ECN5 TOPIC 6 – SOOT
SUBMISSION GUIDELINES

Table of Contents

1 INTRODUCTION

Experimental submissions will focus largely on new soot data acquired for Spray C and Spray D at IFPEN, CATERPILLAR (CAT), and Sandia (SNL). Spray A data from SNL will be revisited for a comparison with data collected at General Motors Research (GMR)

Differences in soot data measured in pre-burn chambers with that measured in constant pressure vessels warrants further study on the effect of water and carbon dioxide in the ambient gases prior to fuel injection. Therefore a comparison of "Spray A" data collected at General Motors with data collected at Sandia and a comparison of "Spray C/D" data collected at CAT with that collected at IFPEN and Sandia will be presented.

Simulations are requested for Spray A with and without pre-burn products using the mechanism and soot model of your choice. All model input conditions should be identical except for the composition of the ambient gases.

2 OBJECTIVES

2.1 EXPERIMENTAL

Spray A: To understand and disseminate to the community the observed differences in soot data collected in pre-burn vs. constant pressure vessels.

Spray C/D: To compare soot measurements acquired at IFPEN, SNL, and CAT and understand the sources of any observed differences. Disseminate information to the community.

2.2 MODELING

Spray A

1) To simulate soot formation in Spray A with and without pre-burn combustion products and understand how water and carbon dioxide may influence soot and soot precursor formation and oxidation.
2) To compare observed trends with experimental results.

3 TARGET CONDITIONS (SIMULATIONS)

The baseline target condition and parametric variants are defined in the recently finalized Topic 4/5 guidelines. All are specified in terms of a nozzle, injection, and ambient condition. Simulations based on Spray A nozzle 675 or 370 are welcome as both injectors have similar hydraulic characteristics. Soot submissions are requested for only **two** conditions—the baseline Spray A LONG (5 ms) injection condition with the standard pre-burn products as ambient gases and the baseline Spray A LONG (5 ms) injection condition with 15% O_2 (by volume) and 85% N_2 (by volume) comprising the ambient gases. Overlapping with Topic 3, non-reacting vapor penetration and non-reacting 2D time-resolved maps of mixture fraction are requested. See Table 1 below (or for more detail see Table 1 in the Topic 4/5 Guidelines).

ACRONYM	O_2 [vol. %]	Amb. Comp.	T_{amb} [K]	ρ_{amb} [kg/m^3]	P_{inj} [MPa]	Inj Duration
AI	0	--	900	22.8	150	LONG (5 ms)
AR	15	Pre-burn	900	22.8	150	LONG (5 ms)
AN	15	O_2/N_2	900	22.8	150	LONG (5 ms)

Table 1 – Nomenclature for Spray A parametric variations

To minimize efforts, previously submitted results for the baseline Spray A case with pre-burn products are welcome as long as the simulation without pre-burn products was carried out with the exact same model and input parameters. Time resolved 2D data with the same grid resolution and step size are requested for both pre-burn and O_2/N_2 results.

When submitting results, the file naming convention should be consistent with the Topic 4/5 guidelines. For example, the nomenclature in Table 2 below describes the three Cases requested for Topic 6.

Case	Nomenclature	Description
Case 1	**A-AI-LONG**	**Spray A 675, Inert ambient 0% O_2, 900 K, 22.8 kg/m^3, 150 MPa injection pressure, Long (5 ms) injection duration**
Case 2	**A-AR-LONG**	**Spray A 675, Reacting ambient 15 vol.% O_2 pre-burn products, 900 K, 22.8 kg/m^3, 150 MPa injection pressure, Long (5 ms) injection duration**
Case 3	**A-AN-LONG**	**Spray A 675, Reacting ambient 15 vol.% O_2 85 vol.% N_2, 900 K, 22.8 kg/m^3, 150 MPa injection pressure, Long (5 ms) injection duration**

Table 2 – Naming convention for three cases requested in Topic 6 (Soot)

4 SPECIFIC RECOMMENDATIONS FOR SIMULATIONS

Consistent with the Topic 4/5 Guidelines, please adhere to the following recommendations for simulation submissions.

- 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. **If time allows, it is highly recommended** that groups submit results with the reference mechanism defined below (available by contacting Evatt Hawkes, evatt.hawkes@unsw.edu.au). Results using one additional alternative mechanism are welcomed, but not required.

  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): The effect of TCI on combustion will be investigated in Topic 4/5. For Topic 6 (Soot), the use of a TCI model is recommended; however, if previously submitted Spray A (pre-burn) data will be used without TCI, the O_2/N_2 simulation should also NOT include TCI so that the effects of water and carbon dioxide can be isolated.

5 DATA TO BE SUBMITTED

Reference operating conditions are summarized in Table 1 and Table 2. The following data are requested for these cases. See Table under heading 7.2 for a detailed list with required and optional data from Topics 4/5/6. Please provide data in the order provided in the Table under Section 7.2 for ease in post-processing. Please follow the guidance provided in Topic 5 Guidelines for the naming of files and directories and the data structure. Also, please provide the associated modeling setup description as requested in the Topic 5 Guidelines Table 9.

- Case 1 A-AI-LONG
  - Global
    - Vapor penetration
  - 2D Time-resolved maps
    - mixture fraction
- Case 2 & 3 A-AR-LONG and A-AN-LONG
- Global
  - Ignition Delay
  - Quasi-steady lift-off length
  - Time-resolved lift-off length
  - Time-resolved reacting spray penetration
  - Time-resolved total soot mass
  - Time-resolved soot onset location (i.e., axial position where SVF first exceeds 0.5 ppm as a function of time)
- Topic 6 Required 2D Time-resolved maps (see Table under heading 7.2 for full list in Topics 4/5/6)
  - Mixture fraction
  - Temperature
  - Fuel (n-dodecane) mass fraction
  - O_2 mass fraction
  - O mass fraction
  - CO mass fraction
  - CO_2 mass fraction
  - H_2O mass fraction
  - OH mass fraction
  - H mass fraction
  - CH_2O mass fraction
  - C_2H_2 mass fraction
  - H_2 mass fraction
  - SVF
  - Benzene and/or any other aromatic mass fraction
  - NO mass fraction (if available)

- 2D maps of production/destruction rate at a single time associated with quasi-steady period
  - Fuel (n-dodecane)
  - O_2
  - O
  - H_2O
  - CO
  - CO_2
  - H_2O
  - OH
  - H
  - C_2H_2
  - H_2
  - SVF
  - Benzene and/or any other aromatic
  - NO (if available)

NOTE: Consistent with Topic 4/5 the time-resolved 2D maps should be provided at 10μs time steps from the beginning of injection until end of combustion

6 DEADLINES

- **Monday 13th March 2017**. Provide to Scott Skeen a sample set of data, not necessarily the final one and all time steps, such that Scott can check data format.
- **Sunday 19th March 2017**. Final data uploaded to IFPEN server or transmitted to Scott Skeen via Sandia Managed File Transfer. Please note, due to the proximity of ECN5 on 31 March, **this is a hard deadline**.

7 SUBMISSION OF MODELING RESULTS

7.1 Global and time-resolved combustion indicators

The following definitions will be used for the modeling-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. +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%
	Total soot mass	Ms	SVF	Total integrated mass of soot within the entire simulated volume **up to 70 mm downstream** of the injector tip at each time step. Use 1.8 g/cm^3 as soot density.
	Soot onset location	Ls	SVF	Axial position where SVF first exceeds 0.5 ppm at each time step

Table 3—Definition of modeling based combustion/emissions 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.
  Example: ECN5M_GLOBAL_[GROUP]_[CHEM]_[TCI]_[VAR]_[INJECTOR]_[COND]_[DUR].txt
- **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:
  Example: 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 3.

- [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 Table 1 (requesting on LONG for Topic 6).
- [CHEM] denotes the chemistry model (e.g. Cai, Yao, Polimi)
- [TCI] denotes the TCI model, (e.g. WM, TPDF/CMC, etc)

7.2 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	Topic 4/5 (optional Topic 6)
Radial velocity (m/s)	V	Topic 4/5 (optional Topic 6)
Mixture fraction	Z	Topic 4/5 & 6
Temperature (K)	T	Topic 4/5 & 6
Density (kg/m^3)	RHO	Topic 4/5 (optional Topic 6)
n-Dodecane Mass Fraction	YC12	Topic 4/5 & 6
O_2 Mass Fraction	YO2	Topic 4/5 & 6
O Mass Fraction	YO	Topic 4/5 & 6
CO Mass Fraction	YCO	Topic 4/5 & 6
CO_2 Mass Fraction	YCO2	Topic 4/5 & 6
H_2O Mass Fraction	YH2O	Topic 4/5 & 6
OH Mass Fraction	YOH	Topic 4/5 & 6
H Mass Fraction	YH	Topic 4/5 & 6
CH_2O Mass Fraction	YCH2O	Topic 4/5 & 6
C_2H_2 Mass Fraction	YC2H2	Topic 4/5 & 6
H_2O_2 Mass Fraction	YH2O2	Topic 4/5 (optional Topic 6)
H_2 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
RO_2 Mass Fraction	YRO2	Optional
OH* Mass Fraction	YOHs	Optional
NO Mass Fraction	YNO	Optional
Mixture fraction variance	Zvar	Optional
Turbulence kinetic energy (m^2/s^2)	K	Optional
Turbulence kinetic energy dissipation rate (m^2/s^3)	EPS	Optional
Viscosity (molecular, kg/m/s)	VIS	Optional
Scalar dissipation rate (1/s)	CHI	Optional

7.3 SPATIAL QUASI-STEADY PRODUCTION/DESTRUCTION RATES (Topic 6)

Provide a 2D map of the time-averaged production/destruction rates of the following species. The time-average should be performed from 2 ms before EOI until 0.5 ms before EOI. The units should be in µg/second. If a time-average cannot be provided, provide the data at the time step corresponding to 2 ms before EOI.

Data (prod/des trate µg/s)	ACRONYM	Comments
n-dodecane	pC12	Optional Topic 6
CO	pCO	Optional Topic 6
H_2O	pH2O	Optional Topic 6
O_2	pO2	Optional Topic 6
O	pO	Optional Topic 6
OH	pOH	Optional Topic 6
H	pH	Optional Topic 6
H_2	pH2	Optional Topic 6
C_2H_2	pC2H2	Optional Topic 6
Benzene and/or other aromatics	pA1, pA2, etc.	Optional Topic 6
Soot volume fraction	pSVF	Optional Topic 6