Engine Combustion Network

ECN 6 - Diesel Combustion Comittee

UNIFIED GUIDELINES FOR:

- Topic 4. Reactions that lead to ignition
- Topic 5. Combustion (lift-off, flame structure) **B Somers (TUe)**, JM Garcia-Oliver (CMT)
- Topic 6. Emissions (soot, NOx, UHC)
- Topic 7. Spray B (diesel) in engines

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Louis-Marie Malbec (IFPEN)

- Topic 8. Fuel effects on compression ignition Yuanjiang Pei (Aramco)





• INTRODUCTION

• TOPICS

- 1. IGNITION SEQUENCE
- 2. FLAME STRUCTURE
- 3. HEAT RELEASE RATE
- 4. MULTIPLE INJECTION
- 5. SOOT
- 6. ENGINES
- 7. FUELS
- OPERATING CONDITIONS
- SOME WORDS ON CFD
- DEADLINES & PARTICIPANTS
- APPENDIX: SUBMISSION INSTRUCTIONS



- General guidelines to include different ECN groups working on **Diesel combustion** topics
 - For each topic:

motivation – objectives – requested info

- Main drivers for ECN6 compared to previous ECN
 - Merging SA/SC/SD analyses
 - How large are differences among modellers regarding HRR?
 - What improvements does LES bring?
 - Consideration of multiple injections under reacting conditions, a highly transient problem



- SA: Large experimental and modelling database
- SC/SD: Experimental database is already available
 - No CFD modelling up to now
 - Interesting test cases due to interaction between evaporation and combustion
- For ECN6, a comparison of SA/SC/SD should be carried out
 - Nozzle diameter could be considered just another parametric variable
 - To keep a reasonable effort, only reference conditions are requested for SC/SD nozzles





- TOPICS
 - 1. IGNITION SEQUENCE
 - 2. FLAME STRUCTURE
 - 3. HEAT RELEASE
 - 4. MULTIPLE INJECTION
 - 5. SOOT
 - 6. ENGINE
 - 7. FUELS



1. IGNITION SEQUENCE

MOTIVATION

- ECN5 has shown important differences among models on ignition location and sequence
- Experiments have shown higher probability for ignition in radial periphery. Head-on view shows a "ring" of ignition for Spray A (C/D as well). What does model show from "head-on" view?
- What is the impact of slight changes in cone angle on early penetration, mixing and therefore ignition?
- Does LES bring new info into the game?

ECN4-Ignition Probability



ECN4-Ignition CFD

Base(**900K**, 15%) Same time instances





OBJECTIVE

- Evaluation of ignition location & timing
 - How similar/different is this picture among nozzles?
 - Sensitivity to cone angle in the spray modelling
- A comparison of Z field before ignition will be carried out (topic 3)

REQUESTED INFO (detailed instructions in appendices)

- Experiments
 - Mixture fraction, location and timing at ignition
 - IFPEN experiments for ECN5 available
 - Other groups doing similar things are welcome
 - Review of ECN experimental database to derive line-of-sight ignition locations
 - Detailed penetration measurements are needed, especially at early timings.
- Model
 - Ignition delay timing
 - Field variables: Time- and spatially resolved species from SOI (Start of Injection) to slightly after SOC (start of combustion)
 - Small variation of cone angle to check sensitivity of ignition to mixing field



2. FLAME STRUCTURE

SA

MOTIVATION

- SA flame structure analysed in detail in past ECN workshops
- Can models capture
 - the transition from SA to SD?
 - Differences between SC/SD?
- Does LES bring in new info?

OBJECTIVE

- Evaluation of accuracy of models for flame structure definition in both small and large nozzles
 - LOL
 - Detailed spatial structure: CH2O, OH fields
 - Z field under reacting conditions



N. Maes et al. / Combustion and Flame 174 (2016) 138-152



- **REQUESTED INFO (**detailed instructions in appendices)
 - Experiments
 - SA/SC/SD: LOL from OH*
 - Time-resolved high-speed OH*, comparison among ECN facilities in progress
 - SC/SD: Detailed spatial structure: CH2O, OH fields
 - Modelling
 - Time-resolved LOL
 - Field variables: Time- and spatially resolved species from start of combustion (SOC) until end of injection (EOI)



MOTIVATION

- How accurate/similar are our modelling approaches in terms of heat release rate (HRR) predictions
 - Important for industry
- Introduced at ECN3, but never considered again
 - Have we improved this picture?



Source: ECN3, Combustion indicators



OBJECTIVE

- Quantification of HRR in SA/SD conditions
 - Comparison among vessels
 - Evaluate differences among models in chemical HRR
- Coordination with Topic 7 (engines)
- **REQUESTED INFO (**detailed instructions in separate doc**)**
 - Experiments
 - Measurements of pressure in constant-volume cells.
 - Modelling
 - Time-resolved chemical HRR (and Pressure, if a constant-volumen vessel is simulated)
 - A coordinated routine has been prepared and will be used to derive HRR from pressure



MOTIVATION

- Usual injection strategy in Diesel engines
- Highly transient compared to single-pulse cases used until now
- Major role of combustion model (mech + TCI) because of the interaction between pulses

• OBJECTIVE

- Evaluation of predictibility of current models with a split injection strategy
 - Pilot 0.5 ms , dwell 0.3/0.5/0.7 ms, main 0.5 ms
- Coordination with Topic 3 (spray mixing)



4. MULTIPLE INJECTION

- **REQUESTED INFO (**detailed instructions in appendices**)**
 - Experiments
 - Detailed penetration (schlieren)
 - LOL/ID as from OH*
 - Simulations
 - Time-resolved LOL
 - Field variables: Time- and spatially resolved species from start of combustion (SOC) until end of second injection (EOI2)



MOTIVATION

- Expanding on work from ECN5 with O2/N2 vs EGR (pre-burn) conditions for Spray A
- **REQUESTED INFO (**detailed instructions in appendices)
 - Time-resolved field variables (consistent with Ignition/Flame structure submission)
 - Everyone must use the SAME chemical mechanism for their primary submission of the Standard Spray A condition and the O2/N2 condition.



MOTIVATION

- Progress towards predictive models in engine environment.
- Understand and model the effects of confinement, aerodynamics, and real engine opration (Diesel fuel, multihole nozzles, multi injections) on mixing and combustion processes.

• OBJECTIVE

- Study the effect of geometry and flow on mixing /combustion processes
- **REQUESTED INFO** (detailed instructions in appendices)
 - Basic metrics of the spray in engine: liquid length, vapor penetration, lift-off length, ignition delay.
 - Additional: same data in free jet configuration.
 - CFD: Time resolved fields variables



7. FUELS

MOTIVATION

 Understand the fuel effects on spray at CI conditions as an additional dimension for model development and validation

• OBJECTIVE

Summarize the available experimental and computational fuel effect studies for future directions

REQUESTED INFO

 For both experiments and simulations for two or more fuels (different physical or/and chemical properties) at one of the following conditions - Spray A, C or D





REQUESTED INFO

- Fuels used, with physical and chemical (e.g., cetane or RON number) properties
- In nozzle flow:
 - Needle lift for different fuels
 - Cavitation comparison (mainly for simulations)
- Non-reacting spray at different ambient T conditions:
 - liquid length/vapor penetration length vs. time
 - Mixing field (fuel mass fraction) at different timing if available
- Reacting spray at different ambient T conditions:
 - Ignition delay and lift-off length
 - OH* contour
 - Soot mass vs. Time or other available data
- Please use the ECN definitions, if different, please specify



• NOMINAL TEST MATRIX

PARAMETRIC		02	Та	Dens	Pinj	Inj Duration
VARIABLE	ACRONTIVI	[%]	[K]	[kg/m3]	[MPa]	
Standard Spray A	Ai	0	900	22.8	150	LONG
Stanuaru Spray A	Ar	15	900	22.8	150	LONG
Temperature	T2	15	800	22.8	150	LONG
	11	15	900	22.8	100	LONG
injection pressure	12	15	900	22.8	50	LONG
	MAI/MAI2	0	900	22.8	150	0.5 ms pulse - 0.5/0.7 ms dwell - 0.5 ms pulse
	MAR/MAR2	15	900	22.8	150	0.5 ms pulse - 0.5/0.7 ms dwell - 0.5 ms pulse

– Ambient composition:

- Non-EGR: XO2=15%, XN2=85%
- EGR(pre-burn): XO2= 15%, XN2=75.15%, XCO2=6.23%, XH2O= 3.62%

Combustion Committee Guidelines – ECN6



- SPRAY IN VESSELS
 - Long injection (except for multiple injection): 5 ms
 - Priorities for each topic
 - IGNITION SEQUENCE / HRR / Soot
 - Nozzle: SA/SC/SD
 - Conditions: SA (EGR/non-EGR) + T2 (800K)
 - FLAME STRUCTURE / Soot
 - Nozzle: SA/SD
 - Conditions: SA (EGR/non-EGR)
 - MULTIPLE INJECTIONS
 - Nozzle: SA
 - Conditions: MAI/MAR



• SPRAY IN ENGINES

- Injection duration: 1.5ms
- Spray B
- Variations
 - Temperature: 800K and 1000K
 - Injection pressure: 50 and 150MPa
 - Density: 15.2kg/m3
 - %O2: 13% and 21%
 - Swirl or engine speed
 - Notes:
 - These conditions are for TDC
 - SOI: near TDC
- Geometry: engine (+free jet if possible)
- If possible, variable liquid angle



- TCI model
 - Reference well-mixed
 - Each participant can additionally submit calculations with a particular TCI closure

Chemical mechanism

– Reference (ALL groups should use):

T. Yao, Y. Pei, B.-J. Zhong, S. Som, T. Lu, et al., A compact skeletal mechanism for n-dodecane with optimized semi-global low-temperature chemistry for diesel engine simulations, Fuel 191 (2017) 339-349.

 Additional submissions with a different chemical mechanism are welcome, but not required.



- RANS vs LES
 - Reference RANS
 - LES submissions are welcome
- Soot models
 - Reference (ALL groups should use):
 K.M. Leung, R.P. Lindstedt, W.P. Jones, A simplified reaction mechanism for soot formation in nonpremixed flames, Combustion and Flame (1991) 87(3–4) 289-305



SOME WORDS ON CFD

SUBMISSION OF MODELLING FIELD VARIABLES

- Field variables to be reported:

Data	ACRONYM	
Axial velocity (m/s)	U	
Radial velocity (m/s)	V	
Mixture fraction	Z	
Temperature (K)	Т	
Density (kg/m ³)	RHO	
Mixture fraction variance	Zvar	OPTIONAL
Turbulence kinetic	К	OPTIONAL
energy (m ² /s ²)		
Turbulence kinetic	EPS	OPTIONAL
energy dissipation rate		
(m²/s³)		
Viscosity	VIS	OPTIONAL
(molecular, kg/m/s)		
Viscosity	VIST	OPTIONAL
(turbulent, kg/m/s)		
Scalar dissipation rate	CHI	OPTIONAL
(1/s)		

MORE DETAILS IN APPENDICES

Data	ACRONYM
	YC12H26
	YO2
	YCO2
	YH2O
	YCO
Species mass fraction	YCH2O
Species mass fraction (kgi/kg)	YOH
	YCH
	YH
	YO
	YC3H3
	YHCO
	YC2H2
	ώC12H26
	ώYO2
	ώYCO2
	ώYH2O
	ώYCO
Production/destruction rate	ώYCH2O
of species (kgi/m3/s)	ώYOH
	ώYCH
	ώYΗ
	ώYO
	ώYC3H3
	ώΥΗϹΟ
	ώYC2H2
Soot Volume Fraction	SVF

Combustion Committee Guidelines – ECN6



SOME WORDS ON CFD

SUBMISSION OF MODELLING FIELD VARIABLES

MORE DETAILS IN APPENDICES

- Time discretization:
 - From Start of Injection (SOI) until 100 μ s after Start of Combustion (SOC+100) field variables should be reported with $\Delta t = 10 \ \mu$ s
 - From 100 μ s after SOC until End of Injection (EOI) field variables should be reported with $\Delta t = 50 \ \mu$ s
- Spatial resolution: Uniform Cartesian mesh
 - 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).



- SUBMISSION DEADLINES
 - All the requested information should be submitted by Monday June 18th 2018
- PARTICIPANTS

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Engine Combustion Network

APPENDIX: SUBMISSION INSTRUCTIONS ECN6 TOPIC 4/5/6/7/8

The following Appendix complements the Guidelines document with the instructions related to the submission of data for ECN6 related to the following topics:

- Topic 4: Reactions that lead to ignition.
- Topic 5: Combustion (lift-off length, flame structure).
- Topic 6. Emissions (soot, NOx, UHC).
- Topic 7. Spray B (diesel) in engines.
- Topic 8. Fuel effects on compression ignition.

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1 TARGET CONDITIONS

Target conditions for experiments will be defined in terms of a nozzle, injection and ambient conditions. The reference ambient conditions will be the same as in ECN4/5.

PARAMETRIC VARIABLE	ACRONYM	O2 [%]	Та [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
Standard Spray A	Ai	0	900	22.8	150	LONG
Stanuaru Spray A	Ar	15	900	22.8	150	LONG
Temperature	T2	15	800	22.8	150	LONG
Injection pressure	l1	15	900	22.8	100	LONG
	12	15	900	22.8	50	LONG
Multiple injection	MAI/MAI2	0	900	22.8	150	0.5 ms pulse - 0.5/0.7 ms dwell - 0.5 ms pulse
Multiple injection	MAR/MAR2	15	900	22.8	150	0.5 ms pulse - 0.5/0.7 ms dwell - 0.5 ms pulse

Table 1 – Nomenclature for submission of Spray A parametric variations. Conditions with acronym in smaller font are low priority, which will be mainly used to assess global combustion indicators (i.e. ID/LOL), but no 2D data will be requested.

Naming for the injection actual duration will be:

• LONG = 5.0 ms; This will be the reference for the analysis of flame evolution, so that steady flame conditions are achieved.

Target injectors (characteristics and reference data in Table 2)

- For Spray A cases the target will be nozzle 675 or 370 in terms of modeling efforts, which have similar injection characteristics. However, experimental contributions from other injectors are also welcome.
- For Spray C and D cases the target injector are respectively Nozzle #037 and #134.

To simplify data handling, the nomenclature of a given experimental condition for single injection cases will be:

NOZZLE – OPERATING CONDITION – INJECTION DURATION While for multiple injection cases the nomenclature will be simplified to: NOZZLE – OPERATING CONDITION

For example, a test with Spray A injector for the reference inert/reacting condition will be named as:

A-Ai-LONG A-Ar-LONG



While the same operating conditions for Spray C injector will be named as: C-Ai-LONG D-Ar-LONG

More specific directions on file naming conventions can be found in Appendices.

Nozzle Type	Ref Nozzle	Ref Nozzle Diameter	Ref Mass Flow Rate	Hydraulic parameters (Ca, Cv)	Reference results (VP, LP, velocities, Mixing)
Spray A	675	93 (APS 7BM) 89.4 (μscope)	CMT VIM	Available and described in AAS 22(12), 1011-1052	VP and LP available from Sandia/IFPEN CMT/Tue etc. Available mixing field for 677 and velocities for (IFPEN exp to be checked).
Spray C	037	207 (APS 7BM) 208 (µscope)	Measured by CMT Payri et al, Fuel 180 (2016) A reference educated injection rate can be downloaded from CMT website.		Available VP and LP in Westlye et al SAE 2016-01- 0860
Spray D	134	188 (APS 7BM) 188 (µscope)			

Table 2 – Reference nozzle and data.



1.1 Specificities for TOPIC 7: Spray B in Engines

For this topic, the target conditions are specific. Also, to clarify, the following acronyms will be used regarding injection parameters:

- Start of Solenoïd Energizing (SSE): crankangle (absolute values, combustion TDC at 360cad) of the electric command of the injection.
- Start of Injection (SOI): crankangle (absolute values, combustion TDC at 360cad) of the effective fuel delivery (when liquid first exits the orifice).
- Duration of Solenoïd Energizing (DSE): Duration (in ms) of the electrical command of the injection.

PARAMETRIC VARIABLE	REACTIVITY (Inert or Reacting)	ACRONYM	O2 [%]	Ta [K]	Dens [kq/m3]	Pinj [MPa]	DSE (DOI) [ms]	SSE ¹ [cad]
Standard Spray	I	STAND	0	900	22.8	150	0.795 (1.5)	355
B	R	STAND	15	900	22.8	150	0.795 (1.5)	355
	I	TEMP0800	0	800	22.8	150	0.795 (1.5)	355
Tomporaturo	I	TEMP1000	0	1000	22.8	150	0.795 (1.5)	355
remperature	R	TEMP0800	15	800	22.8	150	0.795 (1.5)	355
	R	TEMP1000	15	1000	22.8	150	0.795 (1.5)	355
Donaity	I	DENS15.2	0	900	15.2	150	0.795 (1.5)	355
Density	R	DENS15.2	15	900	15.2	150	0.795 (1.5)	355
	I	PRAIL100	0	900	22.8	100	0.795 (1.5)	355
Injection	I	PRAIL050	0	900	22.8	50	0.795 (1.5)	355
pressure	R	PRAIL100	15	900	22.8	100	0.795 (1.5)	355
	R	PRAIL050	15	900	22.8	50	0.795 (1.5)	355
Oxygen	R	O13	13	900	22.8	50	0.795 (1.5)	355
concentration (%vol.)	R	O21	21	900	22.8	50	0.795 (1.5)	355
Engine speed / swirl	No targe mod	t value, but the dification of the	ese pa e flow a	rameter affects r	s can be v nixing and	aried in c	order observe ion processes	how a

• Duration of Injection (DOI):in ms, effective duration of the fuel delivery.

Table 3 - Nomenclature for submission of Spray B parametric variations.

- Requirements:
 - The thermodynamic conditions are targeted at TDC. On the engine, the recommended method to estimate TDC temperature / density is to consider an isentropic compression between BDC and TDC.

¹ This is indicative : the idea is to have start of combustion near the TDC, and can be adapted depending on the engine speed.



- Nozzle tip temperature: in the absence of adapted cooling system => no requirement
- Initial velocities: depend upon the engine speed and intake port geometry => no requirement.
- If possible, variable liquid angle should be specified as a boundary condition for modelers (see image below, from SAE paper 2015-01-0946)

For modeling, in order to use modeling results to bring a better understanding to experimental results, the injector to be modeled is the one that was installed on the engine. All the information can be found here: <u>https://ecn.sandia.gov/diesel-spray-combustion/target-condition/spray-b-nozzle-geometry/</u>.



Also, for a better comparison between engine and vessel, institutions are asked to perform their experiment / simulations both in engine and vessel configuration, when possible.



2 SUBMISSION OF EXPERIMENTAL RESULTS

2.1 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
		tSOC	Pressure	First time with a filtered speed- of-sound corrected pressure increase larger than a threshold of 0.025 bar
	Ignition Delay		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)
GLOBAL	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 4 – 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 (<u>http://www.sandia.gov/ecn/cvdata/expDiag.php</u>).



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:

ECN6E_[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:

ECN6E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR].txt

The following nomenclature has been applied for file names

- \circ ECN6E identifies the information as an experimental contribution for ECN6.
- 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 4.
- [INJECTOR] is a string for the Nozzle + Injector reference 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 1 (LONG/SHORT/SHORT2).

Examples:

- ECN6E_CMT_GLOBAL_SA210675.XLS would be a submission from CMT of global indicators obtained in experiments with SA nozzle, injector number 675.
- ECN6E_CMT_GLOBAL_SC210003.XLS would be a submission from CMT of global indicators obtained in experiments with SC nozzle, injector number 210003.
- ECN6E_CMT_Sr_SA210675_AR_LONG.txt would be a submission from CMT of the reacting tip penetrtion for Spray A injector 675, nominal operating conditions (ambient conditions AR in Table 1) and LONG injection duration.
- ECN6E_CMT_Sr_ SC210003_AR_LONG.txt would be a submission from CMT of the reacting tip penetration for Spray C injector 210003, nominal operating conditions (ambient conditions AR in Table 1) and LONG injection duration.



2.2 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 j
- 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

ECN6E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t].png

ECN6E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t].txt

The following nomenclature has been applied for file names

- ECN6E identifies the information as an experimental contribution for ECN6.
- o [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 Nozzle + Injector reference 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 1 (LONG/SHORT/SHORT2).
- \circ [t] is a string for the particular timing, in μ s after Start of Injection (ASOI).

Examples:

• ECN6E_CMT_T2C_SA210675_1_LONG_4000.txt would be a submission from CMT of the 2C temperature at 4000 us for Spray A injector 210675, nominal



operating conditions (ambient conditions AR in Table 1) and LONG injection duration.

• ECN6E_CMT_T2C_SC210003_1_LONG_4000.txt would be a submission from CMT of the 2C temperature at 4000 us for Spray C injector 21003, nominal operating conditions (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.



2.3 Specificities for TOPIC 7: Spray B in Engines

In addition to reactive conditions data described in Table 4, some additional data relative to inert conditions are demanded and listed in Table 5. File name will follow almost the same convention:

ECN6E_[FACILITY]_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t]

- [FACILITY] ENG for engines, VSL for vessels
- [COND]: is a string for the ambient condition according to Table 3 (examples: reacting .condition at 800K gives R_TEMP0800; inert condition at prail 100MPa and 15.2kg/m3 gives I_PRAIL100_DENS15.2). If relevant, engine speed and swirl values can be added (_SP1200_SW2.5 for example)

Note: Injection duration (DOI) is 1.5ms, corresponding to SHORT.

TYPE	COMBUSTION INDICATOR	ACRONYM	TECHNIQUE	DEFINITION
GLOBAL	Liquid length (steady) [mm]	LL	Mie scattering	Pickett, Lyle M, et al. (2011) Measurement Uncertainty of Liquid Penetration in Evaporating Diesel Sprays. In : ILASS Americas, 23rd Annual Conference on Liquid Atomization and Spray Systems.
			Diffused backlit illumination	Extinction profile of the average image + Extinction decay extrapolation. As described by Manin et AL COMODIA 2012 Averaging time window 2-4 ms ASOI
TIME- RESOLVED	Liquid phase penetration [mm]	LP	Mie scattering	Pickett, Lyle M, et al. (2011) Measurement Uncertainty of Liquid Penetration in Evaporating Diesel Sprays. In : ILASS Americas, 23rd Annual Conference on Liquid Atomization and Spray Systems.
		LP	Diffused backlit illumination Light extinction threshold (0.6) Leading edge of the contour.	Liquid phase penetration [mm] LP Diffused backlit illumination Light extinction threshold (0.6) Leading edge of the contour.
	Vapor	Si/Sr	Schlieren	Image processing available on ECN web page
	penetration	10/10	Volume LIF / IR imaging	No standardization yet.

Table 5 – Additional experimental date required for TOPIC 7.



3 SUBMISSION OF MODELLING RESULTS

3.1 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	tSOCOH	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. +axial, radial and mixture-fraction location of this point.
		tSOCT	Temperature	Time of maximum rate of temperature rise, + axial, radial and mixture-fraction location of this point.
TIME- RESOLVED	Lift-off-length	LOL	OH mass fraction	Location where Favre-average OH mass fraction reached 14% its maximum in the domain (instantaneous maximum). Please submit axial, radial, and mixture- fraction location of this point + axial velocity.
	Reactive spray penetration	Sr	Mixture fraction	Maximum distance from the nozzle outlet to where mixture fraction is 0.1%

Table 6 - Modeling 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:** Provide in any format that is easy to understand. It should clearly identify which condition is modeled, what model, and what group.
- **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:

ECN6M_[GROUP]_[CHEM]_[TCI]_[VAR]_[INJECTOR]_[COND]_[DUR].txt

The following nomenclature has been applied for file names

• ECN6M identifies the information as a modeling contribution for ECN6.



- 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 the corresponding tables defining the combustion indicators (ID, LOL...).
- [INJECTOR] is a string for the Nozzle + Injector reference number.
- [COND] is a string for the ambient condition according to Table 2.
- [DUR] is a string for the injection duration coding as indicated in Section 1 (LONG/SHORT/SHORT2).
- o [CHEM] denotes the chemistry model (e.g. Cai, Yao, Polimi)
- [TCI] denotes the TCI model, (e.g. WM, TPDF/CMC, etc)



3.2 Spatial- (and time-) resolved variables

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

Data	ACRONYM	Comments
Axial velocity (m/s)	U	
Radial velocity (m/s)	V	
Mixture fraction	Z	
Temperature (K)	Т	
Density (kg/m ³)	RHO	
	YC12H26	
	YO2	
	YCO2	
	YH2O	
	YCO	
	YCH2O	
Species mass fraction (kgi/kg)	YOH	
	YCH	
	YH	
	YO	
	YC3H3	
	YHCO	
	YC2H2	
	ώC12H26	
	ώYO2	
	ώYCO2	
	ώYH2O	
	ώYCO	
	ώYCH2O	
Production/destruction rate of	ώYOH	
species (kgi/m3/s)	ώYCH	
	ώYΗ	
	ώYO	
	ώYC3H3	
	ώYHCO	
	ώYC2H2	
Soot Volume Fraction	SVF	Required for topic 6,
		optional for 4/5
Mixture fraction variance	Zvar	Optional
Turbulence kinetic energy (m ² /s ²)	K	Optional
Turbulence kinetic energy	EPS	Optional
dissipation rate (m ² /s ³)		-
Viscosity	VIS	Optional
(molecular, kg/m/s)		
Viscosity	VIST	Optional
(turbulent, kg/m/s)		
Scalar dissipation rate (1/s)	CHI	Optional

Table 7 - 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 10µs step in the following intervals:
 - \circ For LONG injection cases to 7000µs After Start of Injection;
 - \circ For SHORT injection cases to 2500µs After Start of Injection.

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 7. 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],RHO[kg/m3],YC12H26,YO2,YCO2,YH2O,YCO,YCH2O,YOH,YH,YO,YC3H3,YC 2H2, optionals (SVF, WC12H26[kg/m3/s], WO2[kg/m3/s], WCO2[kg/m3/s], WH2O[kg/m3/s], WCO[kg/m3/s], WCH2O[kg/m3/s], WOH[kg/m3/s], WH[kg/m3/s], WO[kg/m3/s], WC3H3[kg/m3/s], WC2H2[kg/m3/s]...)

x1,r1,u,v,Z,T,RHO, YC12H26,YO2,YCO2,YH2O,YCO,... optionals (e.g. SVF...) **x2,r1**,u,v,Z,T,RHO, YC12H26,YO2,YCO2,YH2O,YCO,... optionals (e.g. SVF...)

xn,r1,u,v,Z,T,RHO, YC12H26,YO2,YCO2,YH2O,YCO,... optionals (e.g. SVF...) **x1,r2**,u,v,Z,T,RHO, YC12H26,YO2,YCO2,YH2O,YCO,... optionals (e.g. SVF...) ...

Files are expected to be organised in directories such as:

ECN6M_[GROUP]_[CHEM]_[TCI]_[INJECTOR]_[COND]_[DUR] within which individual files should be named:

ECN6M_[GROUP]_[CHEM]_[TCI]_[INJECTOR]_[COND]_[DUR]_[t].txt The following nomenclature has been applied for file names

- ECN6M identifies the information as a modeling contribution for ECN6.
- [GROUP] is a string for the submitting group acronym.
- [INJECTOR] is a string for the Nozzle + Injector reference number.
- [COND] is a string for the operating condition according to Table 2.
- [DUR] is a string for the injection duration coding as indicated in Section 1 (LONG/SHORT).



- \circ [t] is a string for the particular timing, in μ s after Start of Injection (ASOI).
- o [CHEM] denotes the chemistry model (e.g. Cai, Yao, Polimi)
- [TCI] denotes the TCI model, (e.g. WM, TPDF/CMC, etc)

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

Examples of directory/file names:

- ECN6M_TUE_CAI_FGM_SA210675_AR_LONG/ECN5M_TUE_675_SA210675_AR_LONG_100 0.txt
- ECN6M_TUE_CAI_FGM_SA210675_AR_LONG/ECN5M_TUE_SA210675_AR_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 2 and LONG injection duration).



3.3 Specificities for TOPIC 7: Spray B in Engines

In addition to reactive conditions data described in Table 6Table 4, some additional data relative to inert conditions are demanded and listed in Table 8.

File name will follow almost the same convention:

ECN6E_[FACILITY]_[GROUP]_[CHEM]_[TCI]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t]

- [FACILITY] ENG for engines, VSL for vessels
- [COND]: is a string for the ambient condition according to Table 3 (examples: reacting .condition at 800K gives R_TEMP0800; inert condition at prail 100MPa and 15.2kg/m3 gives I_PRAIL100_DENS15.2). If relevant, engine speed and swirl values can be added (_SP1200_SW2.5 for example)

Note: Injection duration (DOI) is 1.5ms, corresponding to SHORT.

TYPE	COMBUSTION INDICATOR	ACRONYM	DEFINITION
GLOBAL	Liquid length (steady) [mm]	LL	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). Time average between 2-4 ms ASOI
TIME- RESOLVED	Liquid phase penetration [mm]	LP	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 [mm]	Si/Sr	Definition: furthest axial position from the nozzle where the fuel mass fraction is 0.1%.
	Apparent Heat release rate [W]	AHRR	Computed from pressure.
	Chemical Heat Release Rate [W]	ChHRR	Computed from reaction rate

Table 8 - Modeling definition of mixing/combustion indicators added for TOPIC 7.



3.4 Modelling setup description

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

PARAMETER	DESCRIPTION EXAMPLES			
Code name	KIVA, OpenFOAM, CONVERGE, Fluent,			
Turbulence chemistry interaction model	e.g. well-mixed, PDF method, CMC, UFPV, FGM-PDF, if you have TCI variants, describe each			
Turbulence model	RANS, k-ε, LES etc.			
Sub-grid or turbulent scalar transport; provide Sc_t	gradient transport, 0.7			
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			
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			
Туре	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 – Modeling setup description table