Modeling of Diesel Combustion, Soot and NO Emissions Based on a Modified Eddy Dissipation Concept

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Abstract

A three-dimensional reacting flow modeling approach is presented for predictions of compression ignition, combustion, NOx and soot emissions over a wide range of operating conditions in a diesel engine. The ignition/combustion model is based on a modified eddy dissipation concept (EDC) which has been implemented into the KIVA 3V engine simulation code. The modified EDC model is used to represent the thin sub-grid level reaction zone and the small scale molecular mixing processes. In addition, a realistic transition model based on the local normalized fuel mass fraction is implemented to shift from ignition to combustion. The modified EDC model is combined with skeletal n-heptane chemistry and a soot dynamics model which includes nucleation, surface growth and oxidation and coagulation processes. The NO formation and destruction processes are based on the extended Zeldovich reaction mechanism. The modeling results are calibrated against experimental engine data taken at benchmark conditions. The model is subsequently used to conduct parametric studies of the effects of injection timing and exhaust gas recirculation (EGR) on engine combustion and emissions. Predictions of cylinder pressure traces and heat release rates are in very good agreement with the experimental data (e.g. pressure predictions within 3 bar of the experimental data) for a range of injection timings, EGR rates and speeds. The experimental trends observed for the soot and NO emissions are also reproduced by the modeling results. Overall, the modeling approach demonstrates promising predictive capabilities at reasonable computational costs.
Introduction

High-fidelity numerical simulations of physical and chemical processes within a diesel engine remain a challenge due to the many complexities associated with modeling spray dynamics, turbulent mixing, auto-ignition, premixed and diffusion-controlled combustion phases, and pollutant formation. These processes are highly transient, nonlinear, and multi-dimensional, involving a large number of chemical species. Recent studies have made substantial progress by integrating improved sub-models into overall engine modeling frameworks (Reitz and Rutland, 1995). Examples include advanced spray models (Béard et al., 2000; Hasse and Peters, 2002; Von Berg et al., 2003), improved turbulent mixing models (Subramaniam and Haworth, 2000; Lee et al., 2002) and integration of detailed reaction mechanisms (Pitsch et al., 1996; Kong and Reitz, 2000; Gill et al., 1996; Agarwal and Assanis, 1998; Ishii et al., 2001; Pitsch et al., 1995) into combustion and emission models. Nevertheless, more work is required to test the synergy of sub-models which have been developed independently in integrated frameworks (e.g. for prediction of shock tube ignition delay time data or flame species concentration data) for practical engine modeling. Furthermore, the more physically and chemically realistic representation of the engine processes should not introduce computational burdens beyond the capacity of existing computational resources. Therefore, there is a strong need to develop a comprehensive modeling tool that can reproduce desired key characteristics without being cost-prohibitive.

One of the most critical components in compression-ignition engine modeling is the prediction of auto-ignition and combustion. It is well known that both processes are strongly affected by the fuel-air mixing and chemical reactions (Henein and Bolt, 1969; Mastorakos et al., 1997; Naber et al., 1994). Previous compression-ignition modeling efforts often considered
these two aspects separately by describing the ignition/combustion process as a sequence of homogeneous chemical ignition, followed by a diffusion-controlled combustion phase in which turbulent mixing is the primary rate-controlling parameter. Both one-step (Emerson and Rutland, 1999; Dillies et al., 1997; Kong et al., 1995) and detailed reaction mechanisms (Agarwal and Assanis, 1998; Kong and Reitz, 2000) have been used for the prediction of auto-ignition. Kong and Reitz (2000) have attempted to integrate the two effects by defining characteristic time scales for the turbulence and kinetics, based on the eddy break-up and the chemical equilibration of a reference species, respectively. The expression for the species reaction rate is then modified from a chemistry-only structure to include contributions from the two time scales.

An alternative mixing/combustion model was proposed in previous studies of natural gas, direct-injection, compression-ignition engines (Hong et al., 2002a 2002b) as an attempt to simultaneously account for the effects of chemistry and mixing on ignition delay. This hybrid model employs a combination of the chemistry-controlled ignition submodel and a combustion submodel based on a modified eddy dissipation concept (EDC). A transition between the ignition and combustion phase was determined by the amount of residual fuel mass, which was monitored in each computational cell during the calculation.

Predictive engine modeling also needs accurate reaction mechanisms that describe the pollutant formation processes, primarily NOx and soot. In diesel engines, thermal NOx is considered the primary path for the NOx formation, so that variants of the extended Zeldovich mechanism (Lavoie et al., 1970) are found to be adequate. The soot model, on the other hand, is far more complex and requires in-depth understanding of numerous chemical paths. A few attempts have been made to apply detailed multi-step kinetic mechanisms for soot formation and
oxidation (developed by groups such as Frenklach and Wang, 1994; Appel et al., 2000; Mauss et al., 1994; Fairweather et al., 1992) in closed-cycle engine simulations (e.g. Karlsson et al., 1998; Pitsch et al., 1996; Kitamura et al., 2002). However, these detailed models involve an excessive number of species and reactions such that their application in extensive multi-dimensional simulations is not feasible. In contrast, the current status of full-cycle engine simulations relies heavily on empirical models, such as Hiroyasu and Kadota (1976) and its variants (Hampson and Reitz, 1998; Wadhwa et al., 2001; Mather and Reitz, 1998), or the three-stage model with refined rate constants (Nagle and Strickland-Constable, 1962; Tesner et al., 1971; Surovikin, 1976; Haynes and Wagner, 1981). This class of models considerably oversimplifies the gas-phase combustion chemistry and neglects particle dynamics. In an effort to bridge the gap, a soot model has been recently developed (Hong et al., 2004b) that properly reflects advanced knowledge and yet is amenable to large-scale simulations such as KIVA 3V. The model was derived based on a skeletal n-heptane mechanism, integrated with existing submodels that capture the essential physics of the soot formation processes. The model was calibrated with data from well-controlled shock tube studies (Kellerer et al., 1996) and was shown to be valid over a wide range of engine operating conditions.

The primary objectives of the present study is to integrate and extend advanced models of ignition, combustion, NOx and soot formation into the KIVA-3V platform so as to develop a comprehensive tool for direct-injection diesel engine application. The basis of the combustion modeling is the modified EDC concept. The present study extends the previous work by incorporating a more physically realistic transition between ignition and combustion, dictated by the amount of reactants remaining in each cell. The second significant contribution is the use of n-heptane as a surrogate for diesel fuel within the EDC modeling framework. The third major
enhancement is the application of a recently developed soot model (Hong et al., 2004b).

In the following sections, the basic concept of the EDC model is described first, with emphasis on the extensions from our previous studies. The calibration of the new model input parameters and the sensitivity of the modeling results to these parameters are compared against cylinder pressure data acquired in a modern light-duty diesel engine for a benchmark set of operating conditions. Once the new input parameters are set at the optimized values, a parametric study of injection timings, Exhaust Gas Recirculation (EGR) loads and engine speeds is undertaken to evaluate the predictive capabilities over a broad range of conditions. For the parametric studies, cylinder pressure data, heat release rates, and soot and NOx emissions are compared with experimental measurements. Thus, the potential of the present model for high-fidelity predictions of combustion and pollutant formation processes in practical diesel engines is explored.

Model Development

For this work, the KIVA 3V (Amsden, 1977) computational fluid dynamics simulation is used as the modeling platform. In the following sub-sections, our enhancements to critical sub-models including Ignition, Turbulent combustion, Ignition-combustion transition, NO Emissions and Soot emissions are described.

Ignition

The key assumption used in the ignition model is that in each computational cell, turbulent mixing is sufficiently rapid (i.e. the Damköhler number is small) during the ignition stage, such that ignition is controlled by chemical reaction with minimal effects due to mixing. Therefore, the reaction rate for each species $m$ in each cell is computed based on the cell-averaged
temperature and species concentration using:

\[ \bar{a}_{m,\text{Ignition}} = \sum_{n=1}^{L} \left( \nu''_{mn} - \nu'_{mn} \right) \left( k_f \prod_{m=l}^{N} \frac{X_m}{X_m} \nu''_{mn} - k_r \prod_{m=l}^{N} \frac{X_m}{X_m} \nu'_{mn} \right) \]  

(1)

where \( \nu''_{mn} \) and \( \nu'_{mn} \) are the stoichiometric coefficients of the reactions, \( k_f \) and \( k_r \) are the forward and reverse rate constants, respectively, and \( X_m \) is the molar concentration of species \( m \).

For the ignition chemistry calculations, KIVA-3V is modified to incorporate CHEMKIN-II (Kee et al., 1991) for evaluation of the reaction source terms. A stiff ODE solver, LSODE, is linked to KIVA-3V to integrate the species and energy equations involving the detailed chemical reactions and transport. The skeletal mechanism for n-heptane developed by Pitsch (see Hong et al., 2004b and references therein) is used as a surrogate for diesel fuel, due to its similar cetane number. The mechanism includes 44 species and 113 reactions. Additional reaction mechanisms for n-heptane were considered; however, the Pitsch mechanism yielded the best combination of accuracy and computational costs. A comparison of the mechanism results for ignition delay time predictions and further details on the benchmarking of the n-heptane mechanism can be found in Hong et al. (2004a, 2004b).

**Turbulent Combustion**

As mentioned in the introduction, a modified EDC model has been previously developed in our group based on work by Magnussen (1981). The EDC model has been implemented as a physical sub-grid level model to account for the effects of turbulent mixing on combustion for computational studies in a direct-injected, compression-ignited natural gas engine (Hong et al., 2002b). A detailed description of the formulation and relevant parameters can be found in that work. Key steps and new enhancements are summarized here.

Recognizing that chemical reaction occurs within a thin confined reaction zone which is
typically smaller than the size of the numerical grid, the original EDC model (Magnussen, 1981) divides the computational cell into two sub-zones: the fine structure and the bulk gas zone. Figure 1 shows a schematic of a computational cell based on the EDC model. Chemical reactions occur only in the fine structure where reactants are mixed at the molecular level at sufficiently high temperatures. In the bulk gas zone, only turbulent mixing takes place (without chemical reaction), thereby transporting the surrounding reactant and product gases to and from the fine structure. The coupling between the fine structure and the bulk gas zone interactively affects the overall combustion rate. The fine structure is not resolved in detail. Only the size of the fine structure is calculated using a prescribed equation proposed by Magnussen. Therefore, the EDC model effectively captures the two essential characteristics of the combustion process: chemical reaction and mixing, without having to resolve the sub-grid scale fine structures.

The time integration of the conservation equations proceeds as follows. At the beginning of each time step, all scalar variables in the fine structure are set at conditions determined using an adiabatic equilibrium calculation. The CEA equilibrium code (McBride and Gordon, 1996) is integrated into KIVA 3V for the equilibrium calculations. The initialization conditions are obtained using the cell-averaged values for the initial composition and temperature of the equilibrium calculation. The product composition and temperature determined by the equilibrium calculation are then used as the initial conditions in the fine structure. Thus, complete combustion and locally high temperatures are realized in the fine structure. This procedure is based on the assumption that the fine structure in each cell represents a flame that converts the bulk gas in the cell into the equilibrium products. The effects of the initial conditions used for the fine structure are discussed further below.

All the scalar variables in the bulk gas zone are determined based on the cell-averaged
conditions. The interaction between the fine structure and the bulk gas zone is integrated using
the governing equations of the EDC model. At the end of each time step, the states of the fine
structure and the bulk gas zone are updated.

The original EDC model developed for steady state conditions has been extended to
incorporate unsteady terms into the governing equations for the fine structure and the bulk gas
zone (Hong et al., 2002b). The modified EDC governing equations for the fine structure are:

\[
\frac{dY^*_m}{dt} = -\frac{1}{\tau_r} (Y^*_m - \bar{Y}_m) + \frac{\dot{\omega}^*_m W^*_m}{\rho^*}, \tag{2}
\]

\[
\frac{dT^*_m}{dt} = \frac{1}{C_p} \left[ \frac{1}{\tau_r} \sum_{m=1}^{M} \bar{Y}_m (h^*_m - h^*_m) - \sum_{m=1}^{M} h^*_m \dot{\omega}^*_m W^*_m \right], \tag{3}
\]

where * represents the fine structure and bar represents the cell-averaged values. \(Y_m\), \(h_m\), \(\dot{\omega}_m\),
and \(W_m\) are the mass fraction, the enthalpy, the reaction rate, and the molecular weight of species
\(m\), respectively. \(C_p\) is the heat capacity, and \(\rho\) is the density of the gas mixture. The residence
time, \(\tau_r\), during which the species remain in the fine structure is expressed as:

\[
\tau_r = \frac{(1 - \gamma*)}{\dot{m}^*}, \tag{4}
\]

where \(\dot{m}^*\) is the mass exchange rate between the fine structure and the bulk gas zone, \(\gamma^*\) is the
mass fraction occupied by the fine structure, and \(\chi\) represents the fraction of the fine structure
that reacts. The mass exchange rate, \(\dot{m}^*\), and mass fraction, \(\gamma^*\), are calculated using the
following equations,

\[
\dot{m}^* = 2.43 \left( \frac{\varepsilon}{V} \right)^{1/2}, \tag{5}
\]
\[
\gamma^* = \left[ 2.13 \left( \frac{\nu \varepsilon}{k^2} \right)^{1/4} \right]^3,
\]

where \( k \) is the turbulent kinetic energy, \( \varepsilon \) is the dissipation rate of turbulent kinetic energy, and \( \nu \) is the kinematic viscosity of the gas.

The solution to Eqs. (2) and (3) determines the state conditions of the fine structure. Assuming that chemical reactions take place only in the fine structure, the net mean species reaction rate for the transport equation is given by:

\[
\overline{\omega}_{m}^{*}_{EDC} = \frac{P \chi \nu^{*}}{W_{m} \tau_{r}} \left( \gamma^{*} - \overline{\gamma}_{m} \right).
\]

The reaction rates in the fine structure are determined using the CHEMKIN-II subroutines that are interfaced with the KIVA-3V code. In the present study, n-heptane is being used as a surrogate for diesel fuel in the EDC modeling framework. Further, it is assumed that the entirety of the fine structure reacts, hence \( \chi \) is set to unity in Eqs. (4) and (7).

**Ignition-combustion transition**

Both the ignition and combustion models described above are used in the determination of the reaction rates in the current work. It is anticipated that the reaction rate is dominated by the ignition process during the early ignition phase. After the initial ignition transient is complete, the turbulent combustion model should dominate. The transition from ignition to combustion is expected to occur when sufficient radical growth and thermal runaway are achieved (Varatharajan and Williams, 2000). Using the reaction rate for species \( m \) determined by the ignition and the EDC turbulent combustion models (Eqs. (1) and (7)), the transition parameter, \( \alpha \), is introduced such that the overall reaction rate is determined as a linear combination of the two
reaction rates,

\[ \bar{\omega}_m = (1 - \alpha) \cdot \bar{\omega}_{m,\text{Ignition}} + \alpha \cdot \bar{\omega}_{m,\text{EDC}}. \]  

(8)

The transition parameter \( \alpha \) represents the progress of the ignition-controlled reaction (\( \alpha = 0 \)) towards the combustion-controlled reaction (\( \alpha = 1 \)). In our previous work, an abrupt transition between the ignition and turbulent combustion models was used (Hong et al., 2002a). In this study, the transition is dictated by the amount of the reactants remaining in each cell. Based on this approach, a normalized fuel mass fraction, \( \beta \), is introduced as

\[ \beta = \frac{\bar{Y}_{f} - \bar{Y}_{f,\text{eq}}}{\bar{Y}_{f,\text{mix}} - \bar{Y}_{f,\text{eq}}} \]  

(9)

where \( \bar{Y}_{f,mix} \) is the cell-averaged fuel mass fraction assuming only mixing occurs with no fuel oxidation. \( \bar{Y}_{f,eq} \) is the cell-averaged fuel mass fraction when the same mixture is allowed to reach an equilibrium state at the cell-averaged state conditions. \( \bar{Y}_{f,eq} \) is calculated using the CEA equilibrium code. \( \bar{Y}_{f,mix} \) is a function of the equivalence ratio only, while \( \bar{Y}_{f,eq} \) depends additionally on temperature and pressure.

For a given cell, during the course of ignition and combustion, the fuel mass fraction can have a value between the two limiting conditions defined by the unburned fuel (i.e. \( \bar{Y}_{f,mix} \)) and the complete combustion (i.e. \( \bar{Y}_{f,eq} \)) cases. The two limits correspond to the normalized fuel mass fraction of \( \beta = 1 \) and \( \beta = 0 \), respectively, according to Eq. (9).

Based on the definition of \( \beta \), the transition parameter \( \alpha \) is defined as:

\[ \alpha = \begin{cases} 
0 & \text{if } \beta > \beta_i \\
\frac{\beta - \beta_i}{\beta_f - \beta_i} & \text{if } \beta_i > \beta > \beta_f \\
1 & \text{if } \beta < \beta_f 
\end{cases} \]  

(10)
where $\beta_i$ and $\beta_f$ represent the starting and ending points of transition, respectively. The values for $\beta_i$ and $\beta_f$ are numerical constants, and appropriate values for $\beta_i$ and $\beta_f$ are explored as part of this study. Figure 2 shows how the transition parameter, $\alpha$, varies as the normalized fuel mass fraction, $\beta$, varies for arbitrary values of $\beta_i$ and $\beta_f$. If $\beta_i$ is set equal to $\beta_f$, the transition from the chemistry-only to the chemistry-plus-mixing approach is abrupt and will occur from one time step to the next in a computational cell. The transition model is considered an appropriate statistical description of the turbulent ignition and combustion processes because it represents the fact that the role of mixing becomes progressively more important as the overall reaction rate becomes dominated by the transport-limited flames.

**NO emissions**

NO emissions depend strongly on the history of the heat release rates and the major and minor species concentrations. In this work, NO predictions are determined using the extended Zeldovich mechanism. Since the extended Zeldovich mechanism is not included in the n-heptane mechanism by Pitsch, the prediction of NO is performed in a different manner compared to the prediction of other species. By assuming that NO formation is slower than other species, NO concentrations are predicted as a post-processing procedure at each time step. The NO production rates are computed using the extended Zeldovich mechanism for both the bulk gas zone and the fine structure based on the corresponding conditions (e.g. temperature, composition, etc.). The two contributions are added as a weighted sum according to the mass fraction of the fine structure, $\gamma^\star$.

**Soot emissions**
The soot model used in this study includes representation of soot nucleation, oxidation, surface growth and growth by collision. A detailed description of the soot model development and validation can be found in Hong et al. (2004b). Briefly, a moment method is used to monitor the evolution of the soot properties in the cylinder, i.e., the soot number density, the soot volume fraction and the deviation from the average volume. A log-normal particle size distribution is assumed to reduce computational costs. The soot sub-models include (a) direct linking with the n-heptane skeletal reaction chemistry to calculate the formation rate of soot precursor species (C2H2); (b) nucleation of soot primary particles; (c) soot coagulation based on collision theory; (d) soot oxidation by O2 and OH; (e) soot surface growth using a modified HACA mechanism; and (f) soot particle transport. Because acetylene is considered a primary contributor to soot nucleation and the C2H2 detailed kinetics are well represented in the skeletal n-heptane mechanism, soot monomers are assumed to form directly from acetylene. The nucleation rate for the primary soot particles is given by the expression reported by Leung et al. (1991), which was developed to represent direct formation of soot primary particles from acetylene. The soot particle transport includes size-dependent effects such as velocity slip between the soot particles and the gas medium.

**Engine Simulation Details**

Using the skeletal kinetic mechanism for n-heptane, the ignition model combined with the modified-EDC model, and the NO and soot emissions models, KIVA 3V simulations were performed for a light-duty diesel engine operating at steady state conditions. The engine geometry is provided in Table 1. All simulations used the TAB spray breakup model with modified coefficients (Assanis et al., 1993), the RNG-based k-ε turbulence model and a specified
wall temperature for estimating the heat flux into the combustion chamber. To increase computational efficiency, a 60°-sector computational mesh with a single fuel spray was used to model the six-hole injector used in the experiments. Periodic boundary conditions were assumed in the azimuthal direction. The calculations were performed using a three-dimensional sector that consisted of 5340 cells at top dead center (TDC), corresponding to a maximum cell wall dimension of approximately 1.5 mm.

The calculation procedure is modified from the traditional KIVA 3V simulation procedure (described in Amsden, 1997) to accommodate the integration of the sub-models. The modified EDC model parameters are evaluated at each time step if the EDC model is invoked based on the transition parameter $\alpha$. At each time step, the detailed reaction mechanism is used to account for chemistry in the ignition and combustion calculations and in the soot calculations. Thus, the soot sub-models use the kinetically-determined values for the species concentrations. The soot and NOx emissions calculations are made as post-processing steps after the ignition and combustion calculations are completed at each time step.

The simulation conditions considered in the study are listed in Table 2. A broad range of injection timings (as indicated by the start of injection, SOI), EGR content (% mass basis) and engine speeds were investigated. The exact simulation conditions were selected to match the conditions of the corresponding experimental data. The EGR gases were considered to consist of final products of combustion, (CO$_2$, H$_2$O, O$_2$, and N$_2$). The specific distribution of the EGR gases for each case was determined using the fuel equivalence ratio and the percent EGR determined experimentally (based on measured CO$_2$ emissions described below). No trace species were included in the EGR in these studies due to the lack of any experimentally determined means to set the composition and amount of trace species.
Figure 3 shows the conditions studied on EGR versus SOI and equivalence ratio versus engine speed coordinates. Cases 1-4 represent a study of the effects of changing the EGR levels while maintaining constant intake manifold conditions and fuel input rates. Cases 4-8 study the effects of changing the injection timing while fixing all other engine conditions at constant values. For Cases 1-8, 30 mg of fuel is injected. Cases 9 and 10 explore speed and load variations where 20 and 42 mg of fuel are injected, respectively.

**Engine Experimental Details**

A schematic of the experimental engine facility (located in the dynamometer wing of the Ford Research Laboratories) used for model validation is shown in Fig. 4. The experimental set-up featured a single-cylinder engine with the same bore and stroke as noted in Table 1, with a nominal compression ratio of 18:1. The engine speed was controlled using a General Electric AC motor/generator dynamometer. The facilities allowed control of intake pressure and temperature, as well as exhaust pressure in order to simulate turbocharged conditions, and were capable of exhaust gas recirculation. Data acquired in the facility include gaseous emissions measurements (including NOx) using an emissions bench (Horiba MEXA 7000), condensed phase particle measurements using a smoke meter (AVL 415), in-cylinder pressure time-histories using a pressure transducer (AVL GU12P) which was installed in the engine using a glow plug adapter, and various other pressures and temperatures throughout the engine system. Fuel injection timing was monitored via an injector current measurement probe. EGR levels were determined using a ratio of the CO2 emissions in the intake and the exhaust, and mass of fuel injected was monitored using a low-flow measurement cart (Pierberg PII 609).

The fuel system provided diesel fuel at an injection pressure of 100 MPa. A six-hole
injector was used to deliver the fuel at 16 cm³/sec. The injector hole diameter was 0.179 mm, with an included angle of 154° and protrusion of 0.8 mm from injector holes to flame deck. The intake manifold pressure and temperature were 120 kPa and 354 K, respectively. The intake valve closing occurred at -133° after top dead center (ATDC) and exhaust valve closing occurred at 122° ATDC.

Experimental data on engine performance and emissions were obtained over a wide range of operating conditions. The conditions for the focus of the computational studies were selected based on the following process. A six-mode mini-map (used to project emissions generated during a driving cycle) was created for the engine configured for application in a vehicle driving the light-duty Federal Test Procedure (FTP) for emissions testing (also known as the FTP75 city cycle) as defined by the United States Environmental Protection Agency (www.epa.gov, 2004). Conditions that have large contributions to NOx and smoke emissions and that are frequently encountered in the FTP were particularly targeted for investigation. Figure 5 shows the relative magnitude of the contributions of each of the six engine modes to NOx and soot emissions. Mode 5 (1500 rpm, 5 MPa BMEP) was found to be the largest contributor to the soot emissions and the second largest contributor to the NOx emissions for this FTP cycle. Due to the high impact on the engine emissions, the Mode 5 operating conditions were the primary focus of the model calibration and validation, although other modes/operating conditions were also examined.

Results and Discussion

Sensitivity analysis and model calibration

The sensitivity of the diesel simulation results to the proposed approach for setting the initial conditions of the fine structure must be evaluated before starting a parametric study of the engine
operating conditions, as the original steady-state EDC model (Magnussen, 1981) has been extended for application to transient combustion systems. In addition, there are two key parameters appearing in the new transition model ($\beta_i$ and $\beta_f$) that need to be optimized before conducting parametric studies. Mode 5 conditions (Case 1 of Table 2: $3^\circ$ ATDC, 0% EGR) were used for these sensitivity and model calibration tests. The results and the method for selecting the optimized transition parameters are presented below. Once a reasonable set of parameters were selected, no further adjustments to model constants were made throughout the remainder of the computational analysis.

One of the first issues encountered in execution of the modified EDC model is the determination of the initial conditions for the fine structure in each cell at the start of each time step. Since the original EDC model was developed for steady-state combustion systems, the initial thermodynamic conditions of the fine structure did not affect the EDC results. In the present transient engine simulations, however, the initial conditions for the fine structure are important as they determine the subsequent reaction rates.

To estimate the initial conditions at each time step for the fine structure, the most accurate method would be to solve additional transport equations for the quantities inside the fine structure. Since this is a computationally demanding process, in the present study the initial conditions were estimated based on the cell-averaged quantities provided by KIVA-3V. This can be accomplished by either using the cell-averaged quantities themselves or, alternatively, using the equilibrium condition based on the cell-averaged quantities. The former effectively implies a rapid mixing model, i.e. the fine structure conditions are completely homogenized with the bulk gas zone at every time step. The latter implies that the fine structure experiences vigorous combustion (a rapid chemistry model), which appears to be a more reasonable assumption. Note
that these estimates are used to initiate the conditions in the fine structure. The conditions in the fine structure are allowed to evolve from these initial conditions during the modified EDC model calculations which occur between KIVA time steps. Depending on the magnitude of the differences between the properties of the bulk and fine structure and the size of the KIVA time step, the bulk and fine structure can reach equilibrated conditions.

The two initial condition strategies are compared in Fig. 6, where the cylinder pressure variation is plotted through a cycle. The results show that the initial conditions based on the cell-equilibrium conditions yield better agreement with the experimental data, supporting the assumption that the fine structure maintains a near equilibrium condition. Note that, since the fine-structure conditions will eventually approach those of the final equilibrium product, the two initial conditions will not affect the long-time behavior of the solution. However, in engine simulations the duration of the chemistry and mixing events is finite, hence the initial conditions affect the overall outcome of the predictions as demonstrated in Fig. 6.

The next important parameters are associated with the transition model. As expected from Eqs. (8)-(10), changes in the starting and ending points of transition, $\beta_i$ and $\beta_f$, can affect the overall reactivity of the system. To evaluate the effects of the transition parameters on the reaction rates during the combustion process, the cylinder pressure variations predicted for different values of $\beta_i$ and $\beta_f$ were explored. To isolate the effects of each parameter, one parameter was set at a constant value while the other was varied for this exercise. Recall that $\beta_i$ represents the point at which the turbulent mixing starts to affect the reaction rates, and $\beta_f$ represents the end of the ignition model, after which combustion is entirely controlled by the interaction between the fine structure and the bulk gas zone. The formulation for the reaction rate based on the transition parameter (Eqs. (8)-(10)) allows a numerically smooth and physically
realistic transition process from ignition to turbulent combustion.

It was found that the results for cylinder pressure were little affected by different values of $\beta_f$. On the other hand, the onset of the turbulent combustion model, $\beta_i$, had an impact on the overall predictions. To explore this effect further, three values for $\beta_i$ were tested while $\beta_f$ was fixed at 0.1. The results are presented in Fig. 7. Note that ignition, characterized by the rapid pressure rise, occurs earlier as $\beta_i$ increases, because the intense turbulent mixing and combustion are initiated at an earlier time. Since the initial conditions for the fine structure are determined by the equilibrium calculations, an earlier action of the combustion model always tends to reduce the ignition delay and expedite the start of combustion. It is of interest to note that a slightly higher peak pressure is achieved with a higher value of $\beta_i$. This results from the fact that a longer ignition delay causes a higher heat release rate during the premixed combustion phase.

To assess the effect of $\beta_i$ on heat generation, the computed heat release rate is compared with experimental determinations. Since the heat release rate is difficult to measure, a net apparent heat release rate is defined from the experimentally and computationally measured pressure time histories and the piston displacement profile:

$$
\frac{dQ_n}{dt} = \frac{\gamma}{\gamma-1} p \frac{dV}{dt} + \frac{1}{\gamma-1} V \frac{dp}{dt}
$$

(11)

where $Q_n$ is the net apparent heat release rate, $p$ is the cylinder pressure, $V$ is the cylinder volume and $\gamma$ is the specific heat ratio. Equation (11) is taken from Heywood (Heywood, 1988), in which $\gamma = 1.35$ is recommended as an appropriate value at the end of the compression stroke, and $\gamma = 1.26 - 1.3$ is recommended for the burned gas. In this study, $\gamma = 1.325$ was used.

The comparison of the net apparent heat release rate with the predicted heat release rate is shown in Fig. 7(b). The results clearly show that the point of maximum heat release occurs
earlier as the value for $\beta_i$ is increased, consistent with the behavior of the pressure trace as $\beta_i$ is varied. On the other hand, the predicted maximum heat release rate decreases as $\beta_i$ increases. It appears that this behavior is strongly related to the ignition delay. A longer ignition delay implies a longer time for mixing of the fuel injected into the cylinder chamber with the surrounding air. The degree of this premixing determines the strength of the premixed combustion phase after it is ignited. Therefore, the case with $\beta_i$ of 0.5 produces a higher peak value for the heat release rate compared to the case with $\beta_i$ of 0.7.

Based on the sensitivity analysis and model calibration studies, two decisions were made regarding the model parameters. The initial conditions of the fine structure were set as the equilibrium values at each time step, and the transition parameters were set as $\beta_i = 0.7$ and as $\beta_f = 0.1$. These parameter values were adopted for the remainder of the simulations without any further modification.

*Parametric studies – engine performance*

With all values of the model parameters fixed, a range of engine conditions were simulated. Figure 8 compares measured and predicted cylinder pressure traces for Cases 2, 3 and 4 of Table 2. Along with Case 1 shown in Fig. 7, these cases represent approximately the same injection timing with increasing EGR levels varying from 0-25%. Overall, the modeling predictions are in excellent agreement with the experimental data.

Figure 9 compares measured and simulated cylinder pressure traces for Cases 5-8 of Table 2. Along with Case 4 shown in Fig. 8, these cases represent approximately the same EGR level with advancing injection timing from $3.0^\circ$ ATDC to $-20^\circ$ ATDC. Again, the simulation results are in satisfactory agreement with the experimental data for all conditions except the
earliest injection timing, where the peak pressure is over-predicted by ~10 bar.

In general, the predictions for Cases 1-8 were within 0.5 °CA of the experimental data for ignition delay and within 3 bar of the experimental data for peak pressure (with the exception noted above for the earliest injection timing). This level of agreement was also observed even when speed and load conditions were varied, as seen in Figure 10 which compares measured and simulated cylinder pressure traces for Cases 9 and 10 of Table 2.

Using the procedure described above for Case 1, the apparent heat release rates for Cases 2-10 are calculated using Eq. (11). The results are compared with experimental data in Figure 11. As in the comparison with the pressure data, the largest discrepancy between the prediction and measurement is found in Case 8, where the injection timing is significantly advanced. Nevertheless, the comparison over a broad range of conditions demonstrates a remarkable level of predictability of the present model in terms of capturing the correct ignition delay timing and peak heat release rate.

**Parametric studies – NO and soot emissions**

Figures 12 (a) and (b) show the predicted and measured NO mole fractions, \( \chi_{NO} \), as a function of EGR level and injection timing, respectively. All experimental data are normalized by the maximum value for \( \chi_{NO} \) (the experimental value measured for Case 8) and all numerical data are normalized by maximum value for \( \chi_{NO} \) (the NO value predicted in Case 8). It is clearly demonstrated that the present model is capable of capturing the trend for NO emissions, such as the decrease in NO mole fraction with an increase in EGR amount (Fig. 12 (a)). Similarly, the trend of increasing NO with advancing injection timing (Fig. 12 (b)) is also reproduced by the model. This level of fidelity is achieved by consideration of fundamental chemical and turbulent
mixing characteristics.

As a demonstration of the quantitative accuracy of the model results, Fig. 13 shows the predicted NO mole fractions for all cases, where each data point is normalized by the corresponding experimental measurement. For all cases examined, the predicted NO mole fractions are lower than the experimental measurements by 30%. Note the level of agreement is consistent throughout the broad range of operating conditions considered, further demonstrating the robustness of the model.

Figures 14 (a) and (b) show the predicted and measured soot emissions as a function of EGR level and injection timing, respectively. The experimental soot measurements are presented as normalized soot mass based on the measured AVL smoke number, where the AVL correlation for converting smoke number to soot mass concentration has been used (Christian et al., 1993). All experimental data are normalized by the maximum value for Case 5. Similar to the NO emissions, the trends for the soot emissions are well reproduced by the model predictions, although the decrease in soot emissions is more rapid compared to the experimental measurements for decreasing EGR loadings (see Fig. 14 (a)). Specifically, the model captures the increase in soot with increasing EGR and the relatively complex variation in soot with advanced fuel injection timing. Note that advancing the injection timing does not lead to a consistent increase or decrease in the soot as was observed with the NO emissions (i.e. increasing NO with more advanced injection timing).

Figure 15 summarizes the simulation and experimental results for the soot emissions, including the results for Cases 9 and 10. As in Fig. 14, the normalized experimental data are compared with the normalized model results, where the maximum values for soot emissions (Case 5 for both the experimental and modeling soot data) have been used for the normalization.
The simulation results are in excellent agreement with the trends observed in the experimental diesel engine study. In particular, note that the model captures the soot-NOx trade-off observed as EGR loadings are increased as seen in Figure 16.

**Conclusions**

An advanced KIVA 3V simulation capability has been developed by incorporation of a sub-grid level combustion mixing model based on a modified version of the eddy dissipation concept. The combustion model represents chemical processes in diesel engines by implementing a more physically realistic transition between ignition and combustion and skeletal n-heptane chemistry. Additionally, the capabilities for predicting soot emissions have been enhanced by accounting for the critical processes of soot nucleation, growth, oxidation and transport. The soot model also assimilates the n-heptane chemistry. These more physically- and chemically-based sub-models have led to an overall engine model capable of high fidelity predictions of the compression ignition combustion processes as demonstrated by the model validation studies.

Comparison of the model results with the experimental data at a specific set of engine operating conditions led to identification of optimal values for the model parameters regarding the initial conditions for the fine structure in the modified-EDC calculations and the transition from the ignition to combustion regime. Subsequent engine studies were conducted using the set values of the model parameters, and the results were in excellent agreement with the experimental data. Specifically, a range of injection timings (-20° to 2° ATDC), EGR loadings (0 to 26%, mass basis) and three engine speeds/loads (1250/20, 1500/30, 1780/42 rpm/mg) were examined. The predicted and measured in-cylinder pressures and apparent heat release rates were in excellent quantitative agreement for all conditions, except the early injection timing of -
20° ATDC. Trends for NO and soot emissions were also well reproduced by the model predictions. In particular, the soot-NOx trade-off observed experimentally for increasing EGR loadings was clearly replicated in the modeling results. In general, the parametric studies demonstrate the potential of the current modeling approach as a powerful new tool in diesel engine design and development.

Next steps to improve the model fidelity include exploring the potential of integrating this modeling approach with a model that can be used to represent flame propagation. Flame propagation can play a role in systems where significant premixed combustion occurs. Other areas for investigation include exploring the effects of nonuniform reaction rates within the flame and the transition model parameters on the predicted results. In the present model, \( \chi \) represents variations in the reaction rate within the flame due to the external effects, such as flow strain or curvature. While these effects are considered of secondary importance in this study based on the assumption that most of the diffusion flames are far from extinction conditions, it may be more appropriate for a wide range of engine conditions to allow \( \chi \) to vary throughout the cycle as combustion progresses and the flow turbulence level changes. Additionally, the transition model parameters \( \beta_i \) and \( \beta_f \) identified as optimal for the simulations investigated in this work may not be universal, as the transition from one reaction regime to another may occur more rapidly or more slowly for different engine operating modes. Altering the values used for \( \chi, \beta_i \) or \( \beta_f \) may yield improved agreement between the experimental data and the modeling results for conditions such as Case 8 of this study (the earliest injection timing considered), where there is time for significant fuel-air mixing to occur.

Acknowledgements
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Table 1. Geometry of simulated engine.

<p>| | |</p>
<table>
<thead>
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<tr>
<td>Bore [cm]</td>
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<tr>
<td>Stroke [cm]</td>
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<td>Connecting rod length [cm]</td>
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<td>Piston bowl shape</td>
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<td>Compression ratio</td>
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Table 2. Engine simulation conditions.

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<tr>
<th>Case</th>
<th>SOI (°ATDC)</th>
<th>EGR (% mass basis)</th>
<th>Speed (RPM)</th>
<th>φ*</th>
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<td>10</td>
<td>0.5</td>
<td>11.68</td>
<td>1750</td>
<td>0.79</td>
</tr>
</tbody>
</table>

*Here, the equivalence ratio is defined based on the fuel-to-air ratio in the fresh-air charge only and does not include the effect of EGR addition.
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