

A CFD Study of Post Injection Influences on Soot Formation and Oxidation under Diesel-Like Operating Conditions

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ABSTRACT

One in-cylinder strategy for reducing soot emissions from diesel engines while maintaining fuel efficiency is the use of close-coupled post injections, which are small fuel injections that follow the main fuel injection after a short delay. While the in-cylinder mechanisms of diesel combustion with single injections have been studied extensively and are relatively well understood, the in-cylinder mechanisms affecting the performance and efficacy of post injections have not been clearly established. Here, experiments from a single-cylinder heavy-duty optical research engine incorporating close-coupled post injections are modeled with three dimensional (3D) computational fluid dynamics (CFD) simulations. The overall goal is to complement experimental findings with CFD results to gain more insight into the relationship between post-injections and soot.

This paper documents the first stage of CFD results for simulating and analyzing the experimental conditions. In this stage, an engineering CFD model with a two-stage soot sub-model facilitates development of new and appropriate analysis methods. The methods include new ways to visualize and quantify soot formed, soot oxidized and net soot. Parameters used to evaluate formation and oxidation, like fuel and oxygen concentrations, are also visualized and quantified to provide a deeper understanding of the in-cylinder evolution of soot.

Experiments found and CFD replicated a trend where engine-out soot first decreases, then increases with increasing postinjection duration when both the main injection duration and dwell between injections are held constant. To help understand this trend, a number of factors that influence soot formation and oxidation are analyzed, including changes in temperature, pressure, oxygen, fuel vapor and soot distributions. Fuel vapor distribution and burn rate variation appear to be dominant factors in determining whether soot increases or decreases with post injections.

The prime conclusion regarding the in-cylinder mechanism of soot reduction by post injections is that the simulations predict that short post injections increase the rate of fuel burning, thereby reducing the soot precursor species (vapor fuel) concentration, leading to lower soot formation. The model does not predict any appreciable increase in soot oxidation with a short post injection. Indeed, late in the cycle, soot oxidation with a short post injection is slower than with only the main injection because less oxygen is available for soot oxidation after combustion of the larger injected fuel mass and because there is less soot to oxidize.

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INTRODUCTION

Ever-tightening pollutant emissions standards for diesel engines, coupled with regulatory drivers and market demands for lower carbon dioxide emissions and/or lower fuel consumption, motivate the development of strategies to lower pollutant emissions while maintaining fuel efficiency. In recent years, a multitude of in-cylinder and exhaust aftertreatment strategies have been explored, and most current production engines use a combination of both strategies. One in-cylinder strategy of current interest for reducing engine-out soot emissions while maintaining fuel efficiency is the use of close-coupled post injections. Post injections are small injections of fuel that follow a conventional main fuel-injection in a diesel engine, and they are "close coupled" if the dwell between injections is relatively short (typically a few crank angle degrees).

A number of experimental and modeling studies have demonstrated the effectiveness of post injections, and have provided some insight into the in-cylinder mechanisms that may be responsible (see recent review paper [1]). While experimental studies are valuable for establishing the net result of post-injection strategies, the data often do not provide sufficient insight into the in-cylinder mechanisms that yield the global observations. Even in optical engines that provide visualization of in-cylinder processes, experimental uncertainties and optical access constraints leave some aspects unclear. Multi-dimensional reacting flow simulations, by contrast, provide much greater spatial and temporal resolution that can yield greater insight into the in-cylinder fluid mechanical and chemical kinetic mechanisms occurring with post injections.

Two significant factors that limit the utility of simulation predictions are the validity of the simulations, and the ability to extract insight from the massive dataset provided by the simulations. Here, we take steps to address both of those limitations. We use an optical engine to validate the model predictions to the degree possible. The effort is expected to span multiple years and publications, starting with the current study, which reports initial comparisons between model and experiment. The bulk of the current study, however, focuses on the development of new tools and techniques for analysis of model predictions to provide understanding of in-cylinder processes and complements observations from various optical diagnostics. The new insight reported herein also builds on previous simulation studies of post-injections, several of which are reviewed in the following paragraphs.

First, Han et al. [2] concluded from the predictions of their CFD modeling study that splitting up the fuel injection event disrupts the replenishment of rich soot-forming regions that develop in long single injections. They simulated the in-cylinder evolution of soot (and NO_x) in a heavy-duty diesel engine with multiple injections and a Mexican-hat shape piston-bowl under conventional high-temperature diesel combustion (no dilution by EGR). Han et al. used the CFD solver KIVA-II [3] with the

Shell ignition [4], characteristic time combustion [5,6,7], Hiroyasu soot formation [8] and Nagle-Strickland-Constable (NSC) soot oxidation [9] models. The amount of fuel in the first pulse varied from 10 to 75% of total injected fuel, and dwells between pulses ranged from 3 to 8 crank angle degrees. With split injections, the model predicted that replenishment of fuel-rich soot-forming regions from the first injection is terminated, and the subsequently injected fuel burns rapidly and does not contribute significantly to soot production. In-cylinder pressure traces and the derived apparent heat release rate curves matched experiments very well and engine-out soot trends compared reasonably well.

Under low-temperature combustion conditions achieved by EGR dilution, Yun et al. [10] concluded that post-injections were effective when they were directed into fuel-lean pockets between fuel-rich zones created by the first injection. The fuel-lean pockets are created in part by an engine's swirl flow as the fuel-rich zones are transported azimuthally about the combustion chamber. They used a later version of the KIVA code, which is based on KIVA3V-R2 [11] with various submodel improvements, two of which are especially relevant to in-cylinder soot modeling. First, the CHEMKIN II [12] chemistry solver with a reduced n-heptane mechanism with 35 species and 77 reactions [13] replaced the Shell ignition and CTC combustion models. Second, rather than using vapor fuel as the soot precursor species, Yun et al. [10] used acetylene (C₂H₂), which is predicted by the reduced reaction mechanism. The simulated operating condition was low-temperature combustion at 1500 RPM, 3 bar gIMEP and 50% exhaust gas recirculation in a high-speed, direct-injection diesel engine. At equivalent load for single- and double-injection conditions, they found that smaller post-injections reduced soot more effectively because they directed fuel into lean air pockets that were located between fuel-rich zones of neighboring sprays generated by the first fuel pulse. By distributing the fuel more broadly, the small post-injections created in-cylinder mixtures with less fuel-rich soot-forming regions.

While single-precursor soot models can provide useful insight into in-cylinder mechanisms of post-injection effects on soot emissions, they do not account for details of the complex reactions that form ever larger precursor species on the synthesis path to soot. The chemical kinetics of large soot precursor species could be very important for soot and condensed species prediction under certain operating conditions, especially low-temperature combustion conditions where soot and soot precursor formation is extended in both space and time compared to conventional conditions [14]. One example of a semi-detailed soot model is that of Vishwanathan and Reitz [15], who also used KIVA3V-R2 [11] in their study. The model framework is based on four fundamental steps: soot inception through a four-ring polycyclic aromatic hydrocarbon species; surface growth through acetylene; soot coagulation; and oxygen- and OH-induced soot oxidation. Combustion was simulated with a reduced n-heptane mechanism and the model was applied to conventional diesel and low temperature combustion regimes, with some operating conditions using

multiple injections. For the conventional diesel case, pressure and heat release comparisons to experimental data were good. Also, Vishwanathan documented an important method for comparing in-cylinder soot mass, as estimated using a two-color optical method [Singh et al. 16], to in-cylinder CFD soot distribution. The model demonstrated the ability to capture, in general, in-cylinder soot variation with crank angle. The start of soot accumulation, the rate of soot increase and the crank angle location of peak soot were all well captured by the model, but the rate of soot decrease was much faster than in the experiments. Vishwanathan suggested the rapid soot decrease was due to faster simulated soot oxidation. But, according to conclusions based on Han et al. [2], as well as conclusions from the current study, the rapid soot decrease also could be due to over-estimated model heat release rate (HRR), which consumes fuel faster, thus reducing the amount of soot formed in the model compared to the experiment. Using the analysis tools developed in this paper one can more precisely assess the cause and effect of such observations.

The above studies demonstrate a progression of improved internal combustion engine modeling in general, with application to soot and multiple injections specifically. To summarize, Han et al. [2] demonstrated the ability to model combustion very accurately in terms of pressure and heat release rate. They also postulated a method of soot reduction for their operating conditions, which was based on sound interpretations of model results and engine-out emissions data. Contributions of Yun et al. [10] include, in part, a CFD solver upgrade, incorporating a fundamentally based combustion model and transitioning to a more well-accepted soot precursor, C_2H_2 . Vishwanathan et al. [15] contributed a soot model that not only accounted for formation and oxidation, but also included surface growth, coagulation, oxidation by OH as well as O_2 , and an additional equation for transport of soot number density.

One important analysis capability not employed in the above studies is local identification and quantification of the formation and oxidation contributions to net soot throughout the computational domain. Such analysis would provide greater insight into the chemical, fluid-mechanical, and thermal mechanisms by which post-injections may affect the in-cylinder soot evolution.

In the current study, that capability is developed and applied to close-coupled post injection schedules under conditions relevant to current production diesel engines using moderate exhaust-gas recirculation (EGR) with exhaust aftertreatment to meet pollutant regulations. The bulk of the modeling effort for this initial modeling phase is to develop various CFD tools that facilitate more detailed analysis of the in-cylinder soot evolution. As reported here in this first effort, the focus is not on improving soot or combustion sub-models. Therefore, it is desirable to use a CFD code that executes rapidly and provides predictions of sufficient accuracy. During analysis tool development, a set of simulations often need to be run repeatedly, such that a fast turnaround time is very important.

Therefore, the CFD solver used in the current study is based on KIVA3V-R1 [17] using relatively simple combustion and soot models similar to those used by Han et al. [2]. Run times were approximately 30 minutes on a desktop PC (Intel® Xeon® CPU, 64 bit, 3.33 GHz), where similar simulations with the more advanced sub-models take more than a day on a local Linux cluster (Intel Core2 Quad Q6600, 32 bit, 2.4 GHz).

Phase II of the modeling effort (to be reported in subsequent studies) will transition these tools to a KIVA version that has detailed combustion kinetics and a detailed soot model. It will also include recent enhancements by Perini et al. [18], which have demonstrated significant speedup for engine CFD simulations [19].

Initially, the same experiments modeled in this study will be modeled in phase II. Phase II CFD results, processed with the newly developed visualization tools, are to be compared to recently published soot natural luminosity and planar laser induced incandescence images of O'Connor and Musculus [20] with the goals of validating the models, then using its soot formation and oxidation extraction and visualization capabilities to deepen our understanding of experimentally observed soot phenomena.

EXPERIMENTS

Including the main-injection-only condition, six discrete command durations of the post-injection sweep are modeled, and this section describes only those portions of the experiments that are relevant to the modeling effort. Please see the companion publication for more details of the experimental study [20]. Some model inputs are also found in this section where appropriate.

Engine and Injector

Experiments are conducted on a Cummins N14-based, single cylinder, heavy-duty, and low-swirl research engine. Engine and injector characteristics are listed in [Tables 1](#) and [2](#), respectively.

The piston has a centrally located, optically accessible, right circular cylinder bowl. The injector, also centered on-axis, has eight holes evenly spaced azimuthally.

Operating Conditions

All operating conditions are at 1200 RPM, 18% intake oxygen by volume and slightly boosted ([Table 3](#)). The engine is skip fired, nine motored cycles per fired cycle, to reduce thermal stresses on optical components. As such, real EGR is not available for dilution. Instead, the intake charge is diluted with excess nitrogen. Engine load is between 5 and 7 bar gIMEP; the load increases with increasing post injection duration. Minimum load is with the main-injection-only case and it serves as the reference condition.



Table 1. Engine characteristics.

Engine base type	Cummins N-14, DI diesel, 4 stroke
Swirl ratio	0.5 (approx.)
Bore	139.7 mm [5.5 in]
Stroke	152.4 mm [6.0 in]
Connecting rod length, mm	304.8 mm [12 in]
Geometric compression ratio	11.2:1
Bowl width	97.8 mm [3.85 in]
Bowl depth	15.5 mm [0.61 in]

Table 2. Injector characteristics.

Fuel Injector	Delphi DFI-1.5 (light duty)
Fuel injector type	Common-rail, solenoid actuated
Cup (tip) type	Mini-sac
Number of holes & arrangement	8, equally-spaced
Spray pattern included angle	156°
Nominal orifice diameter	0.13 mm

Table 3. Operating conditions.

Engine Speed	1200 RPM
Engine Load Range	5-7 bar gMEP
Intake O ₂ (volume / mass basis)	18 / 20 %
Fuel Pressure	1200 bar
Nominal TDC Motored Density	16.6 kg/m ³
Nominal TDC Motored Temperature	900 K
Intake Pressure	1.61 bar
Intake Temperature	381 K
Main/Post injection command duration, microseconds	Main/Post injection quantity, mg
1950/000 (M-I-O)	70/0
1950/350	70/3
1950/400 (Short)	70/6
1950/500	70/12
1950/600	70/20
1950/700 (Long)	70/26
Injection timings used in simulations	
Start of main injection, CAD	-10.14
Duration of main injection, °CA	16.44
Dwell between main and post, °CA	2.9
Start of post injection, CAD	9.2

Injection Profiles

As is evident by the injection rates of Figure 1, all profiles input to the simulations have the same main injection, same dwell between injections and hence, same start of post injection timing. The main-injection-only case uses only the main injection profile. Table 3 lists injection timings used in the simulations.

The injection rates were measured using an impingement-based meter, and the dwell between injections was set to the minimum reliably achievable. More injection rate measurement details and design of the injection schedule can be found in [20].

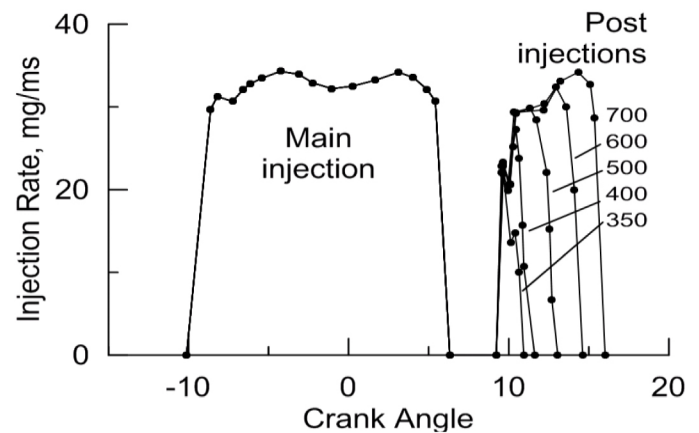


Figure 1. Injection profiles as input to the simulations. Each case uses the same main injection. Post-injection command duration in microseconds is indicated.

Figure 2 compares measured to modeled injection profiles for the 700 microsecond case. There are differences worth mentioning. Start and end crank angles are selected that help with matching the apparent heat release rate (AHRR). As seen in the figure, selected values, i.e., crank angles where model injection rate is 0.0, agree well with the measured injection rate. Other cases compare similarly.

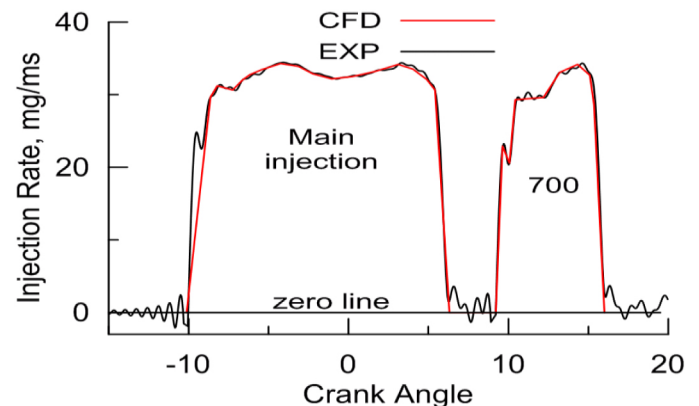


Figure 2. Measured and modeled injection profiles for the 700 microsecond post injection case.

Also, the measured injection rate peak at about -10 crank angle degrees (CAD) is not included in the model, because when including it, the simulated rate of heat release rise was too fast. The peak is believed to exist in the real injection event, but the reason that it causes excessive heat-release in the model is yet to be determined.

Recognizing that integrating the injection rate curves gives the amount of fuel injected, it is apparent that total fueling increases with larger post injections. [Table 3](#) lists the injected fuel mass.

Naming Convention

Six experimental operating conditions are modeled in this study. Experimentally, all have the same control commands to activate the main injection event (1950 microsecond command duration) as well as the same start of the post injection. To explore the influence of the quantity/momentum of the post-injected fuel, the post injection duration is varied from 0 to 700 microseconds. All cases are referred to by their post injection command duration in microseconds. For example, label '350' refers to the operating condition with post injection command duration of 350 microseconds.

Additionally, three particular conditions from the post-injection duration sweep are selected for detailed discussion. These conditions, with post-injection command durations of 0, 400, and 700 microseconds are referred to as the main-injection-only (M-I-O), Short, and Long cases, respectively.

Main injection refers to the first injection pulse, which is the same for all cases. The M-I-O case has only the main injection. Post injection refers to the second injection pulse. All cases other than the M-I-O case have both the main and post injection. More definitions and abbreviations appear at the end of this document.

Measured Trends

In this sub-section, measured trends that instigated this CFD study are presented. [Figure 3](#) plots measured engine-out soot for a series of increasing post-injection durations. Each symbol represents a different post-injection case, and post-injection duration increases from left to right. Leftmost is the main-injection-only case, then the 350, 400, 500, 600 and 700 microsecond post-injection cases. Load monotonically increases as post injection size increases, i.e., with more fueling. The engine-out soot data are from exhaust smoke measurements using a standard correlation [20]. Repeatability of this measurement was tested at several injection schedules; the standard deviation of the carbon volume-fraction measurements at each of these repeated conditions was approximately 0.05 mg/m³ units for continuously fired operation.

Starting from the main-injection-only case, increasing the close-coupled post-injection duration initially lowers the measured engine-out soot, which reaches a minimum near a post-injection command duration of 500 microseconds. Further

increases of the post-injection duration to 700 microseconds more than doubles the measured engine-out soot. A major goal of this work is to understand this soot trend with varying post-injection duration. (Model predictions in [Figure 3](#) will be discussed in a later section.)

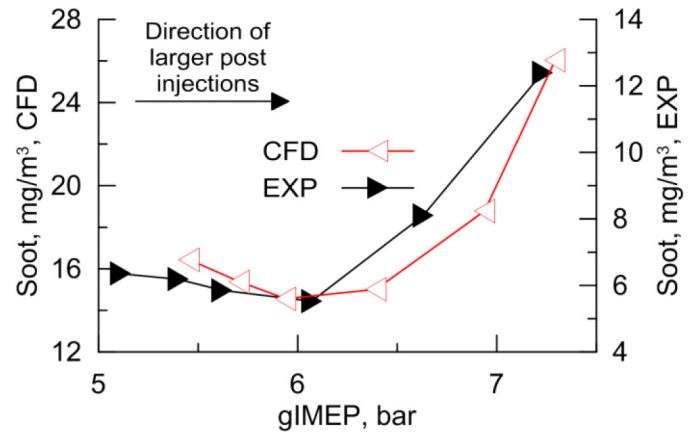


Figure 3. Experimentally measured engine-out soot (EXP, right axis) and model-predicted EVO soot (CFD, left axis) for a post-injection command duration sweep from 0 to 700 microseconds.

Model Setup

This section describes the combustion chamber geometry, models used, initial and boundary conditions, and model assumptions.

Model Geometry

The engine has a centrally mounted injector with eight equally spaced holes, which yields an 8-fold rotational symmetry about the cylinder axis. Hence, to achieve higher spatial resolution for a given number of computational cells, the combustion chamber is modeled with a representative 45° sector, and symmetry assumptions are applied to account for the whole combustion chamber. With this simplification, asymmetries due to valve recesses in the head and material differences due to optical window placement are ignored.

The computational domain ([Figure 4](#), TDC) includes the piston/liner crevice starting at the piston's top surface and extending down to the top ring's top surface. No ring gaps are modeled, so flow does not exit the computational domain via the crevice and no blowby model is used. Crevice depth is adjusted to match motored pressure. The benefit of adjusting crevice depth, as opposed to adjusting squish height to match motored pressure is that the measured TDC squish height can be retained, which should provide better estimates of in-bowl flow structures due to squish flows. Since the crevice is farther from spray and combustion, altering its dimensions should have minimal impact on soot estimates.

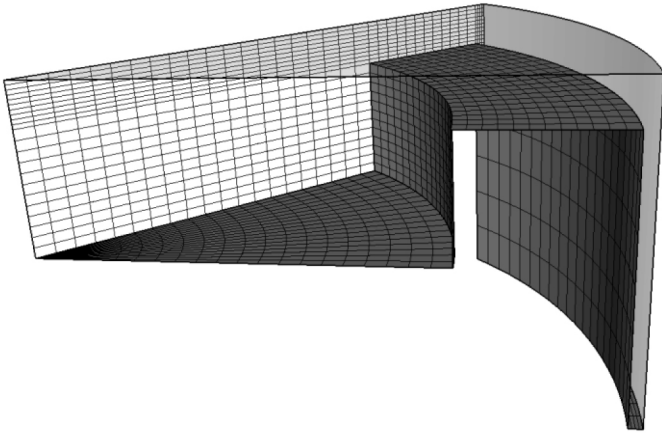


Figure 4. Computational domain at TDC.

Combustion chamber geometry and mesh resolution are summarized in Table 4. The resolution is typical for diesel simulations using CFD solvers like KIVA, although the crevice resolution is relatively coarse. The coarseness does not adversely affect soot results and too much crevice refinement can increase run time substantially.

Table 4. Model dimensions and mesh resolution.

Geometry	Dimension, mm	Number of cells along the dimension	mm/cell
Bowl radius	48.88	20	2.4
Bowl depth	15.5	12	1.3
Crevice radial extent	1.67	4	0.42
Crevice depth	34.51	6	5.75
Squish radial extent (bowl lip to crevice)	19.3	12	1.6
Squish height @ TDC	5.6	10	0.56

Sub-Models

Net soot is the difference between formation and oxidation rates. While a variety of advanced chemistry and soot models are available to model soot formation and oxidation [e.g., 9, 13], a major goal of the present study is to develop analysis tools to understand in-cylinder processes. The added complexity of advanced chemistry models becomes a burden by increasing the model run time, which reduces the number of different analysis techniques that can be tested. Hence, for this effort, simple engineering models can prove valuable for providing short run times with well-tested soot sub-models. Higher fidelity models will be incorporated in the second phase of this project, after the analysis tools have been developed to maturity.

Some of the more important sub-models used in this study are listed in Table 5 and model details can be found in reference [21]. The CFD solver is a version of the Los Alamos National Laboratory KIVA3V code [17], enhanced with sub-models developed at the University of Wisconsin-Madison Engine

Research Center [21]. Ignition is modeled with the Shell model [4] and combustion with the Characteristic Time Combustion model [5].

Table 5. Models used in this study.

CFD solver	KIVA3V-ERC
Ignition	Shell
Combustion	CTC (Characteristic Time Combustion)
Spray breakup	KH-RT (Kelvin-Helmholtz/Rayleigh-Taylor)
Turbulence	RNG k-epsilon
Soot formation	Hiroyasu
Soot oxidation	Nagel-Strickland-Constable

The soot-formation rate is given by the single-equation Hiroyasu model [8]:

$$\frac{dM_{sf}}{dt} = A_f M_{fv} P^{0.5} \exp\left(-\frac{E}{RT}\right) \quad (1)$$

In Eq. 1, M_{fv} is fuel vapor mass (g), P is pressure (bar), and T is temperature (K), all of which are calculated by other KIVA3V-ERC sub-models and supplied to the soot sub-model as formation-equation input values on a per-cell basis. R is the universal gas constant (1.9858 cal/ (g-mole K)). A_f and E are user-supplied model parameters that represent the pre-exponential term and soot activation energy respectively. Here, A_f is 700 (1/ (bar g)) and E is 12500 (cal/mole) [7]. The value of E is not typically changed and the value of A_f is typical of diesel combustion.

The soot oxidation rate is predicted by the Nagle-Strickland-Constable model:

$$\frac{dM_{so}}{dt} = \frac{6Mw_c}{\rho_s D_s} M_{sf}(T, Po_2) \quad (2)$$

In Eq. 2, Mw_c is carbon's molecular weight (12.001 g/mole), M_s is soot mass (g), and ρ_s and D_s are user supplied values for soot density (2 g/cm³) [7] and soot diameter (2.5e-6 cm) respectively. Detailed functional relationships used for the cell gas temperature, T , and oxygen partial pressure, Po_2 , are found in reference [21]. The soot-formation sub-model supplies the soot mass to the oxidation model. Hence, all the dependencies mentioned for the formation model are also dependencies of the oxidation model, as is local oxygen concentration.

Initial and Boundary Conditions

Model in-cylinder initial conditions at intake valve closure (IVC) and surface-temperature boundary conditions for all cases are listed in Table 6. Surface temperatures were not measured directly and are instead estimated based on measured coolant