ECN4 TOPIC 3 – EVAPORATIVE DIESEL SPRAY SUBMISSION GUIDELINES

Version 150525

CONTENTS

1 INTRODUCTION

The main focus of activity in the present topic will be the evolution of the spray, and linking spray breakup outcomes to the initial conditions for combustion via vaporization. Analysis will be focused on details of the spray liquid and vapor morphology during the steady portion of injection and on new ECN injectors and conditions, including multiple injections and Sprays C and D.

Prior experimental ECN workshop activities within this topic area have shown inconsistencies in measuring the liquid penetration, or quasi-steady liquid length, between contributing institutions. At ECN1, traditional Mie-scatter measurements were shown to be sensitive to optical setup and a Diffuse Back Illumination (DBI) method was recommended for adoption by all ECN institutions. DBI was adopted by Sandia for ECN2 and later by IFPen for ECN3. Inconsistencies between DBI measurements at the two different institutions were observed. For ECN4, all experimental measurements of liquid length should be performed using DBI so that we can continue to develop an understanding of these inconsistencies and move towards a more uniform measurement methodology.

Prior computational ECN workshop activities within this topic area have shown inconsistencies in the predicted liquid and vapor fraction morphology in regions near the flame lift-off length and upstream to the injector nozzle, even when downstream axial vapor fraction profiles are well matched between institutes (see ECN3 Proceedings, Topic 1.3, Slides 63-70). For ECN4, further analysis on the detailed spray liquid and vapor morphology will be performed to better understand these differences, their impact on predictions of the downstream vapor mixture field, and resulting combustion outcomes via connection to ECN4 topic 5. Thus, we especially seek contributors to this topic who are also performing simulations for topic 5.

2 OBJECTIVES

2.1 Experimental objectives

After three ECN workshops, the experimental database for some of the spray metrics (liquid penetration (LP), quasi-steady liquid length (LL), vapor penetration (VP), vapor phase fuel-air mixture distributions, and velocity) is already fairly large in terms of Spray A conditions. ECN4 experimental objectives will focus on reducing uncertainties in liquid measurement and extending existing measurements to new spray conditions. Specific objectives for ECN4 will include:

1. DBI measurements of LP and LL for Spray A, B, C and/or D (n-dodecane) at non-reacting standard Spray A conditions (0% O_2, 1500 bar, 900 K, 22.8 kg/m^3) from multiple institutions with 1.5 and/or 5 ms injection durations.
2. Measurements of LP and VP for Spray A (n-dodecane) double injection at

non-reacting standard Spray A conditions from multiple institutions (0.5/0.5 dwell/0.5 ms and 0.3/0.5 dwell/1.2 ms).

3. Measurements of LP, VP, and LL for Spray C and D (n-dodecane) at non-reacting standard Spray A conditions from multiple institutions with 1.5 and 5 ms injection durations.
4. Measurements that elucidate phase-transition behavior under standard Spray A conditions.

2.2 Modeling objectives

The modeling objectives proposed for ECN4 will be focused on comparing liquid and vapor predictions between institutions at a higher level of granularity than in previous workshops and on extending code comparisons to new spray conditions. For consistency with Topic 5 Modeling efforts, modelers should use injector 675 characteristics. Specific objectives for ECN4, ordered by priority, will include:

- Evaluate code-to-code differences in detailed spray morphology predictions of Spray A near the liquid length and lift-off length regions for quasi-steady conditions with long injection duration (5 ms). We also wish to extend this comparison effort to Topic 5 to assess the impact of these differences on predicted combustion metrics and highly encourage institutions to participate in both topic areas.
- Evaluate sensitivity of detailed spray morphology predictions for Spray A to parametric variations in operating conditions (temperature, density, injection pressure) for long injection duration (5 ms).
- Predictions of LP and VP for Spray A (n-dodecane) double injection at non-reacting standard Spray A conditions from multiple institutions (0.5/0.5 dwell/0.5 ms and 0.3/0.5 dwell/1.2 ms).
- Seek computational methods to capture fluctuations in LL observed experimentally for Spray B.

3 TARGET CONDITIONS

3.1 SPRAY A (baseline + parametric variations)

The target injector for Spray A modeling efforts will be nozzle 675. Experimental contributions from other injectors are expected and welcome. Two different injection durations will be targeted, namely the “short” standard Spray A condition and a “long” injection duration to study the quasi-steady spray structure. These injection durations are consistent with those being studied in Topics 5 and 6. The naming structure for employed injection duration will be:

- SHORT = 1.5 ms. This is the standard Spray A injection duration.
- LONG = 5.0 ms. This will be the reference for examining the spray structure and mixing field under quasi-steady injection conditions.

All conditions will be non-reacting (0% O_2). The priority for parametric variations follows the order listed in the below table. The following coding will be used to indicate the ambient conditions:

Parametric Variable	ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
Standard Spray "A"	ASTAND	0	900	22.8	150	SHORT/LONG
Temperature	AT1	0	300	22.8	150	LONG
	AT2	0	700	22.8	150	LONG
	AT3	0	1200	22.8	150	LONG
Density	AD1	0	900	7.6	150	LONG
	AD2	0	900	15.2	150	LONG
Injection Pressure	AP1	0	900	22.8	50	LONG
	AP2	0	900	22.8	100	LONG

Table 1 – Nomenclature for submission of Topic 3 Spray A parametric variations.

3.2 SPRAY A – multiple injections

Multiple injections will be investigated according of the recommendations on Spray A parametric variation in terms of actual injection duration:
http://www.sandia.gov/ecn/cvdata/targetCondition/SprayAParametric.php

The following conditions will be investigated:

ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
AMULT1	0	900	22.8	150	0.5 ms pulse - 0.5 ms dwell - 0.5 ms pulse
AMULT2	0	900	22.8	150	0.3 ms pulse - 0.5 ms dwell - 1.2 ms pulse

Table 2 – Nomenclature for submission of Topic 3 Spray A studies with multiple injections

3.3 SPRAY B

The target injector for Spray B modeling efforts will be nozzle 201. Experimental contributions from other injectors are expected and welcome. Only nominal conditions with the short injection will be investigated, as detailed in the following table:

ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
BSTAND	0	900	22.8	150	SHORT

Table 3 – Nomenclature for submission of Topic 3 Spray B studies.

3.4 SPRAY C/D

The target injectors for modeling efforts of Spray C and D will be nozzle 037 and nozzle 134, respectively. Experimental contributions from other injectors are expected and welcome. Only nominal conditions with the short injection will be investigated, as detailed in the following table:

ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
CSTAND	0	900	22.8	150	SHORT
DSTAND	0	900	22.8	150	SHORT

Table 4 – Nomenclature for submission of Topic 3 Spray C and D studies.

4 PARTICULAR RECOMMENDATIONS FOR CALCULATIONS

When performing calculation, the following recommendations should be followed:

- INJECTION RATE: Standard injection rate profiles will be distributed to interested groups to ensure consistency between contributions. Please contact Caroline Genzale (caroline.genzale@me.gatech.edu) to receive a copy of these profiles.
- MINIMUM GRID SIZE: Each contributing group can use a preferred grid to perform any of the requested calculations. However, a minimum grid size of 0.25 mm is required for all submissions.
- MODEL CONSTANTS: Each contributing group should use the same model constants across all simulations (parametric variations, Spray A, B, C, D, etc.).

4.1 Comparability of liquid and vapor mixture fields for spray A

To enable a meaningful comparison among different modeling submissions, metrics such as liquid penetration and liquid volume fraction must be analyzed using consistent calculation methods. The following detailed spray morphology information and calculation methods are summarized below.

- Each contributing institution will provide 2-D maps of the following spray morphology metrics:

Data	ACRONYM
Vapor Mixture Fraction [-]	Z
Path-Averaged Liquid Volume Fraction [-]	LVF
Path-Averaged Droplet Number Density [1/m^3]	N
Path-Averaged Sauter Mean Diameter [μm]	SMD
Projected Liquid Mass Density [μg/mm^2]	PMD
Axial Velocity [m/s]	U
Temperature [K]	T

Table 5 – 2D-resolved modeling data required for detailed comparison of spray mixture distribution.

- 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, 0.1 mm x 0.1 mm in the axial and radial dimensions, respectively.

- Definitions for liquid and vapor mixture field metrics:
  - **Vapor Mixture Fraction:** Local vapor-phase mixture fraction at a 2-D plane along the spray centerline.
  - **Path-Averaged Liquid Volume Fraction:** Integrate the total liquid volume fraction in each data cell (0.1 mm x 0.1 mm face area) through the depth of the spray, collapsing the liquid volume fraction field to a 2-D map. For 2-D computations, assume axisymmetry and then integrate. The path-averaged liquid volume fraction should then be obtained by dividing the path-integrated liquid volume fraction by the path length along which liquid is present.
  - **Path-Averaged Droplet Number Density:** Integrate the total number of droplets in each data cell (0.1 mm x 0.1 mm face area) through the depth of the spray, collapsing the number density field to a 2-D map. For 2-D computations, assume axisymmetry and then integrate. The path-averaged number density [$1/m^3$] should then be obtained by dividing the path-integrated total number of droplets by the path length along which liquid is present.
  - **Path-Averaged Sauter Mean Diameter:** Integrate the SMD of droplets within each data cell (0.1 mm x 0.1 mm face area) through the depth of the spray, collapsing the SMD to a 2-D map. For 2-D computations, assume axisymmetry and then integrate. The path-averaged SMD [μm] should then be obtained by dividing the path-integrated SMD by the path length along which liquid is present.
  - **Projected Liquid Mass Density:** This quantity is desired for the non-evaporating (300 K) Spray A case, for comparison against x-ray data. Projected mass density [$\mu g/mm^2$] should be calculated by determining the apparent liquid density within each data cell (0.1 mm x 0.1 mm face area), integrated through the depth of the spray.

- Liquid and vapor penetration metrics
    - **Liquid Penetration:**
        - Definition: furthest axial position from the nozzle where the path-averaged liquid volume fraction through a 0.5-mm x 0.5-mm path through the spray is 0.15%.
        - Computation: For each 0.1-mm x 0.1-mm data cell, average the 2-D computed Path-Averaged Liquid Volume Fraction for 2 cells surrounding the target cell in each direction (generating an effective 0.5-mm x 0.5-mm averaging area).
    - **Vapor penetration:**
        - Definition: furthest axial position from the nozzle where the fuel mass fraction is 0.1%.

5 DEADLINES

The following deadlines have been established:

- Experimental and modelling results: June 15th 2015.

6 PARTICIPANT LIST

Name	Affiliation(s)	Email
Lyle Pickett	Sandia	lmpicke@sandia.gov
Julien Manin		jmanin@sandia.gov
Raul Payri	CMT	rpayri@mot.upv.es
Jose Pastor		jopasen@mot.upv.es
Gianluca D'Errico	Polimi	gianluca.derrico@polimi.it
Tommaso Luchinni		tommaso.lucchini@polimi.it
Caroline Genzale (coordinator)	GA Tech	caroline.cenzale@me.gatech.edu
Gina Magnotti		gina.magnotti@gatech.edu
Federico Perini	UW	perini@wisc.edu

Table 6 – Participant list

APPENDICES

7 APPENDIX 1 – SUBMISSION OF EXPERIMENTAL RESULTS – DRAFT (TO BE UPDATED SHORTLY)

7.1 Submission of global and Time-resolved Spray Indicators

The following definitions will be used for some of the experiment-based combustion indicators (for further information check standardization at info at http://www.sandia.gov/ecn/cvdata/expDiag.php):

TYPE	SPRAY INDICATOR	ACRONYM	TECHNIQUE	DEFINITION
GLOBAL	Liquid Length	LL	DBI	
TIME-RESOLVED	Liquid Penetration	LP	DBI	
	Vapor Penetration	VP	Schlieren	

Table 7 – Experimental definition of Combustion Indicators

Whenever possible, combustion indicators obtained after processing of raw information will be submitted. Details on the standard processing routines can be found at the ECN site (http://www.sandia.gov/ecn/cvdata/expDiag.php).

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 three columns, the first one with the time (ms), and the second and third with the average and uncertainty of 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.
- 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 7.
- [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 as indicated in Section 3 (LONG/SHORT/SHORT2).

Examples:

- ECN4E_CMT_GLOBAL_675.XLS would be a submission from CMT of global indicators obtained in experiments with injector 675.

- ECN4E_CMT_Sr_675_AR_LONG.txt would be a submission from CMT of the reacting tip penetration for injector 675, operating conditions of spray A (ambient conditions AR in Table 1) and LONG injection duration.

7.2 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 flame evolution: 0.5 – 2 – 3 ms ¡
- SOC analysis: 0.4 to 0.6 ms in 0.01 ms steps
- After EOI analysis: EOI to EOI+1.0 ms in 0.1 ms steps
- Multiple injections: EOI of the first injection to EOI of the second injection 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 describing the corresponding measured variable. This

should be agreed with the Topic coordinator before submission.
  - [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 as indicated in Section 3 (LONG/SHORT/SHORT2).
  - [t] is a string for the particular timing, in μs after Start of Injection (ASOI).

Examples:

- ECN4E_CMT_T2C_675_1_LONG_4000.txt would be a submission from CMT of the 2C temperature at 4000 us for injector 675, operating conditions of spray A (ambient conditions AR in Table 1) and LONG injection duration.

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

8 APPENDIX 2 – SUBMISSION OF MODELING RESULTS

8.1 Global and Time-Resolved Spray Indicators

The following definitions will be used for the modeling-based spray characteristics:

TYPE	SPRAY INDICATOR	ACRONYM	RELATED VARIABLE	DEFINITION
GLOBAL	Quasi-Steady Liquid Length	LL	LPL	Time-averaged value of the LPL during the quasi-steady period.
			LVF	
TIME-RESOLVED	Liquid penetration	LP	LVF	Furthest axial distance where path-averaged LVF is 0.15%. See recommended calculation method in Section 4.1
	Vapor penetration	VP	vapor fuel mass fraction	Furthest axial distance from nozzle where vapor fuel mass fraction is 0.1%

Table 8 – Modeling definitions for Global and Time-Resolved Spray Indicators

Whenever possible, spray parameters obtained after processing of raw information will be submitted. The file name depends on the type of information to be submitted

- **Global spray parameters:** 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:
  ECN4M_[GROUP]_GLOBAL_[INJECTOR].xls
- **Time-resolved information:** Only one ASCII plain text file per operating condition and spray 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:
  ECN4M_[GROUP]_[VAR]_[INJECTOR]_[COND].txt

The following nomenclature has been applied for file names

- ECN4M identifies the information as a modeling contribution.
- GLOBAL identifies the file as containing Global Spray Indicators.
- [GROUP] is a string for the submitting group acronym.
- [VAR] is a string for the submitted Spray Indicator according to the corresponding Acronym column in Table 8.
- [INJECTOR] is a string for the Spray A Injector number.
- [COND] is a string for the ambient condition according to Table 1 through Table 4.

Examples:

- ECN4M_CMT_GLOBAL_675.XLS would be a submission from CMT of global indicators obtained with simulations from injector 675.

- ECN4M_GATECH_VP_675_AMULTI1.txt would be a submission from GA Tech of the vapor penetration from simulations of injector 675, operating conditions of standard spray A using the multiple injection scheme #1 (as specified in Table 2).

8.2 Spatial- (and time-) resolved variables

Full 2-D (axial and radial) maps of the following variables should be submitted for analyses:

2-D Data	ACRONYM
Vapor Mixture Fraction [-]	Z
Path-Averaged Liquid Volume Fraction [-]	LVF
Path-Averaged Droplet Number Density [1/m^3]	N
Path-Averaged Sauter Mean Diameter [μm]	SMD
Projected Liquid Mass Density [μg/mm^2] (300 K condition only)	PMD
Axial Velocity [m/s]	U
Temperature [K]	T

Table 9 – 2D-resolved modeling data required for detailed comparison of spray mixture distribution.

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, 0.1 mm x 0.1 mm in the axial and radial dimensions, respectively.
- Time discretization:
  - For LONG injection cases from 100μs to 7000μs After Start of Injection, each 100μs.
  - For SHORT injection cases from 100μs to 1700μs After Start of Injection, each 100μs.
  - For multiple injection cases, from 100μs to 2000μs After Start of Injection, each 100μs.

DATA FILE STRUCTURE

The data are to be submitted as ASCII plain text, first line should include the variables name according to the nomenclature in Table 9. To enable post-processing, each file line should contain all variables related to one position. The final structure will be:

x[mm], r[mm], Z[-], LVF[-], N[mm^{-3}], SMD[μm], PMD[μg/mm^2], U[m/s], T[K], …
x1, r1, Z, LVF, N, SMD, PMD, U, T,…

x2, r1, Z, LVF, N, SMD, PMD, U, T,…
…
xn, r1, Z, LVF, N, SMD, PMD, U, T,…
x1, r2, Z, LVF, N, SMD, PMD, U, T,…
…
x1, rn, Z, LVF, N, SMD, PMD, U, T,…

Files are expected to be organized in directories such as:

ECN4M_[GROUP]_[INJECTOR]_[COND]

within which individual files should be named:

ECN4M_[GROUP]_[INJECTOR]_[COND]_[t].txt

The following nomenclature has been applied for file names

- ECN4M identifies the information as a modeling contribution.
- [GROUP] is a string for the submitting group acronym.
- [INJECTOR] is a string for the Spray A Injector number.
- [COND] is a string for the operating condition according to Table 1 through Table 4.
- [t] is a string for the particular timing, in μs after Start of Injection (ASOI).

The previous file directory should be submitted in a single compressed file.

Examples of directory/file names:

- ECN4M_POLIMI_675_ASTAND/ECN4M_POLIMI_675_ASTAND_0500.txt
- ECN4M_POLIMI_675_ASTAND/ECN4M_POLIMI_675_ASTAND_1500.txt

corresponds to a submission from POLIMI of CFD modelling results at 0.5 and 1.5 ms ASOI for injector 675, operating conditions of spray A (ambient conditions ASTAND in Table 1).

MODELING SETUP DESCRIPTION

In addition to the data files, an Excel file should be submitted summarizing the information on the particular model:

Code name	KIVA, OpenFOAM, CONVERGE, Fluent, …
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, …
Max 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…, …
CPU (hours)	

Table 10 – Modeling setup description table