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# Soot and spectral radiation modeling for high-pressure turbulent spray flames

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ABSTRACT

A transported probability density function (PDF) method and a photon Monte Carlo/line-by-line (PMC/LBL) spectral model are exercised to generate physical insight into soot processes and spectral radiation characteristics in transient high-pressure turbulent n-dodecane spray flames, under conditions that are relevant for compression-ignition piston engines. PDF model results are compared with experimental measurements and with results from a locally well-stirred reactor (WSR) model that neglects unresolved turbulent fluctuations in composition and temperature. Computed total soot mass and soot spatial distributions are highly sensitive to the modeling of unresolved turbulent fluctuations. To achieve reasonable agreement between model and experiment and to capture the highly intermittent nature of soot in the turbulent flame, it is necessary to accurately represent mixing and the low diffusivity of soot particles. This is accomplished in the PDF framework using a mixing model that enforces locality in the gas-phase composition space, while not mixing the transported soot variables. The results suggest that mixing is at least as important as kinetics in controlling soot formation and evolution in high-pressure turbulent flames. Regarding radiation, radiant fractions and global influences of radiation in these flames are relatively small. Nevertheless, an examination of spectral radiative heat transfer provides valuable insight into the nature and modeling of radiation in high-pressure turbulent combustion systems. There are complex spectral interactions that are revealed using PMC/LBL. $CO_2$ dominates the total radiative emission and reabsorption, but most of the emitted $CO_2$ radiation is reabsorbed before reaching the walls. On the other hand, most of the emitted soot radiation reaches the walls, but soot radiation is a small contribution overall; $H_2O$ dominates the radiation that reaches the walls. Global turbulence–radiation interactions (TRI) effects are small, but radiative emission from soot increases by approximately a factor two when TRI are considered. Radiative transfer contributes both to energy redistribution in the vessel and to wall heat losses. The results suggest that a simple model that considers soot radiation and the principal $CO_2$ and $H_2O$ spectral bands might be sufficient to capture the key influences of radiation in engine CFD. It is expected that these findings will contribute to the development of truly predictive CFD models for engines and other high-pressure turbulent combustion systems.



## 1. Introduction

Compression-ignition piston engines are widely used in applications including transportation, construction, farming and electric power generation. Increasingly stringent regulations on fuel consumption and emissions are driving the development of next-generation engines that aim to simultaneously achieve high reliability, low maintenance, low fuel consumption and low pollutant emissions [1]. Advanced and truly predictive computational fluid dynamics (CFD)-based models are needed to achieve these goals [2]. Key physical processes to be modeled include liquid fuel injection and spray processes, autoignition and turbulent combustion, heat transfer, and pollutant formation.

In this paper, two important and related aspects are addressed: soot formation/evolution, and spectral radiative heat transfer. Soot modeling for engine-relevant conditions has received considerable attention, because of the importance of soot as a component of particulate matter, a regulated pollutant. However, soot modeling

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remains a weak link in engine CFD. Most soot models are based largely on physical understanding of soot processes derived from experiments at atmospheric pressure or at moderately elevated pressures (usually less than 10 atm) compared to engine-relevant conditions, and the emphasis has been on soot kinetics rather than on turbulent hydrodynamics and mixing. On the other hand, radiative heat transfer modeling in engines has received relatively little attention, although it is increasingly recognized that it can be important both for energy redistribution within the combustion chamber and as a contributor to wall heat losses [3,4]. Conventional wisdom has been that radiative heat transfer in engines is dominated by soot radiation. However, as operating pressures and exhaust-gas recirculation (EGR) levels in engines increase, and as combustion systems are designed to produce less in-cylinder soot, molecular gas radiation (primarily from $CO_2$ and $H_2O$) and spectral radiation properties become more important.

To make progress toward unraveling the complex underlying physical processes and developing reliable CFD models, it is expedient to consider configurations that are more amenable to modeling and experiment compared to a practical engine. To this end, the Engine Combustion Network (ECN) [5] was established to provide an open forum for international collaboration among experimental and computational researchers in engine combustion. One target configuration is a constant-volume turbulent spray combustion chamber that can reach thermochemical conditions (composition, temperature and pressure) that are representative of those in modern direct-injection compression-ignition engines, while allowing a high degree of optical access for advanced experimental diagnostics and well-characterized initial and boundary conditions for CFD, including detailed fuel-injector characterization [5–7].

Here ECN "Spray A" (liquid n-dodecane fuel) is targeted. A transported probability density function (PDF) method is used to account for the influences of unresolved turbulent fluctuations in composition and temperature on chemistry (turbulence–chemistry interactions – TCI) and on radiation (turbulence–radiation interactions – TRI), and a photon Monte Carlo (PMC) method with line-by-line (LBL) spectral resolution is used for spectral radiative transfer. Several earlier modeling studies have been published for Spray A, and an up-to-date summary can be found at [8]. Most relevant to the current work are studies that focused on turbulence–chemistry interactions using transported PDF methods [9–11], including soot and radiation [12]. Results obtained here will be compared with experimental measurements and with results from earlier modeling studies in the Results and Discussion section.

The main contributions of this paper are: 1) to confirm the importance of turbulence–chemistry interactions in high-pressure turbulent flames, and to demonstrate that they are especially important for soot formation and evolution; 2) to show that with appropriate treatment of unresolved turbulent fluctuations, a RANS-based model can capture soot intermittency and related effects; 3) to provide evidence that turbulent transport and mixing are at least as important as kinetics in governing soot formation and evolution in high-pressure turbulent flames, such as in engines; 4) to show that consideration of spectral radiative properties is essential to understanding radiative transfer in engine-relevant environments; and 5) to propose key ingredients that should be included in a CFD-based model for radiative transfer in engines. These are expected to contribute to the development of truly predictive CFD-based models of in-cylinder processes in engines and other high-pressure turbulent combustion systems.

## 2. Target flames

The experimental configuration is a constant-volume, optically accessible, cubic spray combustion vessel with an enclosed volume of 1147 $cm^3$. The vessel is capable of accessing a wide range of engine-relevant thermochemical conditions, allowing initial temperatures up to 1400 K, pressures up to 350 MPa and different levels of oxygen and simulated EGR gases. The desired pre-fuel-injection ("ambient") conditions are varied by preburning a combustible mixture. For this purpose, two spark plugs and a mixing fan are mounted on one wall of the vessel. Further description of the experimental setup can be found in [7]. This is one of the ECN target configurations [5].

Here simulations of ECN Spray A are reported [8]. Liquid sprays of n-dodecane ($C_{12}H_{26}$) are injected using a common-rail diesel-engine fuel injector with a single orifice of nominal diameter 90 μm, located at the center of one vessel wall and injecting toward the center of the vessel. In all cases, the initial chamber gas density is 22.8 $kg/m^3$, the liquid fuel injection pressure is 150 MPa, and the injection duration is 5.5 ms. For reacting cases, the ambient gas composition includes 15% $O_2$ with the remainder being $N_2$ (75.15%), $CO_2$ (6.22%) and $H_2O$ (3.62%), and the ambient temperature ranges from 750 K to 1200 K. The baseline Spray A case corresponds to an ambient gas temperature of 900 K, and this is the condition that is analyzed most extensively in this paper. Reacting experimental data include ignition delays and lift-off lengths, total soot mass as a function of time after start of injection (SOI) and spatial distributions of soot volume fraction [13], and radiant fractions and spatially and spectrally resolved radiative intensities [14].

For the nonreacting case, the ambient gas composition is pure $N_2$ and the ambient temperature is 900 K. In the experiments, the same fuel-injector nozzle was used for all reacting cases (#210370), while a different (nominally identical) nozzle was used for the nonreacting case (#210677). Nonreacting experimental data include liquid and vapor penetration as functions of time, and spatial distributions of mixture fraction (fuel mass fraction) at different times after SOI [7,15].

## 3. Physical models and numerical methods

An unsteady Reynolds-averaged Navier–Stokes (URANS) formulation is adopted, using solvers based on the OpenFOAM v2.3.x toolbox [16]. A segregated pressure-based finite-volume method is used to solve the coupled mean momentum, pressure and enthalpy equations, with second-order spatial discretizations and first-order implicit time discretization. The baseline physical models and model coefficients are summarized in Table 1.

A two-equation $k-\varepsilon$ turbulence model is used [17]. The model coefficients are $C_\mu$ (multiplies $k^2/\varepsilon$ to give the apparent turbulent viscosity), $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and $C_{\varepsilon 3}$ (coefficients in the modeled $\varepsilon$ equation), and $\sigma_k$ and $\sigma_\varepsilon$ (turbulent Schmidt numbers in the $k$ and $\varepsilon$ equations, respectively). Standard values are used for all coefficients except $C_{\varepsilon 1}$, for which a simple round-jet correction has been used (value increased from 1.44 to 1.55 [18]).

The liquid fuel injection and spray evolution are modeled using a stochastic Lagrangian parcel method [21]. The spray is represented by a finite number of parcels, where each parcel represents a group of droplets having the same properties. A simple blob model is employed to represent spray atomization [19,20], and the Reitz–Diwakar model is used for secondary breakup [22,23]. These models are not considered to be truly predictive; rather, the models are tuned to match the measured liquid and vapor penetration rates for the nonreacting case (see Section 4.1 below). The atomization model coefficient *LBU* is related to the distance from the fuel nozzle where the secondary breakup model is switched on, and a standard value of 1.0 has been used. The secondary breakup model coefficients are: critical Weber number for bag-type breakup $C_{bag}$, time factor for bag-type breakup $C_b$, Weber number factor for stripping-type breakup $C_{strip}$, and time factor for