ECN2 Soot Session

Organizers: Emre Cenker (Duisburg/IFPEN), Dan Haworth (Penn State)

Contributors: M. Bolla and Y. Wright (ETH – Zurich); Q. Jiao, H. Wang, L. Qiu and R. Reitz (University of Wisconsin – Madison)

Summary

Soot was a new topic for ECN2, and soot measurement and modeling for ECN configurations are both in their early stages compared to spray and combustion characterization.

On the experimental side, Emre Cenker gave an overview of soot measurement issues and data that are available for the ECN configurations. The experiments targeted soot volume fraction measurements in Spray A, including variations in ambient temperature and ambient oxygen concentration, along the central axial cross section. Experiments also included the standard diagnostics to verify that the conditions corresponded to those of Spray A. A Laser Extinction Method (LEM) and Planar Laser Induced Incandescence (PLII) were coupled for quantitative spatially resolved measurements. LII images were taken after the start of injection where quasistationary combustion was established. In addition, by changing the LII timing relative to the injection timing, the temporal variation of the soot cloud was observed. Lift-off length measurements and flame luminosity imaging were also conducted for each boundary condition to interpret the soot measurements. Due to some inaccuracy in the Spray A characterization measurements, soot results presented at this workshop were acquired under slightly different ambient conditions compared to the nominal Spray A conditions: -1 kg/m³ in ambient density, and +30 K in ambient temperature.

On the modeling side, Dan Haworth gave an introduction to soot physics and CFD-based soot modeling, including radiation heat transfer. Two groups submitted computed mean soot volume fraction data for Spray H (n-heptane). Both used semi-empirical two-equation soot models, but there were several important differences between the two sets of simulations. These included different gas-phase chemical mechanisms, different turbulence-chemistry interaction treatments (TCI neglected versus TCI accounted for using a CMC model), and different radiation models (radiation neglected versus radiation accounted for using an optically thin model), in addition to differences in the soot models themselves. Both models produced reasonable levels of soot compared to the experiments, and both captured the measured trends in soot volume fraction with variations in ambient O_2 level and ambient density.

Conclusions

The results on the experimental side show that Spray A is a moderately sooting jet where signal trapping is not significant, indicating greater potential for quantitative soot diagnostics. Maximum soot volume fractions of approximately 2-4 ppm are measured at near-Spray A conditions (21.8 kg/m³, 930 K, 15% O₂), and are as high as 12 ppm at elevated temperature (1030 K). For the 1.5 ms nominal Spray A injection duration, the soot cloud remains transient. Therefore, a longer injection duration of 4 ms was used to analyze the soot structure in a quasi-steady mode. Variations of ambient temperature and oxygen concentration were carried out, and the effects on soot formation and oxidation were consistent with those in the literature.

On the modeling side, only Spray H soot results were submitted, as reliable gas-phase chemical mechanisms have been available for n-heptane for some time. Existing soot models are able to reproduce measured soot levels and trends with variations in ambient oxygen level and density for Spray H. However, because of the significant differences between the models, no definitive conclusions could be drawn regarding the relative merits of the different modeling approaches or

which physical subprocesses are the most important. Some groups now are beginning to show promising combustion results for Spray A (n-dodecane) in the ignition and liftoff length session, and it is anticipated that soot modeling results should be forthcoming for Spray A.

Recommendations

- It has been shown that accuracy of ambient and boundary conditions in Spray A is crucial. It is therefore recommended that the temperature be characterized carefully and taken into account when monitoring the gas mixture of ECN pre-combustion vessels.
- Significant statistical error was observed in the present LII experiment. It was shown that jitter between the laser and the camera was very probably responsible for the majority of this error. It is therefore recommended for future ECN soot experiments to minimize the jitter and to take it into account in the LII calibration.
- For quasi-steady mode measurements, a longer injection duration such as 4 ms should be employed.
- The focus in soot modeling should shift to injectors and fuels for which new experimental measurements are being made: Spray A, in particular.
- To make progress in physical understanding and modeling, modelers should perform systematic parametric studies to isolate and quantify the effects of individual physical processes. For example, the importance of TCI (or of radiation) can be isolated by comparing results from a model that neglects TCI (or radiation) with results from a model that accounts for TCI (or radiation). The relative importance of individual soot subprocesses (e.g., nucleation, surface growth, agglomeration) can be established by varying soot model parameters.



ECN2: Soot Session Experimental Diagnostics

Session organizers: Dan Haworth Emre Cenker

Second Workshop of the Engine Combustion Network,

Heidelberg, Germany, September 2012

Engine Combustion Network Table of contents

- Introduction and background
- Target ambient and spray
- Standard diagnostics
- Soot volume fraction
- Conclusions and recommendations

Engine Combustion Network Table of contents

Introduction and background

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Engine Combustion Network Introduction and background

• Objective:

- > Collaborative comparisons of **measured and modeled soot** volume fraction (SVF)
 - Comparisons among different institutes
- An increased inter-workgroup communication for phenomena playing key roles in soot processes
 - Concentrations of gas-phase species (e.g., OH, C₂H₂, PAHs)
 - Air entrainment
 - Start of ignition
- > Definition of **best practices** for experimental methods available
- > Definition of **uncertainties**

Strategy:

- > Soot experiments with Spray A
- > Complete **standard diagnostics** for verification
 - > First time ECN experiments at *IFPEn HPHT- Vessel No:2*
- > SVF measurements
- Parametric variations of Spray A

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Spray A – Parametric variation

Engine Combustion Network

Number of holes	single hole – axial (nozzle 678)
Fuel injection pressure	1500 bar, prior to start of injection
Fuel	n-dodecane
Fuel temperature at nozzle	363°K (90°C)
Injection duration	1.5 ms; [4 ms]
Ambient gas temperature	900°K; [800°K, 850°K, 1000°K]
Ambient gas pressure	near 6.0 MPa
Ambient gas density	22.8 kg/m ³
Ambient gas oxygen (by volume)	15% O ₂ ; [0%, 11%, 13%, 21% O ₂]

* Parametric Variations

Engine Combustion Network Table of contents

- Introduction and background
- Target ambient and spray

Standard diagnostics (ECN1 Guidelines-Proceedings)

- > Ambient temperature
- * Soot volume fraction
- Liquid penetration length
 Conclusions and recommendations
 - Vapor penetration length
 - Lift-off length
 - Auto Ignition timing

- ♦ ECN1 (Preburn type vessels) →
 - Global temperature (T_{bulk}) ≠ Local temperature (T_{core}) at spray zone
 - > Non-trivial **density** measurement

T_{core} measurement (radiation corrected thermocouple)

* ρ_{core} computation: $\rho_{core} = \frac{P_{bulk}}{ZT_{core} R_{spesific}}$; Z: compressibility

50 μm-thick Type-K thermocouples (TC):



initial ρ_{bulk} guess:

At
$$ρ_{bulk} = 23.5 \text{ kg/m}^3$$
 → $ρ_{core} ≈ 22 \text{ kg/m}^3 ≠ 22.8 \text{ kg/m}^3$

At
$$ρ_{\text{bulk}} = 24.4 \text{ kg/m}^3$$
 → $ρ_{\text{core}} ≈ 23.8 \text{ kg/m}^3 ≠ 22.8 \text{ kg/m}^3$

• Finally,
$$\rho_{bulk} = 24.0 \text{ kg/m}^3$$

- Could not be verified
 - 25 μm TC measurements (not presented here)

Uncertainties:

 For this study, a total uncertainty of ~±1 kg/m³ in ambient density should be taken into account

Engine Combustion Network Nozzle temperature



Pre-combustion effects on nozzle:

- A TC positioned in the sac volume of the dummy injector (0mm)
- Injector cooler set a value respectively

Remarks:

- Ceramic cover on nozzle for a more stable nozzle temperature
- ~±1°C within the injection range

Engine Combustion Network Liquid penetration

- Non-reacting (~0% O2 concentration)
- Light extinction
 - Diffuse back-illumination imaging
 - Homogenous light background (Fresnel Lens)
 - > Fast Camera at 124k fps



Engine Combustion Network Liquid penetration





- Time-averaged quasi-stationary spray
- Light Extinction at the center-line
- Intersection of linear decay curve-fit and x-axis (following drop-off)

Liquid penetration

Mean LL = 11.00mm, Std LL = 0.35mm Run #1 Run #2 3.5 Run #3 Run #4 3 Run #5 Run #6 2.5 Run #7 Extinction [] Run #8 2 Run #9 Run #10 1.5 Run #11 1 0.5 0 0 5 10 15 20 25 30 Distance from Nozzle [mm]

Engine Combustion Network



✤ LL = 10 to 11 mm

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Engine Combustion Network Vapor penetration

Non-reacting (~0% O₂ concentration)
 Focused shadowgraphy



Engine Combustion Network Vapor penetration



Remarks:

Reproducibility issue

Engine Combustion Network Auto ignition

Direct chemiluminescence

Fast camera, 20k fps

increased gamma correction



Remarks:

- > A single setup (direct visualization) sensitivity to identify 3 mechanisms
- Gamma correction
- Problematic time resolution (50µs)

ECN 2: Soot Diagnostics

Engine Combustion Network Lift-off Length

- OH* chemiluminescence's (line of sight)
- Intensified camera, opened between 2.8ms and 3.3ms aSOI (4ms injection)



Engine Combustion Network LOL vs. O_2



Engine Combustion Network LOL vs. T



Engine Combustion Network LOL vs. T



- Rapid campaign on the IFPEn Vessel #2 before ECN2
- Spray A targeting is not achieved.
- Significant uncertainities on boundary conditions (density, temperature...)
- Additional Spray A targeting campaign will be carried out after ECN2.

Engine Combustion Network Table of contents

- Introduction and background
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Engine Combustion Network Laser Induced Incandescence

Cross sectional information





Single-shot LII image

Assuming homogenous heating

$$f_v = \alpha . I_{LII}$$

λ

Engine Combustion Network Laser Extinction Method

- LEM
 - ✤ Beer's law



Mie theory

$$\overline{\overline{f}}_{v} = \frac{\lambda}{ke}.K$$

 λ : Wavelength [m]

 k_e : Optical extinction coef. [-] ~ 8.7 ^[1]

 k_e is the main source of systematic error (accuracy) !!

[1] Williams T.C. et al; «Measurements of the dimensionless extinction coefficient of soot within laminar difussion flames», Int. Jour. of Heat and Mass Transfer 50:1616-1630.

ECN 2: Soot Diagnostics

Engine Combustion Network LII + LEM coupling

LII + LEM coupling



LEM : information integrated along the line-of-sight

Sector Extended to the entire LII field

$$fv(x, y) = \alpha I_{LII}(x, y) = \frac{\lambda}{ke} \cdot \frac{KL_{LEM}}{KL_{LII}^*} \cdot I_{LII}(x, y)$$

Main work : determining this ratio

Engine Combustion Network LII + LEM coupling

LI signal trapping



Engine Combustion Network LEM coupled PLII setup



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ECN 2: Soot Diagnostics

Laser extinction method

Eliminating natural soot incandescence



- Uncertainities: (at a time-steady environment)
 - 1.3% ΔSignal deviation
 - > Electronics, noise
 - * **1.5%** Mean voltage deviation for I_o
 - > Laser instability, environment dust
 - 2% Day to day deviation

Laser extinction method



$$\frac{I}{I_o} = (-KL)^o$$

$$\frac{K\lambda}{k_{\theta}} = f_{\psi}$$

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ECN 2: Soot Diagnostics

0.9

♦ Spray A – QS (4ms)





Spray A QS (4ms) – Parametric variation



Spray A QS (4ms) – Parametric variation



SVF -- Center line






Engine Combustion Network Table of contents

- Introduction and background
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Engine Combustion Network Recommendations

- Spray A is low sooting
 - Signal trapping is low
- Perform OH* lift-off regularly (simultaneously)
- Long injection duration for quasi stationary soot cloud
- Measure LII gate timing to avoid jitter
- For LEM, Sandia setup is a robust one to minimize beam steering uncertainty

Validation of Soot Model for Spray H



Qi Jiao*, Hu Wang**, and Rolf D. Reitz* *: University of Wisconsin-Madison **: Tianjin University, China



slide 1

Contents

- Current soot model framework
- PRF-PAH mechanism formulation
- Ignition delays for Spray H
- Premixed flames
 - Ethylene (c2h4)
 - N-heptane
- Soot predictions for spray H at ECN website
- Conclusions



Current soot model framework

 $C_{16}H_{10} (A_4) \xrightarrow{\omega_1} 16C(s) + 5H_2$ ([A4]) Soot inception: <u>C₂H₂ assisted surface growth(Leung 1991):</u> $C(s) + C_2H_2 \xrightarrow{\dot{\omega}_2} 3C(s) + H_2$ ([C2H2],S) (N) $nC(s) \xrightarrow{\omega_3} C(s)_n$ Soot coagulation(Leung 1991): 3. $C(s) + \frac{1}{2} O_2 \xrightarrow{\dot{\omega}_4} CO$ ([O2],S) Soot oxidation by O2(NSC model) : 4. **Soot oxidation by OH**(Modified Fenimore and Jones model): $C(s) + OH \xrightarrow{\omega_5} CO + \frac{1}{2}H_2$ ([OH],S) 5. **PAHs surface growth**(Frenklach&Wang, Di Domenico): $C(s) + PAH_{k,j} \longrightarrow C(s+k) + \frac{1}{2}H_2$ ([PAH], S, d_p, d_{PAH}) 6. $S = \pi d_p^2 N \{cm^{-1}\}$ Surface area per unit $Y_{C(S)}$ = soot mass fraction N = soot number density (per cc) volume 6Ya(s) ρ = ambient density Particle size {**cm**} $\rho_{C(S)} = 2.0 \text{ gm/cm}^3$ $M_{C(S)} = MW$ of carbon d_{nuci}=1.25nm (~100 carbon atoms) 7. Two transport eqns.: dp=particle size (1) soot species density; (2) soot number density Gokul Vishwanathan, PhD dissertation, University of Wisconsin-Madison, 2011. (same size for soot in one comp. cell Vishwanathan and Reitz, Comb. Sci. Technol., V.182, 2010. Leung et al., Comb. Flame 87, 1991. d_{PAH}=the PAH collision diameter Frenklach and Wang, In Soot formation in Combustion, 1994 and Di Domenico et al., Comb. Flame, V.157, 2010 slide 3 University of Wisconsin -- Engine Research Center

Primary Reference Fuel (PRF) Mechanism Formulation



References :

[1]. Y. Ra, R.D. Reitz, A reduced chemical kinetic model for IC engine combustion simulations with primary reference fuels, Combustion and Flame, 155 (2008) 713-738.

[2]. N.A. Slavinskaya, P. Frank, A modelling study of aromatic soot precursors formation in laminar methane and ethene flames, Combustion and Flame, 156 (2009) 1705-1722.

[3]. N.A. Slavinskaya, U. Riedel, S.B. Dworkin, M.J. Thomson, Detailed numerical modeling of PAH formation and growth in non-premixed ethylene and ethane flames, Combustion and Flame, 159 (2012) 979-995.

[4]. Y. Shi., H.W.,Ge, J.,Brakora and R.D., Reitz, Energy and Fuels, vol.24, issue 3, pp 1646-1654, 2010.



Ignition Delay for Spray H



Hartmann, I. Gushterova, M. Fikri, C. Schulz, R. Schießl, U. Maas, Auto-ignition of toluene-doped n-heptane and iso-octane/air mixtures: High-pressure shock-tube experiments and kinetics modeling, Combustion and Flame, 158 (2011) 172-178.

K. Fieweger, R. Blumenthal, G. Adomeit, Self-ignition of S.I. engine model fuels: A shock tube investigation at high pressure, Combustion and Flame, 109 (1997) 599-619.

J. Herzler, L. Jerig, P. Roth, Shock tube study of the ignition of lean n-heptane/air mixtures at intermediate temperatures and high pressures, Proceedings of the Combustion Institute, 30 (2005) 1147-1153.

H.-P.S. Shen, J. Steinberg, J. Vanderover, M.A. Oehlschlaeger, A Shock Tube Study of the Ignition of n-Heptane, n-Decane, n-Dodecane, and n-Tetradecane at Elevated Pressures, Energy & Fuels, 23 (2009) 2482-2489.





• Experimental temperature profile was used as input in simulation with CHEMKIN PRO [3].

[1] Slavinskaya, N.A., Frank, P., A modeling study of aromatic soot precursors formation in laminar methane and ethene flames. Combustion and Flame, 2009. 156(9): p.1705-1722.

[2] Inal, F. and S.M. Senkan, Effects of equivalence ratio on species and soot concentrations in premixed n-heptane flames. Combustion and Flame, 2002. 131(1–2): p. 16-28.

[3] CHEMKIN PRO: a chemical kinetics package for the analysis of gas-phase chemical kinetics, Reaction Design, (2008).



slide 6

Sandia_cvb Cases

Table 4.1: Constant volume spray chamber conditions.

Ambient density (ρ)	Vol.% H ₂ O	Vol.% CO2	Vol.% N ₂	Vol.% O ₂
$-kg/m^3$				
14.8	3.77	6.52	89.71	0**
14.8	3.56	6.11	69.33	21*
14.8	3.63	6.22	75.15	15*
14.8	3.65	6.26	78.07	12
14.8	3.67	6.33	80.00	10
14.8	3.69	6.36	81.95	8
30.0	3.63	6.22	75.15	15*
30.0	3.65	6.26	78.07	12
30.0	3.67	6.33	80.00	10
30.0	3.69	6.36	81.95	8*
	Ambient density (ρ) - kg/m³ 14.8 14.8 14.8 14.8 14.8 14.8 14.8 14.8 30.0 30.0 30.0 30.0 30.0 30.0	Vol.% H2OAmbient density (ρ) $- kg/m^3$ 3.7714.83.5614.83.6314.83.6514.83.6714.83.6330.03.6530.03.6730.03.6930.0	Vol.% CO2Vol.% H2OAmbient density (ρ) $- kg/m^3$ 6.523.7714.86.113.5614.86.223.6314.86.263.6514.86.333.6714.86.363.6914.86.223.6330.06.263.6530.06.333.6730.06.363.6930.0	$\begin{array}{ c c c c c c c } Vol.\% N_2 & Vol.\% CO_2 & Vol.\% H_2O & Ambient density (\rho) -kg/m^3 \\ \hline & 89.71 & 6.52 & 3.77 & 14.8 \\ \hline & 69.33 & 6.11 & 3.56 & 14.8 \\ \hline & 75.15 & 6.22 & 3.63 & 14.8 \\ \hline & 78.07 & 6.26 & 3.65 & 14.8 \\ \hline & 80.00 & 6.33 & 3.67 & 14.8 \\ \hline & 81.95 & 6.36 & 3.69 & 14.8 \\ \hline & 75.15 & 6.22 & 3.63 & 30.0 \\ \hline & 78.07 & 6.26 & 3.65 & 30.0 \\ \hline & 78.07 & 6.26 & 3.65 & 30.0 \\ \hline & 80.00 & 6.33 & 3.67 & 30.0 \\ \hline & 81.95 & 6.36 & 3.69 & 30.0 \\ \hline \end{array}$

Ambient temp. (T) = 1000 K, nozzle diameter (d) = 0.1 mm, injection profile – top-hat, injection pressure

Flame lift-off length: First axial location of Favreaverage OH mass fraction reaching 2% of its maximum in the domain.



2-D constant volume chamber mesh,17,000 cells Stretched grid, locally refined near the injector: 0.5mm near the injector, 2.0mm near the walls



slide 7 Engine Combustion Network, http://www.sandia.gov/ecn/.

Spray H Soot Cases

HD/LD_o2%



slide 8

Conclusions

- Firstly, a PRF-PAH mechanism was formulated and validated by ignition delays of n-heptane at equivalence ratios of 1.0 and 0.5.
- Then the mechanism was validated by two premixed flames: c2h4/o2/ar, and n-heptane/o2/n2. Important species for current soot model, such as: c2h2, c2h4, PAHs ranging from benzene to pyrene, were validated as well.
- The model was finally applied to spray H at different conditions, both the averaged soot volume fraction and flame lift-off length could be qualitatively predicted for sweeps of both ambient oxygen content and ambient density.



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The support from CEI, Inc. for visualization from EnSight software.









slide 11



2-equation soot model into CMC framework

- Solve transport equation for soot mass fraction and number density
- Accounts for nucleation, surface growth, coagulation and surface oxidation
- Mono-disperse spherical soot particles assumed
- Optical thin soot model
- Unity Lewis number assumed



2-equation soot model (Leung, C&F 1991)



Source: Bolla, Wright, Boulouchos, Borghesi & Mastorakos, submitted to Comb. Sci. Techn. (2012)



ECN2: Soot session

Session organizers: Emre Cenker Dan Haworth

Second Workshop of the Engine Combustion Network, Heidelberg, Germany, September 2012



- Soot physics and modeling
- Soot modeling results submitted to ECN2
- Modeling issues for discussion

ECN International Sooting Flame (ISF) Workshop

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Current physical understanding of soot formation and oxidation remains limited

- Soot Kinetics (Gas-Phase/Soot Interactions)
 - Nucleation
 - Surface growth
 - Surface oxidation
- Soot-Particle Dynamics (Soot/Soot Interactions)
 - Coagulation
 - Aggregation



Soot Formation in Combustion (1994)

State-of-the-art CFD soot models include many variants

- Nucleation
 - PAH-based
 - Frenklach, Wang in Soot Formation in Combust. (Bockhorn Ed., 1994)
 - C₂H₂-based
 - Leung, Lindstedt, Jones C&F 87:289 (1991)
 - Lindstedt, Louloudi, PCI 30:775 (2005)
- Surface Growth
 - Surface HACA mechanism
 - Frenklach, Wang in Soot Formation in Combust. (Bockhorn Ed., 1994)
 - Surface radicals conserved vs. depleted in C₂H₂-addition step
 - Wang et al. PCI 26:2359 (1996)
 - Steric factor α : fraction of surface sites available for reaction
 - Frenklach, Wang PCI 23:1559 (1991)
 - → Appel, Bockhorn, Frenklach C&F 121:122 (2000): $\alpha = \alpha(T) \rightarrow \alpha_{ABF00}$
 - PAH condensation included vs. excluded
 - Richter, Howard PECS 26:565 (2000)
- Surface Oxidation
 - OH and O₂
 - Neoh, Howard, Sarofim in Particulate Carbon (Smith Ed., 1981)

The first quantity of interest from a CFD-based soot model usually is the total quantity of soot

- Spatial (and temporal) distributions of soot volume fraction
 - Sufficient for computing radiative emission (with appropriate simplifications)





However, it is becoming increasingly important to extract more detailed information, including:

- Particle size distributions
 - Increasing concern about ultra-fine particles
- Particle morphology
 - External structure nonspherical particles
 - Internal structure amorphous versus crystalline
- Particle chemical composition and reactivity

 Health and environment, aftertreatment devices
- Particle absorption coefficient
 - Radiation heat transfer, experimental diagnostics



Different levels of soot modeling are used in CFD

- Correlation-based (zero-equation models)
 - Soot volume fraction specified as a function of local equivalence ratio and temperature
- Semi-empirical (often two-equation models)
 - Modeled equations solved for soot volume fraction and number density
 - Fuel-based (Moss) or acetylene-based (Lindstedt)
- Detailed models
 - Attempt to account explicitly for each key physical processes
 - Require consideration of soot aerosol dynamics
- Soot aerosol dynamics
 - Method of moments with interpolative closure (MOMIC)
 - Discrete sectional method (DSM)
 - MOMIC/DSM variants and hybrids
 - Mueller, Blanquart & Pitsch *C&F* 156:1143 (2009)
 - Stochastic methods

Aspects that are often neglected in CFD-based soot models include:

- Agglomeration into non-spherical particles
- Internal structure of primary particles
 - Crystalline versus amorphous
- Chemical composition of particles
 - Beyond pure carbon
 - Element conservation
- Volume/mass of particles in the multiphase mixture
- "Particulate matter" versus "soot"
 - To compare with experiment



Balthasar & Frenklach *C&F* **140**:130 (2005)





Radiation heat transfer is closely linked to soot

- Radiation is an important mode of heat transfer in many (most?) turbulent combustion systems
- Radiation often has been ignored altogether or has been treated using simple models
 - e.g., optically thin approximation
- Difficulties
 - Strong temperature dependence (T⁴)
 - Mixtures of molecular gases (spectral band radiation) and soot (broadband radiation)
 - Solution of the radiative transfer equation (RTE)
 - Turbulence-radiation interactions (TRI)

Different levels of radiation modeling are used in CFD

- Neglect radiation altogether
- Optically thin radiation
 - No RTE solution required
- Neglect scattering
- Spectral treatments
 - Gray
 - Various spectral approximations
 - Line-by-line (with stochastic RTE solver)
- RTE solution methods
 - Stochastic methods
 - Photon Monte Carlo (PMC)
 - Deterministic Methods
 - Discrete-ordinates method (DOM)
 - Spherical-harmonics methods (e.g., P1, P3)
- Turbulence-radiation interactions
 - Ignored altogether versus emission-only TRI versus full TRI

Turbulence-chemistry-soot-radiation interactions are important in atmospheric-pressure luminous flames





ECN Soot physics and modeling





 Mehta et al., Combust. Flame 157:982 (2010); Mehta et al., Combust. Th. Model. 14:105 (2010)

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 ECN 2: Soot
 12/23

Difficulties in high-pressure flames include:

- Physical modeling uncertainties increase
 - High-fidelity experiments are difficult
- Soot
 - Agglomeration more prominent
 - Soot level scales as p^n , where the value of n:
 - Depends on the specific metric and the configuration
 - Depends on fuel type
 - Is usually between 1 and 2 at low-to-intermediate p (~1-10 atm, say)
 - Decreases to ~0 at very high pressures ("saturation")
- Radiation
 - Optical thickness increases
 - Re-absorption becomes important RTE solution required
 - Scattering may be relatively more important
 - Gas/soot spectral interactions become more complicated
 - TRI become more pronounced
- Sprays
 - High injection pressures that approach or exceed the critical pressure
 - High liquid volume fractions (dense sprays)

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Some modeling aspects may be simpler at high pressure

- Soot
 - Computed soot yields are less sensitive to detailed rate specifications
- Radiation
 - Broadening of spectral lines for molecular gas radiation







Priorities for ECN2

- Mean soot volume fraction (SVF) distributions in the quasi-steady flame
- > Variations in ambient O_2 level for fixed initial ρ and T
- Results for Spray H were submitted by two groups, each for a single model:
 - ETH Zurich (ETH)
 - 14.8 kg/m³, 1000 K: 8%, 10%, 12%, 15% and 21% O₂
 - 30 kg/m³, 1000 K: 8%, 10%, 12% and 15% O_2
 - LOL, axial location of peak mean SVF, value of peak mean SVF
 - Centerline profiles of mean SVF
 - Radial profiles of mean SVF
 - 2D contours of mean SVF
 - University of Wisconsin-Madison (UWM)
 - 14.8 kg/m³, 1000 K: 10% and 21% O₂
 - 30 kg/m³, 1000 K: 10% and 15% $\rm O_2$
 - LOL, axial location of peak mean SVF, value of peak mean SVF
 - Centerline profiles of mean SVF
 - Radial profiles of mean SVF

	MODEL DETAILS SCROLL DOWN TO	ETH		MODEL DETAILS SCROLL DOWN TO COMPLETE	UWM	
ECN	Model number	1		Model number	1	
	Definitions - Ignition Delay				Definitions - Ignition Delay	
		fraction reaches 2% of the maximum in the domain				
		after a stable flame is established. 2. Time of maximum rate of rise of maximum			Time of maximum rate of rise of maximum	
					temperature.	
		temperature.		Definitions Lift off longth		
	Definitions with off loweth			Definitions - Litt off length		
	Definitions - Lift off length	 First axial location of Favre-average OH mass fraction reaching of 2% its maximum in the domain. 			the distance between the injector and the location	
					when temperature reaches 1200K, because sometimes the OH concentration near injector is not continuous for some cases	
	Code name	STAR-CD v4 1	TCI			
	Turbulence chemistry interaction model	CMC		Code name	KIVA	
	Chemistry model	CIVIC		Turbulence chemistry interaction model	well-mixed	
	chemistry model	Pitsch mechanism in Liu et al. CNF 137 (2004) 320:		Chemistry model		
	Dasa mashanism	reduced mechanism with 43 species but only 22			1. TRF mechanism (93species,531reactions) from	
	Base mechanism	transported species and 18 reactions. Other species		Base mechanism	multi-component chemistry mechanism developed by	
	Chamistry dimensional reduction /	are treated with quasi-steady assumption.	Chemical		Ra and Reitz, combustion and flame, 2011.	
	acceleration			Chamistry dimensional reduction /	z. Woulled	
	Turbulence model	RANS K-E-RNG	mechanism	chemistry dimensional reduction /		
	Sub-grid or turbulent scalar transport	Gradient transport	meenamsm	Turbulanca madal	PANS	
	Spray model			Sub grid or turbulant scalar transport	Cradient transport	
	Used Lagrangian discrete phase model			Sub-grid of turbulerit scalar transport	Gradient transport	
	(Y/N), If N, then what method?	Y		Spray model		
	Injection	Blob		N. then what method?	Y	
	Atomization & Breakup	Reitz-Diwakar		Injection	Blob	
	Collision	O'Rourke		Atomization & Breakun	KH-BT (with break-up length)	
	Drag	Dynamic		Collision	O'Bourke	
	Evaporation	Ranz-Marshall		Drag	Dynamic	
	Heat Transfer	Ranz-Marshall			reference Ba and Beitz International Journal	
	Dispersion	Stochastic		Evaporation	of Multiphase Flow, 2009.	
	Grid			Heat Transfer	Ranz-Marshall	
	Dimensionality	2D axisymmetric		Dispersion	Stochastic	
	Туре	structured Cartesian		Grid		
	Grid size range (mm)	0.5 mm hom.		Dimensionality	2D axisymmetric	
	Total grid number	20,000		Type	stretched grid	
	Time advancement	2162		Grid size range (mm)	0.5mm-1.5mm	
	lime discretisation scheme	PISO		Total grid number	17,000	
	lime-step (sec)	1.00E-06	Cast	Time advancement		
	Soot model	comi ompirical Loung et al CNE 97 (1001)	Soot	Time discretisation scheme		
	Description	298-305		Time-step (sec)	5.00E-06	
		298-303	model	Soot model		
	Physics accounted for	C2H2, agglomeration, oxidation by O2 and OH.	← →	Description	semi-empirical, ref:Vishwanathan and Reitz, Comb. Sci. Technol., V.182, 2010.	
	Number of additional equations solved	2			nucleation surface growth agglemoration	
	Quantities solved for	Soot number density and mass fraction		Physics accounted for	oxidation	
	Kadiation model	Y optically thing radiatics have at (14/34	Dadiation	Number of additional equations solved	2	
	Description (if Y) Description (if Y)	Radiation	Quantities solved for	Soot number density and mass fraction		
		Description (if Y) CO2 CO H2O CH4 (Barlow CNE 127 (2001)	n (if Y) CO2 CO H2O CH4 (Barlow CNE 127 (2001)	\longleftrightarrow	Radiation model	N
		2102-2118)	•	Description (if Y)		
	Time after SOI or time interval (if time	_		Time after SOI or time interval (if time		
Sentember 201	averaged) for quasi-steady model results	5 ms	2. Soot	averaged) for quasi-steady model results	2.5ms-7.05ms	
September 20.	Any other important information		2. 5000	Any other important information		





ECN Centerline mean SVF @ 14.8 kg/m³, 1000 K






✤ 10% O₂





ETH



✤ 21% O₂





ECN 2D mean SVF contours @ 30 kg/m³, 1000 K

Experiment

✤ 10% O₂





ETH



ECN Soot modeling issues for discussion

- Influence of variations in soot model parameters
 - > Models calibrated for canonical configurations versus engines
- Correlations with gas-phase quantities
 - Mixture fraction
 - > Key gas-phase species (e.g., C_2H_2 , PAHs, O_2 , OH, . . .)
- Influence of radiation heat transfer
- Influence of turbulent fluctuations
 - > Turbulence-chemistry-soot-radiation interactions
- Beyond time-averaged mean quantities in the quasi-steady flame
 - Transient evolution and "emissions"
 - Rms values, histograms or PDFs
- Beyond soot volume fraction
 - > Particle size distributions
 - Composition and morphology
- Accounting for "phase errors" between simulation and experiment
 - > e.g., from LOL mismatch
- More direct comparisons between simulation and experiment
 - > e.g., direct comparisons of computed and measured radiative intensities