | --- |
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Table 4 – Participant list

**APPENDICES**

# APPENDIX 1 – SUBMISSION OF EXPERIMENTAL AND MODELING RESULTS

## Submission of global and Time-resolved Combustion Emissions

The following definitions will be used for the combustion emission measurements and modeling results (for further information check standardization at info at <http://www.sandia.gov/ecn/cvdata/expDiag.php>). Submissions for Topic 6 should follow the guidance provided in Topic 5 for full submission of necessary combustion indicators. Whenever possible, combustion indicators obtained after processing of raw information will be submitted. Details on the standard methods for such purposes can be found at the ECN site (<http://www.sandia.gov/ecn/cvdata/expDiag.php> ).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| TYPE | COMBUSTION INDICATOR | ACRONYM | TECHNIQUE | DEFINITION |
| GLOBAL | Soot volume fraction | SVF | LII | Ensemble average of individual LII images during quasi-steady period of LONG spray combustion event. LII timing should be after spray head has passed through field of view, but before EOI. |
| Extinction Imaging | Measured SVF during quasi-steady period of LONG injection. Time-averaging of LII or soot extinction images should begin after spray head has passed through field of view and should end just prior to EOI |
| Soot onset time | tSOOT | LII/Extinction Imaging | Time at which total measured soot mass exceeds 0.05 µg |
| UHC after EOI | UHC | PLIF and Gas sampling | PLIF provides a qualitative indication of UHC presence/location. Gas sampling hopes to provide a quantitative measure of UHC remaining after EOI |
| Quasi-steady NOx | NOx | Gas sampling | Gas samples extracted from spray centerline during LONG injection Spray A condition analyzed for presence of NOx. |
| Quasi-steady PAH | PAH | Gas samples extracted from spray centerline during LONG injection Spray A condition analyzed for presence of PAH species. |
| TIME-RESOLVED | Time-resolved Soot | trSVF | LII/Extinction Imaging | Time-resolved SVF or KL as measured by LII or Extinction Imaging. |
| Time-resolved NOx | trNOx | Modeled only | Experimental diagnostics not capable of measuring time-resolved NOx. Modeled NOx to be compared among different institutions. |
| Time-resolved PAH | trPAH | Modeled only | Experimental diagnostics not capable of measuring time-resolved PAH. Modeled PAH to be compared among different institutions. |

Table 5 – Experimental definition of Combustion Indicators

The file name depends on the type of information to be submitted

* **Global combustion indicators:** A template Excel file will be provided by coordinators, where only the corresponding values for experimental indicators will be included. The name of the file will follow the structure:

ECN4E\_[GROUP]\_GLOBAL\_[INJECTOR].xls

* **Time-resolved information:** Only one ASCII plain text file per operating condition and combustion indicator will be sent. It will contain two-columns, the first one with the time (ms), and the second with the corresponding indicator. Name and units should be indicated at the first row. File name should follow the structure:

ECN4E\_[GROUP]\_[VAR]\_[INJECTOR]\_[COND]\_[DUR].txt

The following nomenclature has been applied for file names

* + ECN4E identifies the information as an experimental contribution.
  + ECN4M identifies the information as an experimental contribution.
  + GLOBAL identifies the file as containing Global Combustion Indicators.
  + [GROUP] is a string for the submitting group acronym , e.g. TUE
  + [VAR] is a string for the submitted combustion indicator Acronym according to the corresponding column in Table 5.
  + [INJECTOR] is a string for the Spray A Injector number.
  + [COND] is a string for the ambient condition according to Table 1.
  + [DUR] is a string for the injection duration (LONG/SHORT).

Examples:

* ECN4E\_CMT\_GLOBAL\_675.XLS would be a submission from CMT of global indicators obtained in experiments with injector 675.
* ECN4M\_ANL\_GLOBAL\_675.XLS would be a submission from Argonne National Labs of global indicators obtained from simulations with injector 675.

## Spatial- (and time-) resolved variables

For space and time-resolved information (i.e. imaging experiments) it is suggested that ensemble-averaged information is submitted. If possible, standard deviation and sample size (number of injection cycles) should be delivered for each measured parameter.

Whenever possible, a high acquisition rate for experimental should be used (e.g. high speed imaging at rates higher than 20000 fps) so that information is produced at as many time instants as possible. However, if this is not feasible, acquisition should priorize the following timings (in ms ASOI):

* Steady flame 4.5 ms
* Transient soot evolution at onset for Spray A: 50 µs prior to soot onset, then 50 µs increments until 1.0 ms
* Soot at EOI analysis: EOI to EOI+1.0 ms in 0.1 ms steps

It is recommended that data is submitted following the format employed for Rayleigh scattering results shown in

<http://www.sandia.gov/ecn/cvdata/assets/Rayleigh/bkldaAL4mixing.php>

either as a 16-bit png image (with an indication of the maximum value in Physical Units of the corresponding variable, maxImg) or as a zipped ASCII plain text file with accompanying injector coordinates and a vector of axial and radial positions.

File name will follow the convention

ECN4E\_[GROUP]\_[VAR]\_[INJECTOR]\_[COND]\_[DUR]\_[t].png

ECN4E\_[GROUP]\_[VAR]\_[INJECTOR]\_[COND]\_[DUR]\_[t].txt

The following nomenclature has been applied for file names

* + ECN4E identifies the information as an experimental contribution.
  + [GROUP] is a string for the submitting group acronym , e.g. TUE
  + [VAR] is a string for the submitted combustion indicator Acronym according to the corresponding column in Table 5.
  + [INJECTOR] is a string for the Spray A Injector number.
  + [COND] is a string for the ambient condition according to Table 1.
  + [DUR] is a string for the injection duration coding (LONG/SHORT).
  + [t] is a string for the particular timing, in μs after Start of Injection (ASOI).

Examples:

* ECN4E\_SAN\_trSVF\_370\_AR\_LONG\_4000.txt would be a submission from Sandia of the time-resolved soot volume fraction image 4000 us for injector 675, operating conditions of spray A (ambient conditions AR in Table 1) and LONG injection duration.
* For high-speed imaging submissions where movie files are processed and typically converted into Matlab (.mat) files, the .mat file may be submitted with the following convention: ECN4E\_SAN\_trSVF\_370\_AR\_SHORT\_imgs.mat. This filename represents experimental time-resolved SVF results submitted by Sandia using injector 370 under the standard Spray A (AR) condition with the SHORT injection duration.

Attached to each submission, a text file summarizing the particular experimental techniques that have been used has to be sent.

# APPENDIX 2 – SUBMISSION OF MODELLING RESULTS

**DATA FILE STRUCTURE**

The data are to be submitted as described in the guidelines for Topic 5.

**MODELLING SETUP DESCRIPTION**

Following the guidelines for Topic 5, in addition to the data files an Excel file should be submitted that summarizes the information on the particular model:

|  |  |
| --- | --- |
|  |  |
| Code name | KIVA, OpenFOAM, CONVERGE, Fluent, … |
| Turbulence chemistry interaction model | e.g. well-mixed, PDF method, CMC, UFPV, FGM-PDF,… |
| Chemistry model |  |
| Base mechanism | Luo, Narayanaswamy, Faravelli, Pei, … (if other please send also the mech in CHEMKIN format) |
| Chemistry dimensional reduction / acceleration | e.g. ISAT, flamelets, etc |
| Turbulence model | RANS, k-ε, LES etc. |
| Sub-grid or turbulent scalar transport | gradient transport |
| Spray model |  |
| Used Lagrangian discrete phase model (Y/N), If N, then what method? | Y,N |
| Injection | Blob, |
| Atomization & Breakup | KH-RT (with/without break-up length), Huh, KH, Reitz-Diwakar, ... |
| Collision | None, O’Rourke, … |
| Drag | Dynamic,… |
| Evaporation | Spalding, … |
| Heat Transfer | Ranz-Marshall, … |
| Dispersion | None, Stochastic, … |
| Grid |  |
| Dimensionality | e.g. Full-3D domain, 2D axisymmetric, etc |
| Type | e.g. Block structured Cartesian, structured AMR, unstructured, etc |
| Grid size range (mm) | e.g. 0.25 mm - 5mm, … |
| Total grid number | eg 100,000 |
| Time advancement |  |
| Time discretisation scheme | e.g. SIMPLE, PISO, etc |
| Time-step (sec) | 5e-7, variable with max Courant number equal to…, … |

Table 8 – Modelling setup description table