

Transported Probability Density Function (tPDF) Modeling for Direct-Injection Internal Combustion Engines

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Abstract

Ongoing efforts in applying a “high-end” turbulent combustion model (a transported probability density function - tPDF - method) to direct-injection internal combustion engines are discussed. New numerical algorithm and physical modeling issues arise compared to more conventional modeling approaches. These include coupling between Eulerian finite-volume methods and Lagrangian Monte Carlo particle methods, liquid fuel spray/tPDF coupling, and heat transfer. Sensitivity studies are performed and quantitative comparisons are made between model results and experimental measurements in a diesel/PCCI engine. Marked differences are found between tPDF results that account explicitly for turbulence/chemistry interactions (TCI) and results obtained using models that do not account for TCI. Computed pressure and heat release profiles agree well with experimental measurements and respond correctly to variations in engine operating conditions. Computed CO and HC emissions show large deviations from experiment in some cases; further work is required in emissions modeling. With explicit accounting for TCI, other physical submodels that have been developed and calibrated to give acceptable results without consideration of TCI need to be revisited.

Introduction

Current engine research includes homogeneous-charge compression-ignition (HCCI) and advanced direct-injection spark-ignition (SID) operation [1, 2], advanced engine combustion modes that promise significant gains in thermal efficiency and lower engine-out emissions compared to current state-of-the-art production engines. In the case of HCCI and quasi-HCCI or premixed-charge compression-ignition (PCCI) combustion modes, this efficiency can be gained with a significant reduction in NO_x and soot, a result of lower combustion temperatures and reduced regions of fuel-rich combustion. Efforts to understand and control these modes of operation are being aided by research into the fundamentals of flow structure and combustion behavior through experiments and modeling, from laser diagnostics to high-end

computational fluid dynamics (CFD) [2]. Experimental studies over the past few years have come significantly closer to achieving control of HCCI operation [3, 4]. Numerical studies have made progress towards more comprehensive engine models, including the application of a high-end transported probability density function (tPDF) model to a production engine [5], for example.

Control of HCCI over a wide speed and load range has proven to be difficult and researchers are exploring several strategies to reliably operate an engine in this mode [3, 6–10]. HCCI does not provide a direct mechanism for ignition timing control, which is typically achieved with fuel-injection timing in the case of a conventional diesel engine or ignition timing in the case of a conventional spark-ignition engine. Autoignition processes rely on pressure, temperature, and composition: temperature, in particular. These must be controlled so that the combustion event will be optimally timed for efficiency. Low HCCI operating temperatures can result in incomplete combustion and high engine-out emissions of unburned hydrocarbons (HC) and CO, particularly in the cases where fuel and hydrocarbon species reach the crevice volumes. An optimal temperature range for HCCI combustion is 1500–1800K peak in-cylinder temperature. This is high enough to allow for complete CO-to- CO_2 conversion yet low enough to avoid significant NO_x formation [11].

Technical challenges to bringing HCCI/PCCI combustion to production include [1]: controlling start of combustion and burn-rate; expanding the narrow operating regime (engine speed and load); reducing the detrimentally high rate of heat release at high loading; controlling transient operation; reducing CO and HC emissions; limiting the increase in NO_x at high loads; and managing cold starts. Controlling the engine over a wide range of operating conditions while maintaining low emissions and high efficiency is the goal of the ongoing research.

For numerical studies, sufficiently detailed chemical mechanisms are required to capture autoignition and production of emissions species [12]. Trace emission species, such as carbon monoxide (CO) and NO_x , can be particularly difficult to model. Because of the range

of temperatures and pressures that can be encountered in these combustion modes, mechanisms must be constructed to accommodate these regimes. For example, reaction pathways encompassing lean, low-temperature conditions, such as those that characterize HCCI combustion, must be considered to model NO_x pathways other than thermal NO.

Zonal Models [13] and hybrid CFD/zonal models [14] may be used effectively when flow/chemistry interactions are weak, such as during robust autoignition for nearly homogeneous reactants. However, detailed chemistry and direct consideration of turbulence/chemistry interactions (TCI) are necessary when modeling conditions with less robust performance and/or stronger departures from homogeneity (e.g. late in-cylinder fuel injection) to accurately account for emissions and, in some cases, ignition timing [15]. The strong interaction of turbulence and complex chemistry is an important challenge in turbulent combustion modeling [16].

A high-end CFD-based turbulent combustion model has been developed to accommodate detailed thermochemistry and TCI. Detailed chemical mechanisms have been combined with a consistent hybrid particle/finite-volume composition transported probability density function method [17, 18]. The strength of the tPDF approach is the closed form of the mean chemical source term. A limitation is the high computational cost. One can use either a storage/retrieval-based scheme [19] or parallel computing to accelerate the thermochemistry calculation; here the latter option is employed.

Previous tPDF-based engine modeling [15] has shown that turbulence and turbulence/chemistry interactions always have a strong effect on the computed emissions. Cases with strong in-cylinder flow, strong spatial inhomogeneity, and/or marginal operating conditions also show a strong influence of TCI on the global combustion event. Other studies have looked at the effect of model coefficients [20], the importance of simulating several consecutive engine cycles to achieve a statistically cyclic stationary state [21], and the importance of detailed NO_x pathways [22].

The work presented here builds upon previous work [5] that analyzed global emissions and ignition characteristics. That work demonstrated the significant sensitivity of simulation results to turbulence/chemistry interactions; however, the comparison between simulation and experimental results was not satisfactory. Here, a different n-heptane chemical mechanism is used, sensitivity to variations in engine and model parameters are explored, and quantitative comparisons between computed results and experimental measurements are made.

Physical Models and Numerical Methods

A three-dimensional, time-dependent Reynolds-averaged model is employed within an unstructured, deforming-mesh, compressible finite-volume CFD solver with second-order spatial discretization. We employ a standard $k - \varepsilon$ turbulence model, and a hybrid finite-volume/particle tPDF method is used to capture turbulence/chemistry interactions. Complex thermochemistry is included and liquid fuel spray models are coupled with the gas-phase thermochemistry and tPDF method.

Consistent hybrid finite-volume/particle tPDF method

Several approaches have been implemented to model the effect of turbulence on combustion in internal combustion engine applications [23]. These include flamelet models, conditional moment closure, and tPDF methods. Both Reynolds-averaged Navier-Stokes (RANS) and large eddy simulation (LES) formulations may be used with these combustion models. For example, a Reynolds averaged flamelet model has been used recently [24] to model the same engine configuration that is studied here.

Here a transported composition PDF method is used. One can derive a transport equation for the velocity-composition PDF from the conservation equations for density (continuity), velocity (momentum), composition, and energy [17]. The composition PDF $\tilde{f}_\phi(\psi; \underline{x}, t)$ is derived from the velocity-composition PDF by integrating over velocity space: $\tilde{f}_\phi(\psi; \underline{x}, t) = \int \tilde{f}_{\underline{u}\phi}(\underline{V}, \psi; \underline{x}, t) d\underline{V}$. Here ϕ denotes the vector of composition variables that characterize the thermochemical state (N_s species mass fractions and mixture enthalpy) and tilde ($\sim$) denotes a density-weighted (Favre-averaged) mean quantity. $\underline{x}$ is the position vector, $\underline{u}$ is the velocity vector, and time is t . The result is:

$$\begin{aligned} \frac{\partial[\langle \rho \rangle \tilde{f}_\phi]}{\partial t} &+ \frac{\partial[\langle \rho \rangle \tilde{u}_i \tilde{f}_\phi]}{\partial x_i} + \frac{\partial[\langle \rho \rangle S_\alpha \tilde{f}_\phi]}{\partial \psi_\alpha} \\ &= - \frac{\partial}{\partial x_i} [\langle u_i'' | \psi \rangle \langle \rho \rangle \tilde{f}_\phi] \\ &+ \frac{\partial}{\partial \psi_\alpha} [\langle \rho^{-1} \frac{\partial J_i^\alpha}{\partial x_i} | \psi \rangle \langle \rho \rangle \tilde{f}_\phi] . \end{aligned} \quad (1)$$

Here summation is implied over repeated indices i or α within a term, and $\alpha = 1, \dots, N_s + 1$ (to include enthalpy). $\langle \rangle$ denotes the probabilistic mean. ρ is the density, J^α is the composition variable α 's molecular flux, and S_α is the source term for composition variable α . $\tilde{u}$ is the Favre-averaged mean velocity and $\underline{u}''$ is the velocity fluctuation about $\tilde{u}$. For this implementation, only the *mean* velocity appears in a closed form: the effect of turbulent velocity

fluctuations (“turbulent diffusion”) must be modeled (first term on the right-hand side of Eq.(1)). The other effect that must be modeled (second term on the right-hand side of Eq.(1)) represents molecular transport (“mixing”).

This approach explicitly accounts for the turbulent fluctuations in species composition and enthalpy (hence temperature) relative to the local mean value. A Lagrangian particle Monte Carlo method is used to solve the modeled composition PDF equation using a consistent hybrid particle/finite-volume method [18]. This hybrid scheme is more tractable than grid-based implementations because the increase in computational effort scales linearly with the number of independent variables, rather than exponentially as in the case of grid-based methods. The particles are a discrete, delta-function representation of the composition PDF and evolve by stochastic differential equations that account for changes in particle position and composition. Coupling to the finite volume solver provides the effects due to mean momentum in the particle equations, while models complete the effects of turbulent velocity fluctuations and mixing. A two-equation $k - \varepsilon$ turbulence model and a standard gradient transport approximation is used to account for transport by turbulent velocity fluctuations, and a simple pair-exchange model is used for molecular mixing [25]. This model is a variant of Curl's model [26], where pairs of particles within each finite-volume cell are selected at random for mixing at a rate determined by the local turbulence time scale and the mixing model parameter C_ϕ . The value of C_ϕ is discussed below in the Results section.

Thermochemistry

Chemical kinetics and thermochemistry are handled through the CHEMKIN libraries [27]. In earlier work [5], a 34-species 74-reaction mechanism (including NO_x) was used. That mechanism was based on a 40-species, 165-reaction skeletal mechanism (excluding NO_x) from Chalmers [28–30]. Here the original 40-species mechanism has been retained. Parallel processing is used to reduce the time for chemical reaction calculation.

n-heptane fuel is used as a surrogate for the diesel fuel in the experimental engine because of the absence of a more suitable detailed mechanism for the real fuel. n-heptane will display general characteristics of a diesel-type fuel, but some important details will not be captured, such as ratios between hydrogen and carbon atoms and other structural and chemical differences that can affect combustion behavior.

Fuel sprays

The code uses stochastic Lagrangian models for direct in-cylinder liquid fuel injection based on the KIVA spray formulation [31, 32]. Spray breakup takes into account only secondary breakup through Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) instabilities. A collision model considers particles for interaction within a specified radius. Evaporation is considered for each parcel, each of which is at a uniform temperature (infinitely fast heat transfer within each droplet).

The temperature, mass, physical location, and velocity distributions of liquid fuel are key properties characterizing spray combustion. Because much of sprays and spray combustion is still not understood, model coefficients are adjusted to fit the model's behavior to what is observed in experiments. Key coefficients for the KH-RT spray breakup model are B_1 , B_0 , RT_Tau , and RT_C . These control breakup time and length scales, and are explained further in the Results section.

Use of a tPDF particle model for the gas-phase thermochemistry allows explicit accounting for the locally high levels of temperature and composition fluctuations that occur as a result of vaporization. The Lagrangian parcel spray model is coupled to the gas-phase tPDF particle model through evaporation. Two approaches have been investigated for this coupling. In one, when spray parcels evaporate based on the spray model parameters, their location, vaporized mass, composition (pure fuel), and temperature are assigned directly to new tPDF notional particles. This coupling naturally captures the high levels of local gas-phase fuel concentration and temperature fluctuations that arise from spray vaporization. More conventional treatments must model this effect or ignore it altogether [33,34]. In the other approach, the vaporized spray mass and energy (enthalpy) is distributed among existing tPDF particles within the finite-volume cell. While this attenuates the local fluctuations somewhat compared to the first approach, it is more robust computationally. In particular, it overcomes problems of unrealistically low tPDF particle temperatures that can occur with large computational time steps for the first approach. A comparison of the two approaches is given in the Results section.

Engine Configuration and Operating Conditions

Many advanced diesel engines are utilizing higher fuel injection pressures and multi-hole, axially symmetric configurations to achieve PCCI/HCCI operation. This study looks at one such engine where experimental engine data are available.

Geometry and computational configuration

A 1/7th wedge sector mesh represents a bowl-in-piston diesel engine (see Table 1). The mesh includes a top-ring-land crevice, which can be important in determining HC and CO emissions [15, 35, 36]. Intake and exhaust ports and valves are not modeled. Simulations begin at 138° bTDC (after intake-valve closure) and continue to 90° aTDC.

Parallel computing is performed using up to 32 processors. This provides reasonable runtimes for the accordion-type moving mesh of about 40,000 cells. Moving meshes of this type do not need to account for the addition or removal of cells, but can result in high-aspect-ratio cells. The number of tPDF particles per cell is maintained between 15 and 30 using particle number density control algorithms [18, 25]. The spray is represented by approximately 20,000 parcels.

Exhaust gas recirculation (EGR) is modeled by modifying the initial composition to include appropriate fractions of CO₂, H₂O, O₂, and N₂ for a given EGR percentage. Minor species are not considered.

Operating conditions

Three operating conditions were run to examine the effect of EGR and the response of the models at part load versus full load. The fuel injector is mounted near the top of the chamber on the centerline, with the spray directed along the bisecting plane of the sector mesh and angled down into the bowl. For the part-load cases, the angle of injection is 52.5° and the start of injection (SOI) is 23° bTDC. For the full-load case, the angle of injection is 79.0° and the SOI is 3.5° bTDC.

Results

In the following subsections, examples of results from sensitivity studies are presented first; these are followed by comparisons with experimental data for the three operating conditions specified in Table 1. Two sets of calculations are performed: one with the transported PDF method ('PDF') and one where cell-mean values are used directly in the chemical mechanism ('FV'). Comparison between the two allows for the determination of the importance of turbulence-chemistry interactions.

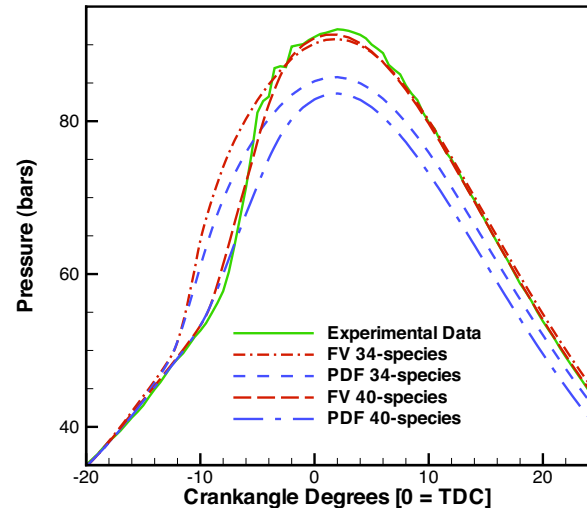


Figure 1: Sensitivity to chemical mechanism and TCI for the 65% EGR case, including comparison with experimental data.

Thermochemical model

Previous results [5] had consistently early ignition timings for both FV and PDF runs compared with the experimental results. The difference between the results of the 34-species and 40-species n-heptane chemical mechanisms (Figure 1) suggests that the discrepancy is largely due to the chemical kinetics. The 40-species n-heptane mechanism has not been tuned with respect to engine data. The significantly better ignition timing of the 40-species mechanism led to the use of this mechanism for the remaining sensitivity studies.

Figure 1 also shows significant differences between the FV and PDF results; this illustrates the importance of TCI. In this case, FV matches the experimental pressure trace better than PDF. This is not unexpected. In the absence of good models for TCI, engine models have been tuned by adjusting parameters in other models to account for this missing physics.

Compression ratio

A second example is sensitivity to engine geometry. The baseline clearance height for this engine configuration is 0.7 mm. An increase or decrease of 0.1 mm causes the geometric compression ratio to change from 16 to 15.8 or 16.2, respectively. The computed peak pressure in-

Table 1: Engine operating conditions for two EGR levels and the full-load case. The bore diameter is 103 mm and the squish height is 0.7 mm.

Engine condition	65% EGR	40% EGR	Full Load
Displacement volume		0.825 l/cyl	
Swirl ratio		1.5	
Engine RPM	1891	1891	3100
Baseline initial pressure (bars)	1.78	1.79	3.285
Baseline initial temperature (K)	400.7	424.7	428.7
Baseline head wall temperatures (K)	500.0	500.0	550.0
Baseline upper bowl wall temperatures (K)	433.0	433.0	433.0
Baseline crevice wall temperatures (K)	433.0	433.0	433.0
Baseline piston wall temperatures (K)	500.0	500.0	550.0
Start of injection	23° bTDC	23° bTDC	3.5° bTDC
External EGR	65%	40%	0%
# of cells in mesh		39483	
Maximum # of tPDF particles		987075	
Equivalence ratio	0.63	0.38	0.53
Baseline compression ratio for 0.7 mm clearance		16:1	

creases or decreases between 2 and 3 bars (Figure 2) in response to this variation, demonstrating a strong sensitivity to this parameter.

Initial and boundary conditions

Changes to initial pressure and temperature were also explored. Changes to initial pressure of 8 kPa resulted in correspondingly higher or lower pressure throughout the cycle with peak pressure changing about 4-5 bars up or down with an increase or decrease of initial pressure, respectively (Figure 3).

Overall the initial and peak pressures for higher initial temperatures are lower, with peak pressure approximately 2 bars lower for each 10 K increase. This is because of the decrease in trapped mass with increasing initial temperature. However, the higher initial temperature gives a steeper rate of pressure rise (Figure 3).

Changes to the wall temperatures, which are set constant throughout the run, showed very little effect on global pressure and heat release for an increase or decrease of 10 K. Changes to swirl, start of injection timing, wall temperature, and fuel temperature were also explored and showed expected but not significant effects on global results.

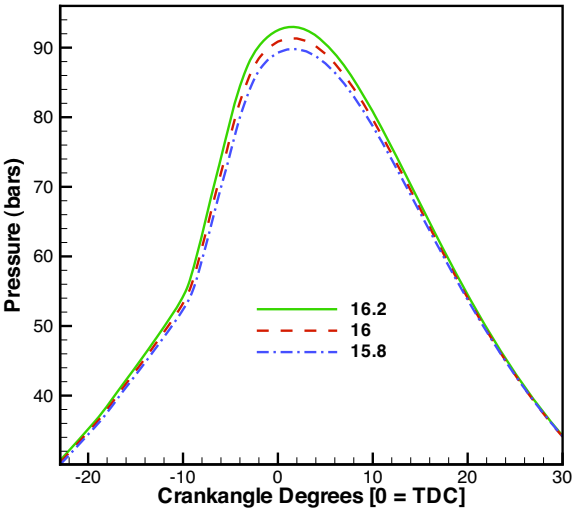


Figure 2: Sensitivity to compression ratio. Clearance height was varied by ±0.1 mm from the baseline case to effect the changes.