ECN5 TOPIC 4/5 – IGNITION AND COMBUSTION SUBMISSION GUIDELINES

Version 170309

CONTENTS

1 INTRODUCTION

These topics are a 'natural' continuation from ECN3-4 diesel combustion topics focusing on ignition and combustion processes.

After four ECN editions, the 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 for the baseline Spray A nozzle. Therefore, for the present workshop, the main effort on the experimental side should be spent on the extension of the activity within the group to Spray C&D nozzles, for which only preliminary work was presented at ECN4.

On the modelling side, at ECN4, significant differences were noted in predictions of ignition delay between different models for Spray A and its parametric variations. There was also a consistent trend of over-prediction of ignition delay with the recommended ECN4 baseline mechanism, while some other mechanisms showed promise. It was recommended to find a new baseline mechanism. Three candidate mechanisms have been identified that seem to be capable of good ID and LOL predictions. The modelling side will therefore focus on the comparison of these mechanisms in terms of the ignition process, and subsequently the resulting flame structure will be compared between mechanisms and turbulence-chemistry interaction (TCI) approaches. Only single injection spray A cases with ambient conditions variations will be considered at ECN5. Hopefully, this session can finally draw a line under ignition of the spray A baseline, enabling future ECN's to focus on C/D, multiple injections, etc.

2 OBJECTIVES

2.1 Experimental objectives

ECN4 Experimental objectives in terms of spray combustion should focus in the following goals:

- Spray C/D: Provide with experimental contributions in terms of main combustion indicators, as well as time- and space-resolved quantitative parameters for flame description.
- Spray A: As the experimental database is fairly large, only time- and space-resolved quantitative parameters for flame descriptions by means of detailed optical techniques (e.g. LIF-type techniques) are requested. Special attention should be paid to the ignition process at nominal and low temperature conditions.

2.2 Modeling and analysis objectives

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

- identify new candidates for a baseline chemical mechanism and select a new baseline mechanism for ECN5 and future ECNs;
- evaluate alternative mechanisms in their predictions of different combustion indicators (ID/LOL/penetration/chemical species profiles);
- understand the differences between models especially with respect to chemical mechanisms and turbulence-chemistry interaction (TCI) approaches;
- identify the reasons for the differences between experimental and modelled ignition delay, lift-off length, and flame structure and improve model performance;
- better understand the processes from ignition through to combustion recession by analysing the experimental and model databases.

The focus remains on spray A with ambient environment variations and effects of the chemistry model and TCI model will be studied.

Interaction with the following topics will be needed:

- Topic 3 (Evaporative diesel spray) to assess spray models predictability in terms of mixing.
- Topic 6 (Emissions) to coordinate submission information.

3 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, as shown in Table 1. Conditions in smaller font are low priority, which will be mainly used to assess global combustion indicators (i.e. ID/LOL), but 2D data will be optional.

PARAMETRIC VARIABLE	ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
Standard Spray A	**Ai**	0	900	22.8	150	LONG
	Ar	**15**	**900**	**22.8**	**150**	**SHORT/LONG/SHORT2**
Injection pressure	**I1**	15	900	22.8	100	LONG
	I2	15	900	22.8	50	LONG
Temperature	**T2**	15	**800**	22.8	150	SHORT/LONG
	T3	15	700	22.8	150	LONG
	T4	15	1000	22.8	150	LONG
Oxygen	**O3**	**21**	900	22.8	150	LONG
High Expansion	EX	15	780	14.8	150	LONG
Multiple injection	**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**

	MAT2	15	800	22.8	150	**0.5 ms pulse - 0.5 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.

<u>For the models</u>, only a subset of the experimental data points are requested, as shown in Table 2. Only the Spray A nozzle will be requested in the models and only single injection cases will be considered. For the conditions in bold font, 2D fields are requested. For the others, only global indicators are requested, though in their place 2D fields could be provided if the time and space resolution, etc., are sufficient to extract the global indicators.

PARAMETRIC VARIABLE	ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
Standard Spray A	**Ai**	0	900	22.8	150	LONG (all submissions must include)
	Ar	15	**900**	22.8	150	**SHORT/LONG** (all submissions must include LONG case; those planning topic 6 contribution should do with and without pre-burn products – see topic 6 guidelines)
Temperature	**T2**	15	**800**	22.8	150	**SHORT**/LONG
	T5	15	**1100**	22.8	150	**SHORT**/LONG
Oxygen	O2	13	900	22.8	150	LONG
	O3	21	900	22.8	150	LONG

Table 2 – Nomenclature for submission of Spray A parametric variations. Conditions with acronym not in bold 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:

- SHORT = 1.5 ms; This is the standard Spray A injection duration, which will be the reference for ignition and end-of-injection recession analysis.
- LONG = 5.0 ms; This will be the reference for the analysis of flame evolution, so that steady flame conditions are achieved.
- Note that since combustion recession will be studied, simulations need to be run out to ~1 ms after end of injection.

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 3 – Reference nozzle and data.

Target injector for Spray A will be nozzle 675 in terms of modeling efforts, although experimental contributions from other injectors are also welcome.

For spray C and D the target injector are respectively Nozzle #037 and #134 the characteristics and reference data are reported in Table 3.

4 PARTICULAR RECOMMENDATIONS FOR CALCULATIONS

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

- INJECTION RATE:
  - Spray A: 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. It is highly recommended however that groups submit results with the reference mechanism defined below (available by contacting Evatt Hawkes, evatt.hawkes@unsw.edu.au), and in addition at least one alternative mechanism. This will enable a comparison of TCI and chemistry sub-models among different groups.

  Recommended mechanisms:
  - Reference mechanism Cai: 57 species mechanism developed by Liming Cai at Aachen. Underpinned by Narayanaswamy mechanism, with reduction and optimisation against experimental targets. Reference: M. Davidovic, M. Bode, T. Falkenstein, L. Cai, H. Pitsch, LES of *n*-dodecane spray combustion and pollutant formation using a multiple representative interactive flamelet model, LES for internal combustion engine flows LES4ICE, Oil & Gas Science Technology accepted for publication (2017).
  - Yao: 54 species reduced mechanism developed by Tianfeng Lu ad co-workers at U. Conn., underpinned by USC-MECH high-temperature path, empirical 4 species low-T path, with reduction and optimisation against large LLNL mechanims and experimental targets. Reference: 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.
  - Polimi: 96 species reduced mechanism, underpinned by Polimi semi-detailed mechanism. Reference: A. Frassoldati, G. D'Errico, T. Lucchini, A. Stagni, A. Cuoci, et al., Reduced kinetic mechanisms of diesel fuel surrogate for engine CFD simulations, Combust. Flame 162 (10) (2015) 3991-4007.

- TURBULENCE-CHEMISTRY INTERACTION (TCI): Each contribution can use a particular TCI model. It is recommended to submit results both with and without contributions of TCI (where without corresponds to a well-mixed model that assumed there are no turbulent fluctuations), such that the importance of TCI can be assessed. Also helpful would be to submit results from multiple TCI approaches (e.g. mixing models, etc) with other factors held fixed.

- DATA TO BE SUBMITTED: Reference operating conditions are summarized in Table 2:
    - Conditions not in bold font are low priority, which will be mainly used to assess global combustion indicators (i.e. ID/LOL), but 2D data is optional.
    - For conditions in bold font the requested information is:
        - combustion indicators (i.e. ID/LOL)
        - 2D maps with a 10μs time step from the beginning of injection until end of combustion

5 DEADLINES

The following deadlines have been established:

- Monday 13th March 2017. Provide to Bart Somers a sample set of data, not necessarily the final one and all time steps, such that Bart can check data format and set up post-processing scripts.
- Sunday 19th March 2017. Final data. Please note, due to the proximity of ECN5 on 31 March, this is a hard deadline.

6 PARTICIPANT LIST

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Table 4 – 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 5 – 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:
  ECN5E_[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:
  ECN5E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR].txt

The following nomenclature has been applied for file names

- ECN5E identifies the information as an experimental contribution.
- GLOBAL identifies the file as containing Global Combustion Indicators.
- [GROUP] is a string for the submitting group acronym , e.g. TUE
- [VAR] is a string for the submitted combustion indicator Acronym according to the corresponding column in Table 5.
- [INJECTOR] is a string for the 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 3 (LONG/SHORT/SHORT2).

Examples:

- ECN5E_CMT_GLOBAL_SA210675.XLS would be a submission from CMT of global indicators obtained in experiments with SA nozzle, injector number 675.

- ECN5E_CMT_GLOBAL_SC210003.XLS would be a submission from CMT of global indicators obtained in experiments with SC nozzle, injector number 210003.

- ECN5E_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.

- ECN5E_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.

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

ECN5E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t].png
ECN5E_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[t].txt

The following nomenclature has been applied for file names

- ECN5E 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 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 3 (LONG/SHORT/SHORT2).
- [t] is a string for the particular timing, in µs after Start of Injection (ASOI).

Examples:

- ECN5E_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.

- ECN5E_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.

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	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:
  ECN5M_[GROUP]_[CHEM]_[TCI]_[VAR]_[INJECTOR]_[COND]_[DUR].txt

The following nomenclature has been applied for file names

  - ECN5M 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 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 3 (LONG/SHORT/SHORT2).
- [CHEM] denotes the chemistry model (e.g. Cai, Yao, Polimi)
- [TCI] denotes the TCI model, (e.g. WM, TPDF/CMC, etc)

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
Axial velocity (m)	U	Topic 4/5 (optional Topic 6)
Radial velocity (m)	V	Topic 4/5 (optional Topic 6)
Mixture fraction	Z	Topic 4/5 & 6
Temperature (K)	T	Topic 4/5 & 6
Density (kg/m3)	RHO	Topic 4/5 (optional Topic 6)
n-Dodecane Mass Fraction	YC12	Topic 4/5 & 6
O2 Mass Fraction	YO2	Topic 4/5 & 6
O Mass Fraction	YO	Topic 4/5 & 6
CO Mass Fraction	YCO	Topic 4/5 & 6
CO2 Mass Fraction	YCO2	Topic 4/5 & 6
H2O Mass Fraction	YH2O	Topic 4/5 & 6
OH Mass Fraction	YOH	Topic 4/5 & 6
H Mass Fraction	YH	Topic 4/5 & 6
CH2O Mass Fraction	YCH2O	Topic 4/5 & 6
C2H2 Mass Fraction	YC2H2	Topic 4/5 & 6
H2 Mass Fraction	YH2	Topic 6 (optional Topic 4/5)
Soot volume fraction	SVF	Topic 6 (optional Topic 4/5)
Benzene and/or aromatics	YA1, YA2, etc.	If available
H2O2 Mass Fraction	YH2O2	Topic 4/5 (optional Topic 6)
RO2 Mass Fraction	YRO2	Optional
OH* Mass Fraction	YOHs	Optional
NO Mass Fraction	YNO	Optional
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 7 – 2D-resolved data required from models

SPATIAL QUASI-STEADY PRODUCTION/DESTRUCTION RATES

At a select time corresponding to the quasi-steady period, provide a 2D map of the production/destruction rate of the following species. The units should be in µg/second.

Data (prod/des trate µg/s)	ACRONYM
n-dodecane	pC12
CO	pCO
H_2O	pH2O
O_2	pO2
O	pO
OH	pOH
H	pH
C_2H_2	pC2H2
Benzene and/or other aromatics	pA1, pA2, etc.
Soot volume fraction	pSVF

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 10µs step in the following intervals:
    - For LONG injection cases to 7000µs After Start of Injection;
    - 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],YC12,YO2,YCO,YCO2,YOH,YCH2O,YC2H2,YH2O2,YRO2,… YC12, YO2, YO, YCO, YCO2, YH2O, YOH, YH, YCH2O, YC2H2, YH2O2, YRO2, optionals (e.g. SVF, production/destruction rates…)
x1,r1,u,v,Z,T,RHO, YC12,YO2,YCO,YCO2,YOH,YCH2O,YC2H2,YH2O2,YRO2,… YC12, YO2, YO, YCO, YCO2, YH2O, YOH, YH, YCH2O, YC2H2, YH2O2, YRO2, optionals (e.g. SVF, production/destruction rates…)
x2,r1,u,v,Z,T,RHO, YC12,YO2,YCO,YCO2,YOH,YCH2O,YC2H2,YH2O2,YRO2,… YC12, YO2, YO, YCO, YCO2, YH2O, YOH, YH, YCH2O, YC2H2, YH2O2, YRO2, optionals (e.g. SVF, production/destruction rates…)
…
xn,r1,u,v,Z,T,RHO, YC12,YO2,YCO,YCO2,YOH,YCH2O,YC2H2,YH2O2,YRO2,… YC12, YO2, YO, YCO, YCO2, YH2O, YOH, YH, YCH2O, YC2H2, YH2O2, YRO2, optionals (e.g. SVF, production/destruction rates…)
x1,r2,u,v,Z,T,RHO, YC12,YO2,YCO,YCO2,YOH,YCH2O,YC2H2,YH2O2,YRO2,… YC12, YO2, YO, YCO, YCO2, YH2O, YOH, YH, YCH2O, YC2H2, YH2O2, YRO2, optionals (e.g. SVF, production/destruction rates…)
...

Files are expected to be organised in directories such as:

ECN5M_[GROUP]_[CHEM]_[TCI]_[INJECTOR]_[COND]_[DUR]

within which individual files should be named:

ECN5M_[GROUP]_[CHEM]_[TCI]_[INJECTOR]_[COND]_[DUR]_[t].txt

The following nomenclature has been applied for file names

- ECN5M identifies the information as a modeling contribution.
- [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 3 (LONG/SHORT).
- [t] is a string for the particular timing, in μs after Start of Injection (ASOI).
- [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:

- ECN5M_TUE_CAI_FGM_SA210675_AR_LONG/ECN5M_TUE_675_SA210675_AR_LONG_1000.txt
- ECN5M_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).

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
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 – Modeling setup description table