



ECN3 TOPIC 2 – MIXING-CHEMISTRY INTERACTION SUBMISSION GUIDELINES

Version 140228



CONTENTS

1	INTRODUCTION.....	4
1.1	OBJECTIVES.....	4
1.2	GENERAL RECOMMENDATIONS FOR EXPERIMENTS.....	5
1.3	GENERAL RECOMMENDATIONS FOR CALCULATIONS.....	6
2	SUBTOPIC 2.1 – COMBUSTION INDICATORS.....	9
2.1	COORDINATORS.....	9
2.2	OVERALL OBJECTIVES	9
2.3	OVERARCHING QUESTIONS TO BE ADDRESSED	9
2.4	COMBUSTION INDICATOR DEFINITIONS.....	9
2.4.1	Experimental definitions.....	10
2.4.2	Modelling definitions	11
2.5	TEST MATRIX	11
2.6	DATA NEEDED.....	12
3	SUBTOPIC 2.2 – FLAME STRUCTURE.....	14
3.1	COORDINATORS.....	14
3.2	OVERALL OBJECTIVES	14
3.3	OVERARCHING QUESTIONS TO BE ANSWERED	15
3.4	TEST MATRIX	15
3.5	DATA NEEDED.....	15
4	SUBTOPIC 2.3 – SOOT FIELD.....	18
4.1	COORDINATORS.....	18
4.2	OVERALL OBJECTIVES	18
4.3	SPECIFIC QUESTIONS	18
4.4	TEST MATRIX	19
4.5	DATA NEEDED.....	19
5	SUBMISSION IN PRACTICE.....	24
5.1	GENERAL ASPECTS	24
5.2	SUBMISSION OF EXPERIMENTAL RESULTS.....	26



5.2.1	Global and Time-resolved Combustion Indicators	26
5.2.2	Spatial- (and time-) resolved variables	26
5.2.3	Raw information.....	27
5.3	SUBMISSION OF MODELLING RESULTS	29
5.3.1	Global and Time-resolved Combustion Indicators	29
5.3.2	Spatial- (and time-) resolved variables	30
6	REFERENCES.....	34
7	APPENDICES.....	36
7.1	CHEMICAL MECHANISM VALIDATION	36



1 INTRODUCTION

The present document summarizes the instructions for contributions to the ECN3 Workshop within Topic 2 'Mixing-Chemistry interaction', which deals with combustion-related processes within Diesel sprays. This session has been divided into the following Sub-topics:

- Subtopic 2.1. Combustion indicators (Section 2):
 - Definition of quantitative parameters that can serve for a global description of the combustion process
 - Ignition Delay
 - Lift-off Length
 - Flame length
 - Reactive Spray Penetration
 - Heat Release Rate
 - Comparison of results obtained for the different quantitative parameters both from experiments and models so that
 - Experiments in different groups can be compared
 - Experiments with different techniques can be compared
 - Modelling approaches can be compared
- Subtopic 2.2. Flame structure (Section 3):
 - Analysis of flame structure in terms of the following stages
 - Ignition and early flame
 - Mature flame
 - Burnout phase
- Subtopic 2.3. Soot field (Section 4):
 - Analysis of soot results within the flame

The document is divided into 5 Sections. This Introduction will describe general issues related to the whole Topic 2. Sections 2 to 4 give an *Extended Definition* of the three Subtopics. Section 5 contains the particular recommendations for the submission of information.

1.1 OBJECTIVES

The definition of the present guidelines should enable reaching the following goals:

- Experiments
 - To enable the comparison (reproducibility, scattering) among the submitted contributions at different levels
 - Experimental facility
 - Injector



- Experimental technique
 - To deliver data to be compared with calculations with a two-fold objective
 - Calibration
 - Validation
- Calculations
 - To enable the comparison (reproducibility, scattering) among the submitted contributions at different levels
 - Numerics
 - Turbulence-Chemistry Interaction (TCI) model
 - Soot model
 - To deliver predictions that should be comparable to experiments
 - Validation of model hypotheses/simplifications
- Both experiments and calculations
 - To deliver information that helps understand physical and chemical phenomena behind flame ignition and evolution

1.2 GENERAL RECOMMENDATIONS FOR EXPERIMENTS

While ignition delay and lift-off length were the main topics related to combustion within ECN2, ECN3 should provide more detailed validation of reacting spray parameters (i.e. spatially-resolved information). The following information is expected to be delivered from the different experimental techniques:

TECHNIQUE	RAW INFO	SPATIAL/TIME RESOLVED	GLOBAL
Pressure signal	Pressure trace	Heat release (t)	τ SOC
Broadband Radiation (PD, PMT/Imaging)	filtered flame PD,PMT record /Image	Radiation (t), LOL(t) Flame-front penetration (t)	τ SOC LOL _{avg} FL
OH*/CH ₂ O* Chemiluminescence	Long exposure/time resolved OH*/ CH ₂ O* rad. image	LOL(t)	LOL _{avg}
Schlieren	Schlieren images	Penetration (t) LOL(t)	τ SOC
OH LIF	OH image	OH(t,x,r)	Flame reaction zone
CH ₂ O LIF	CH ₂ O image	CH ₂ O (t,x,r)	Low Temperature τ SOC
PIV	Velocity field	U,V (t,x,r)	
Extinction (PD/Imaging)	Optical attenuation field	SVF(t,x,r)	
LII	LII signal field	SVF(t,x,r)	



2Color	Incandescence imaging	T(t,x,r) KL2C(t,x,r)	
Soot sampling		Soot morphology	

Table 1 – Overview of experimental contributions to ECN3

Standardization information is available at ECN webpage

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

for the following techniques

- Ignition delay:
 - Light-based (chemiluminescence)
 - Pressure-based
- Lift-off length by OH* imaging
- Soot by laser extinction and LII
- Schlieren under reactive conditions from which penetration, ignition delay and lift-off can be derived
- Extinction imaging

1.3 GENERAL RECOMMENDATIONS FOR CALCULATIONS

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

- INJECTION RATE: For models: rate of injection generated with CMT Virtual Injection Rate Generator should be used (<http://www.cmt.upv.es/ECN03.aspx>). If available, the experimental injected mass should be assigned.
- SPRAY MODEL: The approach to model liquid spray dispersion and evaporation should follow the recommendations in Topic 1.3: Evaporation and Parametric Variations. Please refer to the corresponding guidelines, which should also be valid for calculations within reactive cases.
- CHEMICAL MECHANISM: After some comparisons based on comparisons with shock-tube measurements, two chemical mechanisms are recommended:
 - Narayanaswamy et al.: a 255 species mechanism [1] .
 - Luo et al.: 111 species skeletal mechanism, which was defined as follows:
 - The starting detailed mechanism was Sarathy et al. [2] .
 - This was reduced to a skeletal mechanism as outlined in Luo et al. [3] .
 - To the skeletal mechanism, OH* [4] was added. Precursor species for CH were also added, per [2] .



If another mechanism is used by any contributor, it should be tested (and compared to the reference mechanism) on homogeneous reactors corresponding to the following conditions

- Pfahl et al. [5] : n-decane, pressure = 50 bar, ϕ = 0.67, 1.0 and 2.0
 - Zhukov et al. [6] : n-decane, pressure = 80 bar, ϕ = 1.0
 - Vasu et al.[7] : n-dodecane, pressure = 20 bar, ϕ =1.0. The raw data have to be scaled to 20 bar according to [1].
-
- TURBULENCE-COMBUSTION INTERACTION (TCI) AND SOOT: Each contribution can use a particular TCI and SOOT model.



SUBTOPIC 2.1 – COMBUSTION INDICATORS



2 SUBTOPIC 2.1 – COMBUSTION INDICATORS

2.1 COORDINATORS

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José M García-Oliver, CMT

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2.2 OVERALL OBJECTIVES

Analyse model and experimental results to determine different parameters that can serve for a global description of the combustion process, namely:

- Ignition delay/Ignition Location
- Lift-off Length
- Reactive Spray Penetration
- Heat Release Rate

2.3 OVERARCHING QUESTIONS TO BE ADDRESSED

- What is the measured and computed dependency of the main “combustion indicators” on the recommended parametric variations of the operating conditions?
- What are the differences among experiments, among models and between models and experiments? What are the reasons for these differences?
- What is the influence of the chemical mechanism? What is the influence of the turbulence-chemistry interaction?

2.4 COMBUSTION INDICATOR DEFINITIONS

Both experimental and modelling information to be submitted can be divided into:

- **Global indicators:** single quantitative parameters globally describing a particular aspect of the combustion sequence, (e.g. ignition delay, ignition location, stabilized LOL, stabilized Flame Length...)
- **Time-resolved indicators:** single quantitative parameters describing a particular aspect of the combustion sequence with a time evolution (e.g. reacting spray penetration, heat release rate...). It must be noted that Global combustion indicators can be produced from averaging time-resolved ones (e.g. stabilized



LOL) or by considering particular timings (e.g. spray tip penetration at ignition timing).

2.4.1 Experimental definitions

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	
		OH LIF	Most downstream axial of average OH map with a signal higher than a threshold to be defined.	
TIME-RESOLVED	Reactive spray penetration	Sr	Schlieren	Same as for inert sprays
	Heat release rate	HRR	Pressure measurement	dP/dt

Table 2 – Experimental definition of Combustion Indicators

2.4.2 Modelling definitions

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)	$\frac{dP}{dt}$ P = average pressure in the domain
			ChHRR (Chemical)	$\sum \omega_i h_{f,i}^0$

Table 3 – Modelling definition of Combustion Indicators

2.5 TEST MATRIX

Baseline Spray A is the reference for the analysis. According to that, it will be set as a standard for the comparison of both experiments and calculations.

Recommended parametric variations for combustion indicators are in the following priority list (Spray A reference in bold):

1. Ambient Temperature [K]: **900** – 800 – 1000 – 700 – 1100
2. Injection pressure [MPa]: **150** – 100 - 50
3. Oxygen concentration [%]: **15** – 21 – 17 – 13
4. Ambient density [kg/m3]: **22.8** – 15.2 – 30.4 – 7.6
5. Injector: **210677**, 210675, 210678



For all cases, a long injection duration is needed, to be able to properly investigate the combustion evolution (check at Section 5.1, Injection Duration).

2.6 DATA NEEDED

As stated above, combustion indicators from both experiments and calculations will be confronted to evaluate dependencies from operating conditions, as well as differences between experiments and modelling. Therefore submissions for this Subtopic will consist of all combustion indicators listed in the corresponding table (i.e. τ SOC, LOL, Reactive spray penetration, Flame length, Heat release rate). An Excel file template will be provided to help the data submission, and further details for submission can be found in Section 5.

MODELLING APPROACHES

Although each group should contribute with their particular TCI model, a task for comparison with different models will be undertaken. For that purpose, each modelling contribution should include the combustion indicators from as many configurations as possible from the following prioritized list:

- Spray A with a particular TCI model under reacting conditions
- (optional) Well-mixed models (i.e. source terms are evaluated directly from Favre-averaged species mass fraction and temperature, no TCI).
- (optional) Different TCI models
- (optional) Different chemical mechanisms. In this case, the particular mechanism files should be validated as shown in Appendix 1.

Such variations of modelling approaches should be performed essentially on Spray A conditions and, whenever possible, from extreme conditions from the parametric variation matrix.

SPRAY A UNDER INERT CONDITIONS

Each group should carry out calculations with the same configuration as in Spray A reference case, but inhibiting the activation of the particular combustion model. The main objective is the comparison of the underlying mixing field, which obviously affects the subsequent combustion process. This evaluation will be based upon submitted mixture fraction and temperature fields at $t=1400 \mu\text{s}$.



SUBTOPIC 2.2 – FLAME STRUCTURE

3 SUBTOPIC 2.2 – FLAME STRUCTURE

3.1 COORDINATORS

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 Maarten Meijer, TUE
 Yuri Wright, ETH-Zurich

3.2 OVERALL OBJECTIVES

Analyse model and experimental results to determine characteristics of the flame structure during its stages of evolution. The analysis will focus on the time evolution of some global metrics shown in Figure 1 and detailed 1D and 2D structure analysis based on characteristics profiles and fields for the baseline spray A ambient conditions with a 6.0 ms injection duration. Global metrics are in particular:

- Schlieren-derived tip penetration under reacting (ShadowR) and inert (ShadowI) conditions.
- Flame tip penetration (FTP) from broadband radiation (BBand)
- Lift-Off Length (LOL)

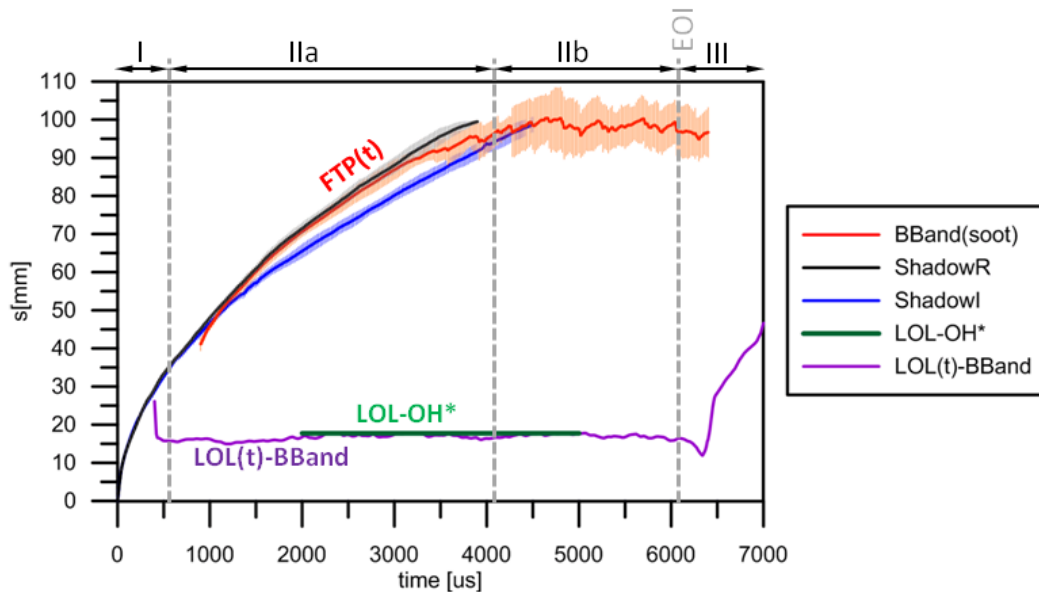


Figure 1 – Definition of flame evolution stages for Spray A (6ms injection)



According to the previous Figure, the following stages have been defined:

I – Ignition and early flame: From start of injection until LOL stabilizes (<0.6ms). Both the cool flame (first stage ignition) and main flame (second stage ignition) will be considered. Cool flame might precede first time FTP is detected.

II – Mature flame: From LOL stabilization until EOI

IIa – Quasi-steady mature flame: Until flame length (FTP) front stabilizes (0.6 to 4.0 ms)

IIb – Steady flame (4.0 ms to End of Injection (EOI))

III – Burn-out phase: After EOI

3.3 OVERARCHING QUESTIONS TO BE ANSWERED

- What is the observed structure of the ignition / flame in experiments?
- What are the differences in ignition / flame structure between models and between models and experiment? What are the reasons for these differences?
- What do the experimental and modelled ignition / flame structures suggest about the underlying physical phenomena governing the evolution of the spray along the different combustion stages?

3.4 TEST MATRIX

Baseline Spray A is the condition for detailed analysis within this subtopic. According to that, it will be set as a standard for the comparison of both experiments and calculations. Compared to the standard Spray A injection duration, a long injection pulse is recommended, to enable the full description of the previously defined phases (check Section 5.1, Injection Duration).

Additionally, analysis of flame structure during the quasi-steady phase will be investigated under Temperature and Oxygen variations according to the following matrices and priorities:

- 1. Ambient Temperature [K]: 900 – 800 – 1000
- 2. Oxygen concentration [%]: 15 – 21 – 13

3.5 DATA NEEDED

As stated in the objectives, the analysis within this subtopic will try to build up a coherent description of the flame evolution along the injection process based upon:

- Analysis of combustion indicators (from Subtopic 2.1).
- Analysis of 2D fields of relevant variables (e.g. mixture-fraction, velocity, turbulence, formaldehyde and hydroxyl) during the various stages

The following table summarizes the contributions from both experiments and calculations that are particularly demanded for this Subtopic:



Data	ACRONYM	Experiments	Models
n-Dodecane Mass Fraction	YC12	-	X
O2 Mass Fraction	YO2	-	X
CO Mass Fraction	YCO	-	X
CO2 Mass Fraction	YCO2	-	X
OH mass Fraction	YOH	LIF	X
OH* Mass Fraction	YOHs	OH* Chemiluminiscence	X
CH2O Mass Fraction	YCH2O	LIF	X
Axial velocity (m)	U	Reacting + non-reacting	Reacting + non-reacting
Radial velocity (m)	V	Reacting + non-reacting	Reacting + non-reacting
Mixture fraction	Z	Non-reacting	Reacting + non-reacting
Temperature (K)	T	-	X
Mixture fraction variance	Zvar	-	Optional
Turbulence kinetic energy (m²/s²)	K	-	Optional
Turbulence kinetic energy dissipation rate (m²/s³)	EPS	-	Optional
Viscosity (molecular, kg/m/s)	VIS	-	Optional
Scalar dissipation rate (1/s)	CHI	-	Optional

Table 4 – Data required from models and experiments

2D maps derived from Experiments should be ensemble averages, while those from Modelling should be Favre averages (except for mixture fraction variance).

The following cases are demanded, in a priority order:

- Baseline with a particular TCI model under reacting conditions
- Baseline under non-reacting conditions
- (optional) Well-mixed models (i.e. source terms are evaluated directly from Favre-averaged species mass fraction and temperature, no TCI).
- (optional) Different TCI models
- (optional) Different chemical mechanisms. In this case, the particular mechanism files should be validated as shown in Appendix 1.

For spatial and temporal positions and file format details, please refer to Section 5.



SUBTOPIC 2.3 – SOOT FIELD



4 SUBTOPIC 2.3 – SOOT FIELD

4.1 COORDINATORS

Contact: Scott Skeen, SNL, sskeen@sandia.gov

Michele Bolla, ETH

Dan Haworth, PSU

4.2 OVERALL OBJECTIVES

- To improve the understanding of the physical/chemical processes of soot formation and oxidation under engine-relevant conditions and to distill this improved understanding into predictive CFD-based models.
- Which is the soot distribution within spray A?
 - How is it modified with different parametric variables?
 - How different measurement techniques compare?
 - How accurate do different modeling approaches predict the soot field?

4.3 SPECIFIC QUESTIONS

- “Soot onset”:
 - Location and timing of soot onset for Spray A.
 - Variation of location and timing for different conditions (temperature and oxygen).
- Quasi-steady soot (long injection):
 - Spatial distribution of Soot Volume Fraction (SVF) or KL at 4.5 ms ASOI
 - Comparison between different measurement techniques: LII, high-speed and single-shot 2C-pyrometry, extinction imaging, laser extinction
 - Imaging extinction experiments will also provide a time- and ensemble-averaged SVF field. The time averaging will be performed during the quasi-steady period of the spray event.
 - Soot precursor C₂H₂ (evtl. PAH) distribution
 - Mean particle size distribution
- Transient soot (short injection):
 - Temporal soot mass (or KL) evolution
 - Soot oxidation behavior



4.4 TEST MATRIX

Baseline Spray A with both nominal and long injection duration (check Section 5.1, Injection Duration) is the reference for the analysis. Changes of operating conditions are considered for the long injection duration case only. The following priority has been defined:

1. Ambient Temperature [K]: **900** – 800 – 1000
2. Oxygen concentration [%]: **15** – 21 – 13

Fuel is n-dodecane only.

4.5 DATA NEEDED

EXPERIMENTS

The following information is requested from experiments

- 1) What is the location and timing of “soot onset” in the spray head for Spray A?
Any injection duration will suffice. The corresponding criterium for the determination of soot onset will be determined based on experimental submissions.
 - a. LII: Measured intensity corresponding to onset must be determined.
 - b. High-speed 2-Color Pyrometry:
 - c. Single-Image 2-Color Pyrometry.
 - d. Imaging Extinction.
 - e. Imaging spectrometer based high-speed pyrometry.
- 2) What is the KL distribution at subsequent timings after soot onset? (1.5, 2, 2.5 ms ASOI).
 - a. See details above.
- 3) What is the quasi-steady distribution of soot (KL or SVF) for Spray A (long injection)? Reference timing will be 4.5 ms
 - a. LII: composite average of multiple images acquired during the quasi-steady period calibrated with laser-extinction data (see detail below).
 - b. High-speed Soot Pyrometry Imaging: composite (ensemble) average of multiple time-averaged images acquired during the quasi-steady period. Tomographic reconstruction of time- and ensemble-averaged images yields soot volume fraction.
 - c. Single-shot Soot Pyrometry Imaging: composite average of multiple images acquired during quasi-steady period. Tomographic reconstruction of time- and ensemble-averaged images yields soot volume fraction.



- d. Extinction Imaging: composite (ensemble) average of multiple time-averaged images acquired during the quasi-steady period. Tomographic reconstruction of time- and ensemble-averaged images yields soot volume fraction.
 - e. Laser-extinction: If measurements are limited to a single axial location, they should be performed 60-mm downstream of the injector orifice.
- 4) How do different soot measurement techniques compare (LII, 2-color pyrometry, high-speed imaging extinction)?
 - 5) How does the location and timing of “soot onset” change with changes in ambient temperature and O₂ concentration? (Parametric variations for both temperature and O₂ concentration have been defined above).
 - 6) How does the particle morphology change along the spray centerline as a function of axial distance from the nozzle for Spray A (TEM measurements)?

The nomenclature for submitted variable should follow the convention in the following table:

	ACRONYM
LII signal	LII
KL as from light extinction method	KLext
KL as from 2C method	KL2C
T as from 2C method	T2C

Table 5 – Nomenclature for variables from Soot experiments

General recommendation for measurements (see section 1.3) should be followed. In addition to soot-related measurements, experimental results will preferably include measurements of lift-off length (OH chemiluminescence or high-speed luminosity), ignition delay time (high-speed luminosity), and vapor penetration (high-speed schlieren during non-reacting conditions) to aid in the interpretation of potential differences in soot results. If such results have been submitted for other subtopics, it should be indicated.

The coordinators may request raw experimental signals if deemed helpful for the coordination and presentation of results. For example, imaging extinction measurement submissions will include the unprocessed movie files. This will facilitate more direct comparisons between the experiment and model. Data submission regarding file naming, formats, etc. should follow recommendations in Section 5.



SIMULATIONS

The following information is requested from calculations for nominal Spray A conditions in terms of time-resolved variables and 2D maps. In the latter case, please refer to Section 5.3 for details on timings and spatial resolution

VARIABLE	ACRONYM	FORMAT
Soot Volume Fraction	SVF	2D maps
C2H2 Mass Fraction	YC2H2	2D maps
Mean Soot Particle Size	SPS	2D maps
Total Soot Mass	TSM	Time-resolved

Table 6 – Data required from soot modelling for nominal Spray A conditions

Regarding parametric studies, the following reduced number of variables is requested:

VARIABLE	ACRONYM	FORMAT
Axial location and magnitude of maximal SVF	Xsm	2D mapas at 4ms ASOI
Mean Soot Particle Size at maximal SVF	SPSXsm	
Total Soot Mass	TSM	Time-resolved

Table 7 – Data required from soot modelling for parametric variations

General recommendation for Spray Modelling (see Topic 1 Guidelines) and Topics 2.1 and 2.2 (see section 1.3) should also be valid here. In particular, the chemical model as suggested in topic 2 should be used when possible. If a different chemical mechanism is used, then homogeneous reactor calculation should be performed as contribution to the sub-topics “Combustion indicators” and “Flame structure”.

The ECN3 soot sub-topic primarily seeks to compare experiments with simulations and to extend insight gained from ECN2. Therefore, there is no strict recommendation about soot model to be used.

Depending on the chemical mechanism used PAH may be included or not. An acetylene-based model can be considered (e.g. Leung et al. Combust. Flame 87 (1991) 289-305).

It is highly recommended for contributors employing a TCI closure to submit also results neglecting TCI (well-mixed model) for an improved analysis of modelling results.



The comparison of different chemical models for soot inception and surface growth is beyond the scope of ECN3.

Data submission regarding file naming, formats, etc. should follow recommendations in Section 5.



SUBMISSION IN PRACTICE



5 SUBMISSION IN PRACTICE

This section contains specific instructions for submission of information. First conventions applicable to both experiments and modelling are presented, while specific requirements to either experiments (Section 5.2) or modelling (Section 5.3) are presented.

5.1 GENERAL ASPECTS

Three types of information to be submitted

- Global combustion indicators: According to definitions in Section 2.4.
- Time-resolved indicators: According to definitions in Section 2.4 and 4.5.
- Space- (and, if possible, time-) variables: 2D maps
- Raw info (for some experiments, as requested).

OPERATING CONDITIONS NOMENCLATURE

The following coding will be used to indicate the ambient conditions:

ACRONYM	O2 [%]	Ta [K]	Dens [kg/m ³]	Pinj [MPa]
AI	0	900	22.8	150
AR	15	900	22.8	150
I1	15	900	22.8	50
I2	15	900	22.8	100
T1	15	700	22.8	150
T2	15	800	22.8	150
T3	15	1000	22.8	150
T4	15	1100	22.8	150
O1	13	900	22.8	150
O2	17	900	22.8	150
O3	21	900	22.8	150
D1	15	900	7.6	150
D2	15	900	15.2	150
D3	15	900	30.4	150

Table 8 – Nomenclature for operating conditions for result submission

Fuel will be n-dodecane. If any other fuel is used, it should be indicated at the end of each corresponding file

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.

CONTACT PEOPLE

Information will be sent to the following coordinators

INFORMATION	CONTACT EXPERIMENTS	CONTACT MODELLING
Global Combustion Indicators	Jose M García-Oliver jgarciao@mot.upv.es	Gianluca D'Errico gianluca.derrico@polimi.it
Time-resolved Combustion Indicators		
Space- (and Time-) resolved maps	Louis-Marie Malbec louis-marie.malbec@ifpen.fr	Bart Somers L.M.T.Somers@tue.nl
Time-resolved Soot Indicators	Scott Skeen sskeen@sandia.gov	Michele Bolla mbolla@lav.mavt.ethz.ch
Space- (and Time-) resolved Soot-related maps		

Table 9 – Reference people for submission of information

DEADLINES

According to the official ECN3 calendar, March 1st is the final deadline for modelling/experimental submissions to ECN3.



5.2 SUBMISSION OF EXPERIMENTAL RESULTS

5.2.1 Global and Time-resolved 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>).

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:
ECN3E_[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:

ECN3E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR].txt

The following nomenclature has been applied for file names

- ECN3E 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 2.
- [INJECTOR] is a string for the Spray A Injector number.
- [COND] is a string for the ambient condition according to Table 8.
- [DUR] is a string for the injection duration coding as indicated in Section 5.1 (LONG/SHORT).

Examples:

- ECN3E_CMT_GLOBAL_675.XLS would be a submission from CMT of global indicators obtained in experiments with injector 675.
- ECN3E_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 8) and LONG injection duration.

5.2.2 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 prioritize 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
- 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

ECN3E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t].png

ECN3E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t].txt

The following nomenclature has been applied for file names

- ECN3E 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 2.
- [INJECTOR] is a string for the Spray A Injector number.
- [COND] is a string for the ambient condition according to Table 8.
- [DUR] is a string for the injection duration coding as indicated in Section 5.1 (LONG/SHORT).
- [t] is a string for the particular timing, in μ s after Start of Injection (ASOI).

Examples:

- ECN3E_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 8) and LONG injection duration.

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

5.2.3 Raw information

In the following cases, raw information can be submitted:



- Soot-related measurements.
- Upon request from ECN3 coordinators, after analyzing submitted Global or Time-resolved Combustion Indicators raw information can be supplied.
- Upon request from ECN3 coordinators, some soot-related measurements may be beneficial to the coordination and presentation of results.

For those cases, please contact the corresponding person in Table 9.



5.3 SUBMISSION OF MODELLING RESULTS

5.3.1 Global and Time-resolved 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:

ECN3M_[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:

ECN3M_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR].txt

The following nomenclature has been applied for file names

- ECN3M 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 2 and soot-derived variables from Table 6 and Table 7.
- [INJECTOR] is a string for the Spray A Injector number.
- [COND] is a string for the ambient condition according to Table 8.
- [DUR] is a string for the injection duration coding as indicated in Section 5.1 (LONG/SHORT).

Examples:

- ECN3E_CMT_GLOBAL_675.XLS would be a submission from CMT of global indicators obtained with simulations from injector 675.
- ECN3E_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 8) and LONG injection duration.
- ECN3E_SAND_TSM_677_AR_LONG.txt would be a submission from Sandia group of the Total Soot Mass for injector 677, operating conditions of spray A (ambient conditions AR in Table 8) and LONG injection duration.



5.3.2 Spatial- (and time-) resolved variables

Full 2D (axial and radial) maps of modelling-derived variables recorded in Table 4 and Table 6 (soot modelling) should be submitted for analyses within Topic 2 according to the following conventions:

- 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 (500 points)
 - Axial: 0 to 100mm; 0.2mm spacing (500 points)
- Time discretization: from 100 μ s to 6000 μ s After Start of Injection, each 100 μ s

DATA FILE STRUCTURE

The data are to be submitted as either ASCII plain text, first line should include the variables name according to the nomenclature in Table 4, Table 6 and 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], 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*, soot-related )
x2,r1,u,v,Z,T,n-dodec,O2,CO,CO2,OH,CH2O,optionals (e.g. OH*, soot-related)
...
xn,r1,u,v,Z,T,n-dodec,O2,CO,CO2,OH,CH2O,optionals (e.g. OH*, soot-related)
x1,r2,u,v,Z,T,n-dodec,O2,CO,CO2,OH,CH2O,optionals (e.g. OH*, soot-related)
...
```

Files are expected to be organised by directories such as:

ECN3M_[GROUP]_[INJECTOR]_[COND]_[DUR]

within which individual files should be named:

ECN3M_[GROUP]_[INJECTOR]_[COND]_[DUR]_[t].txt

The following nomenclature has been applied for file names

- ECN3M 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 8.
- [DUR] is a string for the injection duration coding as indicated in Section 5.1 (LONG/SHORT).
- [t] is a string for the particular timing, in μ s after Start of Injection (ASOI).

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



Examples:

- ECN3M_TUE_677_1_LONG/ECN3M_TUE_677_1_LONG_1000.txt
- ECN3M_TUE_677_1_LONG/ECN3M_TUE_677_1_LONG_4000.txt

corresponds to a submission from TUE of CFD modelling results at 1.0/4.0 ms ASOI for injector 677, operating conditions of spray A (ambient conditions AR in Table 8) 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 10 – Modelling setup description table

CHEMICAL MECHANISM

In addition, if possible the chemical mechanism files should be submitted in CHEMKIN format if they are different from the reference chemical mechanism.



REFERENCES



6 REFERENCES

- [1] K. Narayanaswamy, P. Pepiot, H. Pitsch, (2013), *Combust. Flame* (2013), <http://dx.doi.org/10.1016/j.combustflame.2013.10.012>
- [2] 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) 2338-2357.
- [3] 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.
- [4] 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.
- [5] U. Pfahl, K. Fieweger, G. Adomeit, *Proc. Combust. Inst.* 26 (1) (1996) 781-789.
- [6] V.P. Zhukov, V.A. Sechenov, A.Y. Starikovskii, *Combust. Flame* 153 (1) (2008) 130-136.
- [7] S.S. Vasu, D.F. Davidson, Z. Hong, V. Vasudevan, R.K. Hanson, *Proc. Combust. Inst.* 32 (1) (2009) 173-180.



APPENDICES



7 APPENDICES

7.1 CHEMICAL MECHANISM VALIDATION

A QUICK COMPARISON OF CHEMICAL KINETIC MODELS OF N-DODECANE USING SHOCK TUBE DATA

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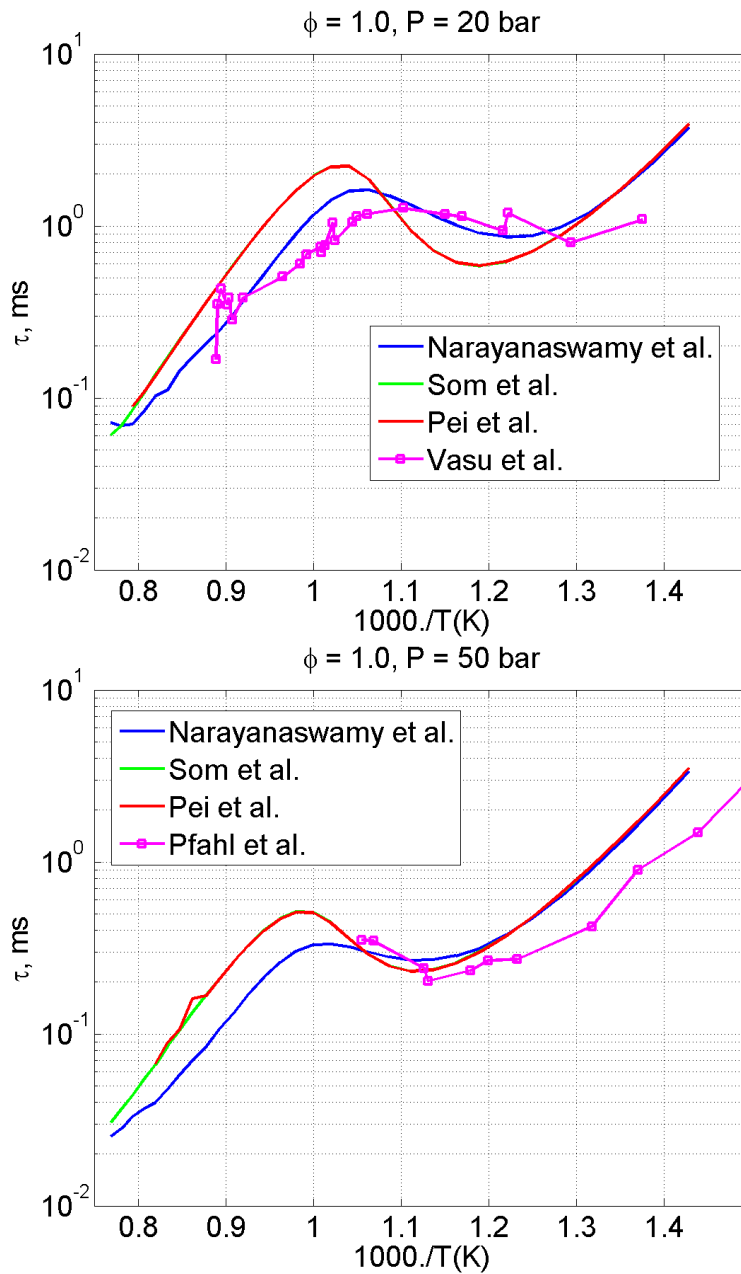
Aim

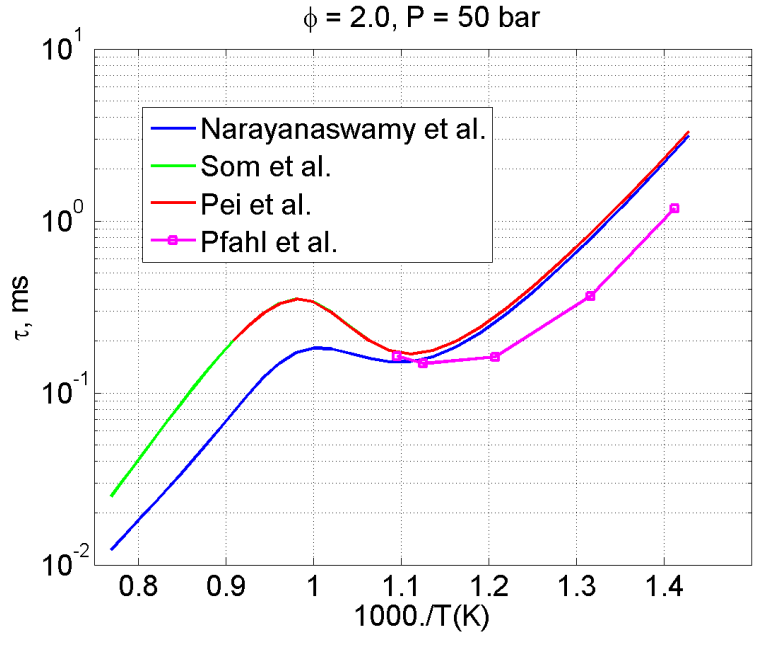
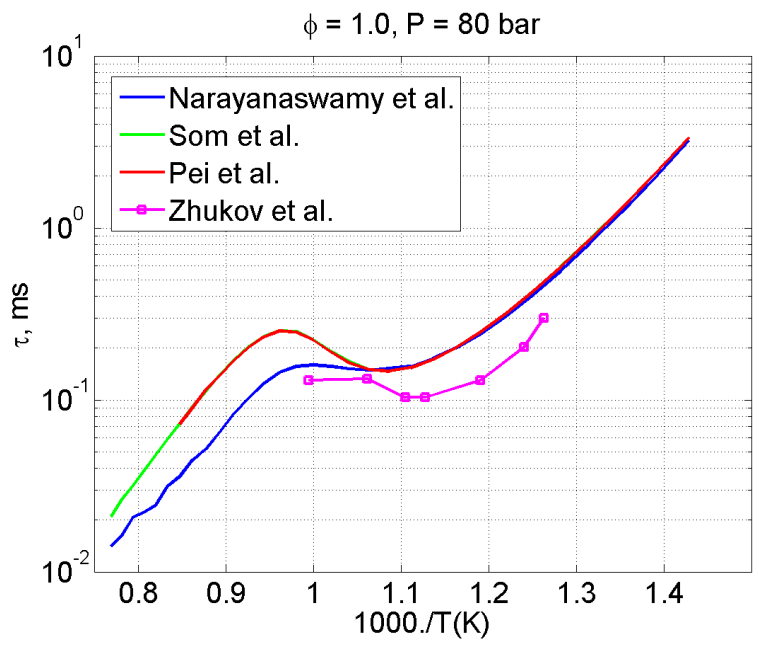
- To determine which chemical mechanism best captures ignition in the Engine Combustion Network (ECN) Spray-A conditions [1].

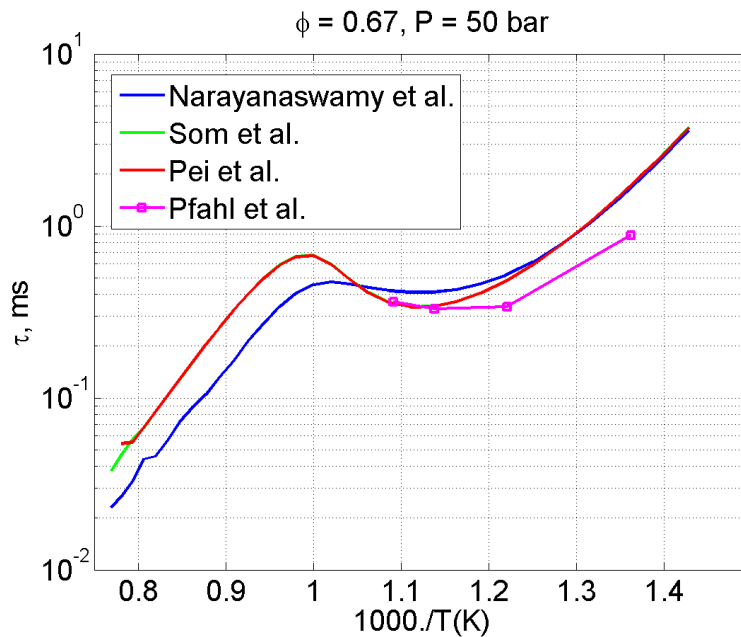
Method

- Constant volume homogeneous ignitions were modelled using SENKIN [2].
- Ignition was defined computationally as the time of the maximum rate of change of temperature. For experiments whatever definition was used in the experimentally reported data was retained.
- The following three chemical mechanisms were compared:
 - Narayanaswamy et al.: a 255 species mechanism [3].
 - Sarathy et al.: 111 species skeletal mechanism, which was defined as follows:
 - The starting detailed mechanism was Sarathy et al. [4].
 - This was reduced to a skeletal mechanism as outlined in Luo et al. [5].
 - To the skeletal mechanism, OH^* [6] was added. Precursor species for CH were also added, per [4].
 - Pei et al.: an 88 species reduced mechanism [7], which resulted from application of quasi-steady state assumptions to the 111 species mechanism described above.
- The model was compared with ignition delays from shock tubes:
 - Pfahl et al. [8]: n-decane, pressure = 50 bar, $\phi = 0.67, 1.0$ and 2.0
 - Zhukov et al. [9]: n-decane, pressure = 80 bar, $\phi = 1.0$
 - Vasu et al. [10]: n-dodecane, pressure = 20 bar, $\phi = 1.0$. The raw data were scaled to 20 bar according to Ref. [3].

Results







Discussion

- Results from Sarathy et al. and Pei et al. are nearly identical.
- The Sarathy et al. mechanism and the Narayanaswamy et al. do not significantly differ at low temperatures. The main difference is in the high temperature range.
- For 50 bar or higher pressure, agreement around 900-1000K (i.e. $1000/T$ around 1.0-1.1) is quite good for all the mechanisms.
- For 50 bar or higher pressure, at temperatures below $\sim 900\text{K}$ the mechanisms all over-predict the ignition delay, and there is little to distinguish between the mechanisms. This is significant because the spray A baseline ignites at a $\phi > 2.0$ where the temperature is under 850K.
- As shown in Narayanaswamy et al, their mechanism mainly improves the high temperature behaviour relative to the starting detailed mechanism of Sarathy et al. [4]. However, these temperatures would only be relevant for ignition in cases where the oxidiser temperature is at least 1100K, and even then it is possible that because of the NTC, the ignition would occur at even richer mixtures, which are also cooler.

Recommendation

- The Narayanaswamy et al. mechanism appears to improve results at high temperature, but it is significantly larger.
- Therefore the Sarathy/Luo/Som et al. based mechanisms are recommended. The Pei et al mechanism gives almost the same results at somewhat reduced cost, so this could also be used.



References

- [1] Pickett, L.M. et al., Engine Combustion Network data archive, available at <http://www.sandia.gov/ecn/index.php> (2013).
- [2] R.J. Kee, F.M. Rupley, J.A. Miller, M.E. Coltrin, J.F. Grcar, E. Meeks, H.K. Moat, A.E. Lutz, G. Dixon-Lewis, M.D. Smooke, J. Warnatz, G.H. Evans, R.S. Larson, R.E. Mitchell, L.R. Petzold, W.C. Reynolds, M. Caracotsios, W.E. Stewart, P. Glarborg, C. Wang, O. Adigun, CHEMKIN collection, release 3.6. Reaction Design, Inc., ISCRE, San Diego, 2000.
- [3] K. Narayanaswamy, P. Pepiot, H. Pitsch, (2013), *Combust. Flame* (2013), <http://dx.doi.org/10.1016/j.combustflame.2013.10.012>
- [4] 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.
- [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.
- [6] 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.
- [7] J.M. Hall, E.L. Petersen, *Int. J. Chem. Kinet.* 38 (2006) 714-724.
- [8] U. Pfahl, K. Fieweger, G. Adomeit, *Proc. Combust. Inst.* 26 (1) (1996) 781-789.
- [9] V.P. Zhukov, V.A. Sechenov, A.Y. Starikovskii, *Combust. Flame* 153 (1) (2008) 130-136.
- [10] S.S. Vasu, D.F. Davidson, Z. Hong, V. Vasudevan, R.K. Hanson, *Proc. Combust. Inst.* 32 (1) (2009) 173-180.