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Large Eddy Simulations for Detailed Soot Investigations

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1 Introduction

Modelling of soot formation in diesel engines is a challenging task, because it depends on the accurate description of a long chain of complex processes such as break-up, atomization and evaporation of the liquid fuel, mixture formation, auto-ignition and combustion in a turbulent flow-field as well as the interaction of chemistry and turbulence with the soot dynamics themselves.

In this study, the spatially filtered conservation equations are solved numerically and a semi-empirical soot model is implemented in order to simulate a reacting n-dodecane spray. The simulation pertains to experiments conducted in the cube-shaped, pre-burn combustion vessel of Sandia National Laboratories¹ (**Fig 1.a**). The corresponding computational grid, which consists of 1.8 million cells, is shown in **Fig 1.b**. The test case considered (**Table 1**) represents engine-relevant conditions with moderate EGR.

Table 1: Operating conditions for Spray A					
Ambient Temperature	900 K	Injection Duration	6 ms		
Ambient O ₂ mol fraction	15%	Fuel Type	n-dodecane		
Ambient Density	22.8 kg/m ³	Fuel Temperature	363 K		
Injection Pressure Difference	150 MPa	Orifice Diameter	0.091 mm		



Figure 1: a) Schematic of the optically accessible high-temperature, high-pressure combustion chamber. b) Cross-section of the computational grid at the midplane of the domain.

2 The Soot Model

The two-equation model originally proposed by Leung² and extended by Kronenburg³ has been employed in this study. Additional transport equations are solved for the soot mass fraction (Y_s) and particle number density (N_s). Monodisperse distribution and spherical shape are assumed for the soot particles.

The model accounts for simultaneous particle inception, surface growth by C_2H_2 adsorption, oxidation by O_2 , oxidation by OH and agglomeration (**Table 2**). Accordingly, the source terms of the two equations read:

• $\omega_{Y_s} = 2R_{INCP} + 2R_{SGRW} - R_{OxO2} - R_{OxOH}$

• $\omega_{N_s} = 2R_{INCP} N_{AV}/n_{C,min} - R_{AG}$

The reaction rate constants in I to IV follow Arrhenius-like expressions of the form: $k = AT^{\beta}e^{-\frac{Ta}{T}}S_{soot}^{c}$. The last term represents the functional dependence of the respective process on soot surface density, S_{soot} .

3 Results and Discussion

Vapor penetration shows excellent agreement with the experiment, while global soot mass is underestimated by one order of magnitude (**Fig 2.a**). This discrepancy can be addressed by tuning A_{SGRW} , which has originally been calibrated for CH_4 -air flames at atmospheric pressure.

The time-averaged⁴ soot volume fraction contours also show a very similar distribution of sooting areas with the experiment (**Figure 2.b**). Soot presence is confined to the fuelrich areas of the spray and downstream of the flame lift-off length, in the vicinity of which formation of C_2H_2 is favored. High intermittency is correctly reproduced.

Conceptually the soot cloud (defined as $2\% fv_{soot,max}$) can be divided in three distinct zones of soot evolution (**Figure 2.c**). The first zone extends from the onset of soot formation until the location of peak net formation. The second zone marks the transition from maximum net formation to maximum net oxidation. The last zone tracks the oxidation of soot, with inception and surface growth fading in the absence of C_2H_2 , as the mixture leans out and the flame tip is approached. Particle inception contributes little to soot mass per se, but it is important for creating the sites where the bulk of formation will take place by surface growth, slightly upstream of peak soot volume fraction. O_2 -oxidation takes place in a very thin layer across the flame, mostly on the fuel-rich side (see also **Fig 2.d**). OH-oxidation extends over a much wider area than O_2 -oxidation because of the greater extent of OH presence in the fuel rich zone and is therefore

	Table 2: Kinetic mechanism of soot					
No	Process Reaction		Reaction Rate			
Ι	Particle Inception	$C_2H_2 \xrightarrow{R_{INCP}} 2C_{(s)} + H_2$	$R_{INCP} = k_{INCP} [C_2 H_2]$			
п	Surface Growth	$C_2H_2 + nC_{(s)} \xrightarrow{R_{SGRW}} (n+2)C_{(s)} + H_2$	$R_{SGRW} = k_{SGRW} [C_2 H_2]$			
ш	Oxidation by O ₂	$C_{(s)} + \frac{1}{2} O_2 \xrightarrow{R_{OxO2}} CO$	$R_{0x02} = k_{0x02}[0_2]$			
IV	Oxidation by OH	$C_{(S)} + OH \xrightarrow{R_{OxOH}} CO + H$	$R_{OxOH} = k_{OxOH}[OH]$			
v	Agglomeration	$nC_{(s)} \overset{R_{AG}}{\longrightarrow} C_{n(s)}$	$R_{AG} = 2C_a \left(\frac{6M_s}{\pi \rho_s}\right)^{1/6} \left(\frac{6k_{Boltz}T}{\rho_s}\right)^{1/6} (\rho N_s)^{11/6}$			



ultimately more dominant.

Analysis of azimuthally and radially integrated quantities along the spray axis (**Fig 2.e**) yields that surface growth rate is affected more by the distribution of soot (correlation coefficient: $\langle r \rangle = 0.876$) than by the soot precursor ($\langle r \rangle = 0.651$), which is itself controlled by mixture with equivalence ratio over 1.5 ($\langle r \rangle = 0.955$). O₂ mass encompassed by the soot cloud agrees very well with O₂-oxidation $\langle r \rangle = 0.879$, even though only 40% takes place within the cloud. Finally, correlation between OH and OH-oxidation is even higher ($\langle r \rangle = 0.964$), because about 90% of soot oxidation by OH takes place within the soot cloud.

Overall, LES offers a framework capable of predicting accurately the spatial distribution of soot as well as capturing transient and intermittent processes with a simple model.

4 Acknowledgements	5	References
Financial support from the Swiss Federal Office of Energy (grant no. SI/500818- 01) and the Swiss Competence Centre Energy and Mobility (CCEM project "ScheDual") is gratefully acknowledged.	1. 2. 3. 4.	 Pickett, L.M., Engine Combustion Network. http://www.sandia.gov/ecn/dieselSprayCombustion.php Leung, K.M., R.P. Lindstedt, and W.P. Jones, A Simplified Reaction-Mechanism for Soot Formation in Nonpremixed Flames. Kronenburg, A., R.W. Bilger, and J.H. Kent, Modeling soot formation in turbulent methane- air jet diffusion flames. Farrace, D., et al., Analysis of Averaging Methods for Large Eddy Simulations of Diesel Sprays.

Large Eddy Simulations for Detailed Soot Investigations

The primary aim of this work has been to assess the predictive capabilities of the LES framework with respect to soot dynamics in a reacting diesel spray. The relatively advanced k-equation LES technique is utilized together with the uninvolved Direct Integration (DI) combustion model[1]. A single but full injection event is simulated with a view to tracking the complete course of the spray evolution and collecting sufficient statistics[2]. A version of Leung's phenomenological soot model has been implemented[3], modified to additionally account for oxidation by OH[4]. The flow field is treated with the commercial CFD code STAR-CD and the computational mesh is three-dimensional, cubic and symmetric over the X and Y planes. It comprises hexagonal, nominally cubic cells. The model corresponds to the "Spray A" experimental data set of the Engine Combustion Network (ECN), obtained from the optically accessible high-pressure and high-temperature constant volume combustion chamber (CVCC) installed at the Sandia National Laboratories (SNL)[5]. The configuration consists of a cubic-shaped, pre-burn chamber with a side of 108 mm, in which normal dodecane is injected. The reference operating condition considered in this work reports a 900 K initial nominal temperature and 15% oxygen volume fraction.



Figure 1: Temporal evolution of vapor penetration and soot mass inside the combustion chamber as measured for the reference case by SNL and as calculated in the simulations

Figure 1 depicts the temporal evolution of vapor penetration and total soot mass inside the combustion chamber. The spray event can be divided into three distinct periods in order to facilitate the analysis. The first period commences with the start of injection and lasts until the soot plateau is established at approximately 3 ms ASOI. The second phase corresponds to the soot plateau observed in the experiments and lasts from 3 to 6 ms ASOI. It mirrors the quasi-steady state of the conceptual spray model [6]. Results referring to this phase will be presented in the form of time mean and standard deviation. These are defined as

$$\langle \widetilde{\phi} \rangle = \frac{1}{N} \sum_{n=1}^{N} \widetilde{\phi}$$
 and $\sigma_{\widetilde{\phi}} = \sqrt{\frac{1}{N-1} \sum_{n=1}^{N} (\widetilde{\phi} - \langle \widetilde{\phi} \rangle)^2}$

respectively, where $\tilde{\varphi}$ represents some time-dependent, Favre-averaged quantity of the flow-field and N is the total number of time-steps. Data have been collected over a period of 3 ms, that is between 3 and 6 ms ASOI, with prescribed generation of output files at intervals of 0.025 ms, which amounts to N = 121 samples. The last phase of the spray event is the transient period that ensues after the end of injection and ends when the soot content inside the combustion chamber is completely oxidized at 7 ms ASOI.

Figure 2 displays the spatial distribution of soot over time at the vertical midplane XZ of the combustion chamber. The spray boundary is defined as an isoline for ξ =0.1%. The stoichiometric level is defined for $\xi = \xi_{stoich}$ and the boundary of the soot cloud is arbitrarily defined at $\widetilde{Fv}_{soot} = 0.02\widetilde{Fv}_{soot}^{max}$, where $\widetilde{Fv}_{soot}^{max}$ equates to the instantaneous peak value of soot volume fraction in the computational domain. Predicted global soot mass is found to be roughly one order of magnitude lower than the experimentally measured, which is attributed to underestimation of the pre-exponential factor in the surface growth step for the fuel under consideration[7-9]. The simulation successfully predicts the time-averaged distribution of soot volume fraction in physical space and it additionally succeeds at capturing the intermittency of soot formation and oxidation in the instantaneous fields and reproducing the mechanisms that drive it.



Figure 2: Top: Instantaneous contours of soot volume fraction at four selected time instants during soot onset and timeaveraged contours of soot volume fraction during the quasi-steady state for LES. Bottom: instantaneous images of soot optical thickness during soot onset and time-averaged over the quasi-steady state, ensemble-averaged over multiple realizations contours of soot volume fraction, as measured by SNL.

Figure 3 shows contour plots of the time-averaged soot volume fraction and kinetic soot source terms during the quasi-steady state. Conceptually the soot cloud can be divided in three distinct zones of soot evolution. The first zone extends from the onset of soot formation (17mm, defined as 5% of the maximum formation rate) until the location of peak net formation rate (39.9mm). The second zone marks the transition from maximum net formation to maximum net

oxidation (60.9mm). The last zone engulfs the oxidation of soot as inception and surface growth fade in the absence of C_2H_2 , as the mixture becomes less rich and the flame tip is approached. It extends up to 80mm from the injector tip, past which no soot particles survive. Note that the absence of large standard deviation regimes at the far end of the computational domain indicates that soot processes are always confined to a section of the domain suitable to time-averaging technique.

Surface growth is strongest at distances between $40 \div 60 \text{ mm}$ from the injector tip. Maximum formation rate is located slightly upstream of peak soot mass, because of the finite rate kinetics in the model and the downstream advection of soot. Inception does not contribute significantly to soot mass, but creates the sites where the bulk of soot formation will take place. The DI combustion model predicts a thin reaction zone that only sees a petty amount of O_2 survive in the fuel-rich side and restricts oxidation of soot by O_2 in a very narrow layer across the stoichiometry. OH exhibits a broader profile with substantial presence in the fuel-rich region, which is the root cause of the predominance of soot oxidation by OH. Standard deviation of both oxidation terms is strong in the third zone, because flame pockets are frequently detached from the main column and oxidized in this area. Mean fields of the kinetic terms become comparable in magnitude to the respective fields of standard deviation because of the high intermittency associated with the soot processes, as is consistent with behavior in soot volume fraction.



Figure 3: Time-averaged contours of Favre-averaged rates of surface growth, oxidation by O₂ and oxidation by OH during the quasi-steady period for RANS (top) and LES (bottom).

Finally, in order to investigate in greater detail the soot transient dynamics, the variation of quantities relevant to soot formation and distribution is analyzed along the spray axis. At each axial distance from the injector, an integration over the transverse cross-sectional plane is performed (Figure 4). Correlation coefficients are calculated for the instantaneous distributions and then averaged over the 121 available time instants during the quasi-steady phase, where the very low standard deviations indicate that a strong correlation exists for each instantaneous field as well. The

enhanced flow structures captured by the LES model affect the distribution and magnitude of soot mass fraction by shaping the chemical and advective terms, which are found to be the most prominent ones. Intermittency in soot is generated by the fact that the advective term and the chemical term do not balance out each other. The same observation holds in a fully 3D analysis. The chemical term is linked to the flow field both on the side of soot formation through surface growth rate, which is in turn determined by existing soot mass ($\langle r \rangle \sim 0.876$) and acetylene ($\langle r \rangle \sim 0.651$), itself determined by fuel-rich gas for $\Phi \ge 1.5$ ($\langle r \rangle = 0.955$), and soot oxidation through O₂-oxidation and OH-oxidation, which are controlled by the respective oxidant ($\langle r \rangle \sim 0.879$ and $\langle r \rangle \sim 0.964$) concentration within the soot cloud.



Figure 4: Axial variation of radially and azimuthally integrated quantities in 0.1mm slice. All integrations are performed over the whole transverse cross-section of the domain at each axial distance, with the exception of the second row of plots, which depicts the mass flow rate and the oxidizers' mass enclosed into the soot cloud.

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