ECN4 TOPIC 5 – COMBUSTION SUBMISSION GUIDELINES

Version 150324

CONTENTS

1 INTRODUCTION

The main focus of activity in the present topic will be the evolution of the flame from the very onset of combustion until End of Injection. Additionally, analysis will be started on After End of Injection (EOI) processes and, if possible, on multiple injections. This topic intends to be a natural continuation from ECN3 Topics 2.1 (Combustion Indicators) and 2.2 (Flame structure). Compared to ECN3, a reduced matrix of conditions has been defined. The objective is trying to minimize the effort for generating the data and improving the analysis on the already existing conditions as well as the comparison between experiments and modelling.

2 OBJECTIVES

2.1 Experimental objectives

After three ECN editions, experimental database for some of the flame metrics (Lift-off Length (LOL), Ignition delay (ID), spray tip penetration (sr), Flame Length (FL)) is already fairly large in terms of Spray A conditions. ECN4 Experimental objectives in terms of spray combustion should focus in the following goals:

- Spray A: Provide with time- and space-resolved quantitative parameters for flame descriptions by means of detailed optical techniques (e.g. LIF-type techniques) for baseline Spray A and simple parametric variations.
- Provide with additional experimental contributions of main combustion indicators for conditions other than parametric Spray A variations, which should be compared to the ones already available
    - Spray A, High expansion configuration (low density, low oxygen)
    - Spray A, Multiple injections and after End of Injection (EOI) processes
    - Spray B/C

2.2 Modelling objectives

In terms of modelling, an effort was achieved at ECN3 to normalize the chemical mechanism. However, discrepancies still existed on the predictions of the models, some of which were probably due to the description of the mixing process. The objectives proposed for ECN4 regarding modelling are:

- Evaluate predictability of CFD for Spray A and additional conditions explored.
- Discern influences on reacting spray evolution due to
    - Spray/mixing models.
    - Turbulence Chemistry Interaction (TCI). Interaction is needed with Topic 4 to use a standard chemical mechanism.

2.3 Analysis objectives

Based upon the interaction between both experiments and modelling, understanding of the combustion process should be gained according to the following objectives:

- Baseline Spray A and simple parametric variations: Improve the understanding of
  - Flame structure, i.e. reacting zone spatial distribution (as from OH/CH2O fields, LOL, FL).
  - Flow evolution along the transient evolution during the autoignition and mature flame stages (transient tip penetration, velocity field as from PIV,…).
  - Comparison between inert and reacting spray evolution.
- Efforts will also be devoted to the comparison of baseline Spray A flame structure with the additional conditions/injectors explored, as defined in 2.1 Experimental objectives.

3 TARGET CONDITIONS

3.1 SPRAY A (baseline + parametric variations)

Target injector for Spray A will be nozzle 675 in terms of modeling efforts, although experimental contributions from other injectors are also welcome. Naming for the injection actual 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 the analysis of flame evolution, so that steady flame conditions are achieved.
- SHORT2 = 0.5 ms This will be used as a reference for multiple injection studies.

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**
I2	15	900	22.8	**100**	LONG
T2	15	**800**	22.8	150	LONG
O3	**21**	900	22.8	150	LONG
EX	15	**780**	**14.8**	150	LONG

Table 1 – Nomenclature for submission of Spray A parametric variations

3.2 SPRAY B

Target injector for Spray B will be 201 in terms of modelling, although experimental contributions from other injectors are also welcome. Only nominal conditions with Short

injection will be investigated, as detailed in the following table:
:

ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
BI	0	900	22.8	150	SHORT
BR	**15**	**900**	**22.8**	**150**	**SHORT**

Table 2 – Nomenclature for submission of Spray B parametric variations

3.3 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
MAI	0	900	22.8	150	0.5 ms pulse - 0.5 ms dwell - 0.5 ms pulse
MAR	**15**	**900**	**22.8**	**150**	**0.5 ms pulse - 0.5 ms dwell - 0.5 ms pulse**

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

4 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: Each contributing group can use a preferred mechanism to perform any of the requested calculations. However, a reference case will be compulsory for all groups, namely a calculation with a reference mechanism as defined for Topic 5:
    - 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.

Such a reference calculation will enable a comparison of TURBULENCE-CHEMISTRY INTERACTION (TCI) among different groups.

- TURBULENCE-CHEMISTRY INTERACTION (TCI): Each contribution can use a particular TCI model.

4.1 Comparability of mixture fields for spray A

To enable a meaningful comparison among different modeling submissions regarding TCI and/or chemistry approaches, an analysis will be performed on the mixture fields. For that purpose, 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/m^3)	RHO
Mixture fraction variance	Zvar
Turbulence kinetic energy (m^2/s^2)	K
Turbulence kinetic energy dissipation rate (m^2/s^3)	EPS

Table 4 – 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)

      (if using a smaller mesh, the spacing should be maintained).
- Time discretization: from 100μs to 1500μs 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.

5 DEADLINES

The following deadlines have been established:

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

6 PARTICIPANT LIST

Name	Affiliation(s)	Email
Sibendu Som	Argonne	ssom@anl.gov
Yuanjiang Pei		ypei@anl.gov
Jose M García-Oliver (*)	CMT	jgarciao@mot.upv.es
Michele Bardi	ETH-Zurich	bardi@lav.mavt.ethz.ch
Yuri Wright		wright@lav.mavt.ethz.ch
Gilles Bruneaux	IFPEN	gilles.bruneaux@ifpen.fr
Hubert Baya-Toda		hubert.baya-toda@ifpen.fr
Louis-Marie Malbec		louis-marie.malbec@ifpen.fr
Gianluca D'Errico	Poli. di Milano	gianluca.derrico@polimi.it
Lyle Pickett	Sandia	LMPicke@sandia.gov
Scott Skeen		sskeen@sandia.gov
Bart Somers	TU/e	L.M.T.Somers@tue.nl
Noud Maes		n.c.j.maes@tue.nl
Michele Bolla	UNSW	m.bolla@unsw.edu.au
Evatt Hawkes		evatt.hawkes@unsw.edu.au

Table 5 – Participant list

(*) Topic coordination

APPENDICES

7 APPENDIX 1 – SUBMISSION OF EXPERIMENTAL RESULTS

7.1 Submission of global and Time-resolved Combustion 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	COMBUSTION INDICATOR	ACRONYM	TECHNIQUE	DEFINITION
GLOBAL	Ignition Delay	tSOC	Pressure	First time with a filtered speed-of-sound corrected pressure increase larger than a threshold of 0.025 bar
			Chemiluminescence	First time with a chemiluminescence signal higher than a threshold of 50% the maximum luminosity
			Schlieren	First positive peak in the intensity increase curve (check standardization info)
	Lift-Off Length	LOL	OH*	First location where OH* intensity profile exceeds a value of 50% the knee
			Schlieren	Location where increase in radial width compared to the inert spray exceeds a value of 25% of the maximum value
			OH PLIF	Most upstream axial location of average OH map with a signal higher than a threshold to be defined.
	Flame length	FL	Broadband flame luminosity	Most downstream axial flame boundary higher than a threshold of 10% of maximum intensity
TIME-RESOLVED	Reactive spray penetration	Sr	Schlieren	Same as for inert sprays
	Heat release rate	HRR	Pressure measurement	dP/dt

Table 6 – 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 6.
- [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 MODELLING RESULTS

8.1 Global and Time-resolved Combustion Indicators

The following definitions will be used for the modelling-based combustion indicators:

TYPE	COMBUSTION INDICATOR	ACRONYM	RELATED VARIABLE	DEFINITION
GLOBAL	Ignition Delay	tSOC	OH mass fraction	First time at which Favre-average OH mass fraction reaches 2% of the maximum in the domain after a stable flame is established.
			Temperature rise	Time of maximum rate of rise of maximum temperature
	Lift-Off Length	LOL	OH mass fraction	First axial location of Favre-average OH mass fraction reaching of 2% its maximum in the domain (instantaneous maximum)
	Flame length	FL	Mixture fraction	Maximum distance where mixture fraction on the axis reaches the stoichiometric value
TIME-RESOLVED	Reactive spray penetration	Sr	Mixture fraction	Maximum distance from the nozzle outlet to where mixture fraction is 0.1%
	Heat release rate	HRR	AHRR (Aparent)	dP/dt P = average pressure in the domain
			ChHRR (Chemical)	$\sum \omega_i h_{f,i}^0$

Table 7 – Modelling definition of Combustion Indicators

Whenever possible, combustion indicators obtained after processing of raw information will be submitted. 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:
  ECN4M_[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:
  ECN4M_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR].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 Combustion Indicators.
- [GROUP] is a string for the submitting group acronym.
- [VAR] is a string for the submitted combustion indicator according to the corresponding Acronym 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 with simulations from 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.

8.2 Spatial- (and time-) resolved variables

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

Data	ACRONYM	Comments
n-Dodecane Mass Fraction	YC12	
O2 Mass Fraction	YO2	
CO Mass Fraction	YCO	
CO2 Mass Fraction	YCO2	
OH mass Fraction	YOH	
OH* Mass Fraction	YOHs	Optional
CH2O Mass Fraction	YCH2O	
Axial velocity (m)	U	
Radial velocity (m)	V	
Mixture fraction	Z	
Temperature (K)	T	
Density (kg/m^3)	RHO	
Mixture fraction variance	Zvar	Optional
Turbulence kinetic energy (m^2/s^2)	K	Optional
Turbulence kinetic energy dissipation rate (m^2/s^3)	EPS	Optional
Viscosity (molecular, kg/m/s)	VIS	Optional

Scalar dissipation rate (1/s)	CHI	Optional

Table 8 – 2D-resolved data required from models

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)
      (if using a smaller mesh, the spacing should be maintained).
- 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 8. To enable post-processing, each file line should contain all variables related to one position. The final structure will be:

```
x[m],r[m],U[m/s],V[m/s],Z[-],T[K], YC12,YO2,YCO,YCO2,YOH,YCH2O,YOHs,SVF,…
x1,r1,u,v,Z,T,n-dodec,O2,CO,CO2,OH,CH2O,optionals (e.g. OH*)
x2,r1,u,v,Z,T,n-dodec,O2,CO,CO2,OH,CH2O,optionals (e.g. OH*)
…
xn,r1,u,v,Z,T,n-dodec,O2,CO,CO2,OH,CH2O,optionals (e.g. OH*)
x1,r2,u,v,Z,T,n-dodec,O2,CO,CO2,OH,CH2O,optionals (e.g. OH*)
...
```

Files are expected to be organised in directories such as:

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

within which individual files should be named:

ECN4M_[GROUP]_[INJECTOR]_[COND]_[DUR]_[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.
- [DUR] is a string for the injection duration coding as indicated in Section 3 (LONG/SHORT).
- [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_TUE_675_1_LONG/ECN4M_TUE_675_1_LONG_1000.txt
- ECN4M_TUE_675_1_LONG/ECN4M_TUE_675_1_LONG_4000.txt

corresponds to a submission from TUe of CFD modelling results at 1.0/4.0 ms ASOI for injector 675, operating conditions of spray A (ambient conditions AR in Table 1) and LONG injection duration.

MODELLING 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 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 9 – Modelling setup description table