ECN4
TOPIC 4 – Chemical reactions that lead to ignition
SUBMISSION GUIDELINES

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CONTENTS

1 INTRODUCTION, OBJECTIVES AND DEADLINE 4
2 CONTRIBUTIONS OVERLAPPING WITH TOPIC 5 4
3 ADDITIONAL CONTRIBUTIONS FOR TOPIC 4 4
3.1 Target conditions 5
3.2 Model variations 5
4 SUBMISSION OF MODELLING RESULTS 7
4.1 Global and Time-resolved Combustion Indicators 7
4.2 Spatial- (and time-) resolved variables 8

1 INTRODUCTION, OBJECTIVES AND DEADLINE

At both ECN2 and ECN3, significant differences were noted in predictions of ignition delay between different models for Spray A and its parametric variations. There was also a general trend of over-prediction of ignition delay. In this context, the objectives of the present session are to:

- identify the reasons for the significant differences between models;
- identify the reasons for the differences between experimental and modelled ignition delay and improve their agreement; and
- better understand the process of ignition by analysing the experimental and model databases.

The focus remains on spray A and effects of the chemistry model and turbulence-chemistry interaction model will be studied.

Important note: Much of the data collection for this session overlaps with topic 5, while the analysis and some parameter variations will be different. It is suggested to first read the topic 5 guidelines before proceeding.

Deadline: 16 August 2015

2 CONTRIBUTIONS OVERLAPPING WITH TOPIC 5

Contributors to topic 4 are requested to please submit all conditions and data requested in topic 5, with all the recommendations that are made in topic 5. For topic 4 I will focus mainly on spray A and the parametric variations of ambient conditions. I am unlikely to look at spray B or the multiple injection cases unless there are several submissions. There is no need to separately submit to topic 4 – I will collect the data from the organisers of topic 5.

There is only one additional request from topic 4, which is to also provide the mass fractions of H2O2 and dodecyl peroxy radical (R-OO) versus time and space in the same way as the other mass fractions requested in topic 5. (R-OO is taken as the sum of its various isomers, i.e. the sum of species C12H25O2-2, C12H25O2-5, and C12H25O2-6 in the recommended Luo et al. chemistry mechanism.)

3 ADDITIONAL CONTRIBUTIONS FOR TOPIC 4

To enable a deeper analysis of chemistry effects on ignitions, groups that have capacity to submit the additional contributions described below by the due date are encouraged to do so. These contributions would require a greatly reduced data-set and would only

need to be run up to the time of ignition.

We already have the results we need from experiments, so these additional contributions are needed from modellers only.

3.1 Target conditions

A small parameter sweep of temperature and oxygen concentration is requested. Note that some conditions overlap with those requested for topic 5.

All other parameters, e.g. injector, injection parameters, etc., should be the same as for topic 5.

ACRONYM	O2 [%]	Ta [K]	Dens [kg/m3]	Pinj [MPa]	Inj Duration
T2	15	800	22.8	150	LONG*
A	15	900	22.8	150	LONG*
T3	15	1000	22.8	150	LONG*
O2	12	900	22.8	150	LONG*
O3	21	900	22.8	150	LONG*

*Table 1 – Nomenclature for submission of Spray A parametric variations; *: It is only necessary to run up to the time of ignition, so the injection just has to go up to this time, whatever that is in your simulations.*

3.2 Model variations

These contributions can be considered optional, but appreciated, for topic 4.

Chemistry sweep
The following chemistry sub-models are now available and contributions with more than one of these models would be appreciated. I would give priority to contributing results without a turbulence-chemistry interaction (TCI) model (i.e. well-mixed), but TCI model contributions are also welcome.

The chemistry models are available in CHEMKIN format from Evatt Hawkes at evatt.hawkes@unsw.edu.au.

- Luo: 106 species (topic 5 baseline)
  Z. Luo, S. Som, S. M. Sarathy, M. Plomer, W. J. Pitz, D. E. Longman and T. Lu, Development and validation of an n-dodecane skeletal mechanism for spray combustion applications, Combustion Theory and Modelling, Volume 18, Issue 2, 2014, pp. 187-203.

- Wang: 100 species
  Wang, H., Ra, Y., Jia M., Reitz, R.D., Development of a reduced n-dodecane-PAH mechanism, and its application for n-dodecane soot predictions, Fuel 136 (2014) 25–36.

- Yao: 53 species
  T. Yao, Y. Pei, B.-J. Zhong, S. Som, T. Lu, A hybrid mechanism for n-dodecane combustion with optimized low-temperature chemistry, 9th U. S. National Combustion Meeting, May 17-20, 2015, Cincinnati, Ohio.

- Polimi: 99 species
  A. Frassoldati, G. D'Errico, T. Lucchini, A. Stagni, A. Cuoci, T. Faravelli, A. Onorati, E. Ranzi, Reduced kinetic mechanisms of diesel fuel surrogate for engine CFD simulations, Combustion and Flame, in press.

- Narayanaswamy: 255 species
  Narayanaswamy, K., Pepiot, P., Pitsch, H., A chemical mechanism for low to high temperature oxidation of n-dodecane as a component of transportation fuel surrogates, Combustion and Flame 161 (2014) 866–884.

TCI sweep

A sweep is requested with and without a model for turbulence-chemistry interactions, where the "without" case corresponds to "well-mixed", "direct integration", etc., i.e. where turbulent fluctuations of chemical species and temperature are neglected and where the "with" case corresponds to e.g. a flamelet, CMC or PDF model. Please use the topic 5 recommended chemistry for this sweep.

4 SUBMISSION OF MODELLING RESULTS

4.1 Global and Time-resolved Combustion Indicators

If there is insufficient time to code new analysis to extract these indicators, I am able to do it if the fields of OH, temperature, and mixture-fraction are all submitted instead, following the guidelines for the 2D, time-resolved data as described in topic 5.

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
TIME-RESOLVED	Ignition location (axial)	IX-OH-2 IX-OH-14 IX-T	OH mass fraction; temperature	First axial location of Favre-average variable reaches a certain value, where IX-OH-2 corresponds to OH mass fraction reaching of 2% its maximum in the domain (instantaneous maximum), IX-OH-14 corresponds to the location of 14% and T corresponds to average temperature reaching 1600K
	Ignition location (radial)	IX-OH-2 IX-OH-14 IX-T	OH mass fraction; temperature	As above, except the radial location of this position
	Ignition location (mixture-fraction)	Z-OH-2 Z-OH-14 Z-T	OH mass fraction; temperature	As above, except the local mixture fraction at this location

Table 2 – Modelling definition of combustion indicators

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

- **Global combustion indicators:** Any format is fine as long as I can clearly see what ignition delay corresponds to what case and model.
- **Time-resolved information:** Only one ASCII plain text file per operating condition and combustion indicator will be sent. It will contain two-columns, the first one with the time (ms), and the second with the corresponding indicator. Name and units should be indicated at the first row. File name should follow the

structure:

ECN4M_[GROUP]_[VAR]_[INJECTOR]_[COND]_[DUR]_[MOD].txt

The following nomenclature has been applied for file names

- ECN4M identifies the information as a modelling 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.
- [INJECTOR] is a string for the Spray A Injector number.
- [COND] is a string for the ambient condition according to Table 1.
- [DUR] is a string for the injection duration coding as indicated in Section Table 1 (LONG/SHORT/SHORT2).
- [MOD] is a string corresponding to the model – i.e. which chemistry and which TCI model. Also please email me a key for the different models.

Examples:

- ECN4E_CMT_GLOBAL_675_M1.XLS would be a submission from CMT of global indicators obtained with simulations from injector 675 using model M1.

- ECN4E_CMT_Sr_675_AR_LONG_M1.txt would be a submission from CMT of the reacting tip penetration for injector 675, operating conditions of spray A (ambient conditions A in Table 1) and LONG injection duration using model M1.

4.2 Spatial- (and time-) resolved variables

Full 2D (axial and radial) maps of following modelling-derived variables should be submitted for analyses. It is only necessary to submit these for the spray A baseline and the parameter variations requested in topic 5. Please see topic 5 for additional information about the data format, etc.

Data	ACRONYM	Comments
H2O2 Mass Fraction	YH2O2	Optional
ROO Mass Fraction	YROO	Optional

Table 3 – 2D-resolved data required from models

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,… (where more than one model is being submitted, include a key here)
Chemistry model	(where more than one model is being submitted, include a key here)
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 4 – Modelling setup description table