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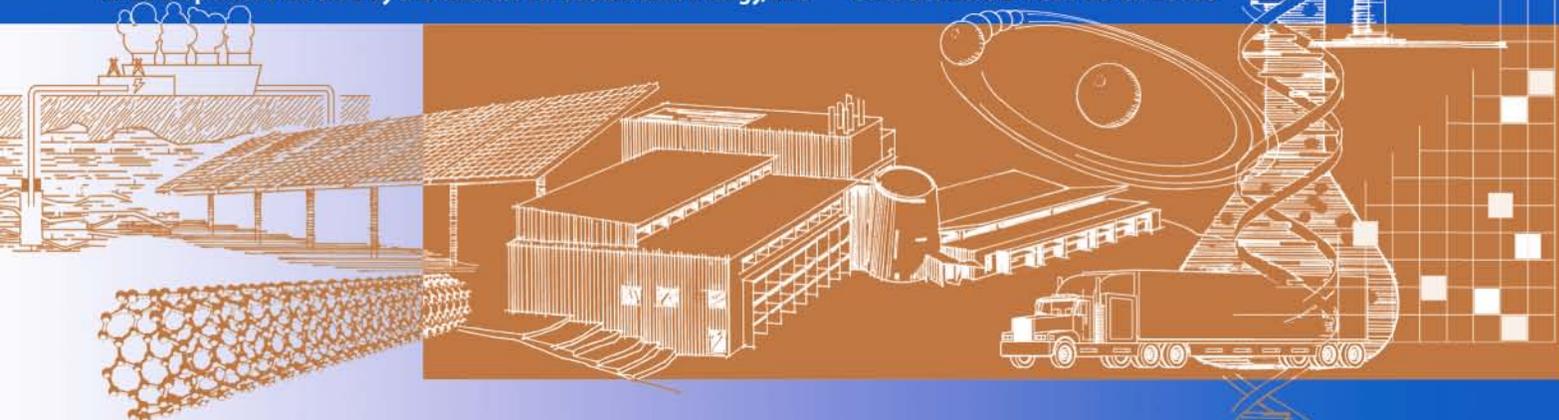
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# Modeling the Fuel Spray and Combustion Process of the Ignition Quality Tester with KIVA-3V

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Development of advanced compression ignition and low-temperature combustion engines is increasingly dependent on chemical kinetic ignition models. However, rigorous experimental validation of kinetic models has been limited as a result of several factors. For example, shock tubes and rapid compression machines are often limited to premixed gas-phase studies, precluding the use of more realistic, low-volatility diesel or biodiesel surrogates. The Ignition Quality Tester (IQT) constant-volume spray combustion system measures ignition delay of low-volatility fuels; therefore, the IQT has the potential to validate ignition models experimentally. However, a better understanding of the IQT's fuel spray and combustion processes is necessary to facilitate chemical kinetic studies. KIVA-3V is utilized in developing a three-dimensional computational fluid dynamics (CFD) model that accurately and efficiently reproduces ignition behavior and temporally resolves temperature and equivalence ratio regions inside the IQT. The model's fuel spray characteristics (e.g., velocity, cone-angle, oscillations) are experimentally validated; n-heptane is initially studied because of the simplicity of its chemical kinetics and use as IQT calibration fuel. Reduced/skeletal n-heptane chemical mechanisms (60, 42, and 33 species) and one-step chemistry are employed. The CFD results indicate combustion is governed by autoignition kinetics, and perturbations/oscillations in the fuel spray have significant effects on the combustion process, as verified experimentally. The CFD model provides insight into the complex interaction between the fuel spray and combustion processes, which is vital to expanding the fuel research capabilities of the IQT.

## 1. Introduction

Enhanced understanding of kinetic pathways to combustion autoignition has become increasingly important to the development of advanced combustion engines and fuels. Homogeneous charge compression ignition (HCCI) and other forms of low-temperature combustion (LTC) strategies rely on fuel autoignition kinetics to control combustion timing [1]. Additionally, the autoignition characteristics of new generation biofuels are of current great interest [2,3]. Development of accurate chemical kinetic models for the ignition of diesel and biodiesel model compounds relies on well-characterized experiments [4]. However, rigorous experimental validation of these kinetic models has been limited for a variety of reasons. Shock tubes and rapid compression machines are typically limited to premixed gas-phase studies, for example [5,6]. Although some progress in studying lower vapor pressure fuels has been made with these devices [7,8], other research platforms may complement this work and extend ignition kinetics studies.

The Ignition Quality Tester (IQT) is a constant-volume combustion chamber experimental apparatus developed to measure ignition qualities of diesel type fuels [9,10,11,12,13]. The American Society for Testing and Materials (ASTM) method D6890-08 was developed around the IQT device to allow rapid determination of derived cetane number (DCN) [14]. The D6890 method calculates DCN for a fuel based on correlation of averaged ignition delay times from a series of IQT injection events, to reference tests using the ASTM D613 engine test method [15]. Since the IQT is a constant-volume spray combustion system that allows ignition and combustion studies of low-volatility fuels, the IQT has potential to generate experimental data relevant to validating kinetic ignition models by virtue of its well-controlled temperature, pressure, and spray fuel injection. IQT-based DCN measurements have been shown to be reliable over a range of cetane numbers for middle distillate and some nonconventional diesel fuels [16,17,18].

The IQT, which burns fuel injected into a high-pressure chamber, conveniently quantifies ignition processes for traditional hydrocarbon fuels through a semi-empirical correlation between measured ignition delay and engine-based cetane number [13]. This correlation will not likely hold for anticipated new fuels derived from biomass, which will have properties that are different from those of traditional fuels. A better understanding of the IQT combustion process may lead to its use as a development and validation platform for kinetic models of novel fuels, as the device provides a well-controlled environment for such tests in comparison to a traditional engine. Experimental parameters such as charge pressure, chamber wall temperature, air temperature, oxygen concentration, and mass of fuel injected are easily quantifiable for model implementation. The IQT offers the additional benefit of a low fuel quantity requirement (capable of testing with approximately 50 mL), increasing its desirability for testing experimental biofuels produced in small amounts.

In this analysis, measurements of IQT spray events at ambient and pressurized conditions are used in retrieving the physical spray characteristics necessary for development of a three-dimensional KIVA-3V numerical model. Values for spray velocity, mass flow rate, droplet size, and other fuel nozzle effects are selected such that the spray model matched measurements from high-speed imaging of ambient spray events. With a valid physical model in place, chemical kinetics are applied to the simulation, and the results of the combustion simulation are compared with pressure rise data from high-pressure IQT events. Simulations uncover the importance of autoignition chemistry on IQT combustion events. Additionally, study of model results allow for comparison of the relative effects of droplet breakup, droplet evaporation, and chemical kinetic delay in contributing to overall ignition delay within the IQT. Such a parametric understanding allows for developing the potential of using the IQT as a chemical mechanism validation tool, filling an experimental void and complementing other research platforms.

## 2. Experimental Setup and Computational Model

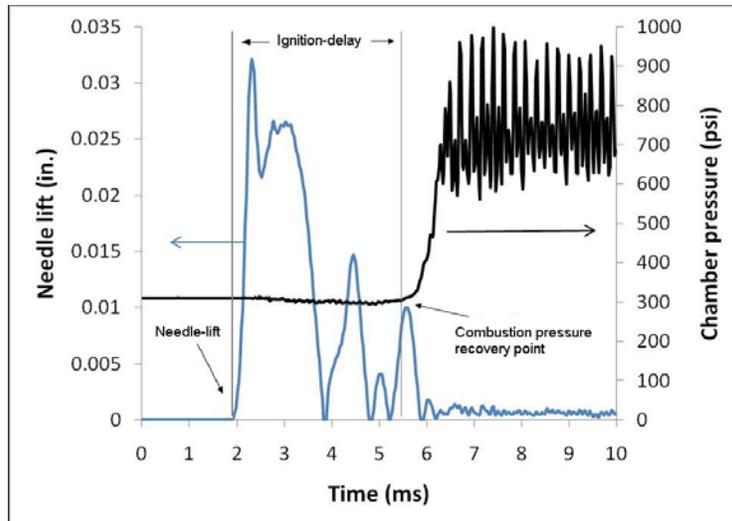
### 2.1 IQT overview

The ignition quality tester (IQT) is a bench-scale, constant-volume combustion device (Figure 1) with a spray injection system designed for the direct measurement of the ignition delay of liquid fuels. Ignition delay is then used to calculate a derived cetane number (DCN) using the ASTM D6890-08 method with high repeatability ( $\pm 0.85$  DCN, 34-61 DCN range) [14], providing high sensitivity for middle distillate fuels. A piezo-electric pressure transducer installed in the combustion chamber measures the pressure rise during the combustion event; the time delay between the start of injection (SOI) and the rise in combustion pressure to the combustion pressure recovery point of injected fuel determines the ignition delay for various fuels [9,10] (Figure 2). The ignition delay comprises both physical processes (e.g., spray breakup, vaporization, air entrainment) and the chemical kinetics of ignition [9]. A pneumatically driven mechanical fuel pump is used for the injection of the fuel along with a single-hole S-type delayed (inward opening) pintle nozzle. The injection pressure, as experimentally determined, is approximately 225 bar during the main injection period; n-heptane ( $\geq 99.5\%$ , Fluka) is used for all experiments in this study and is chosen because of its use as a calibration fuel for the IQT, with a reference ignition delay time of 3.78 ms [14].



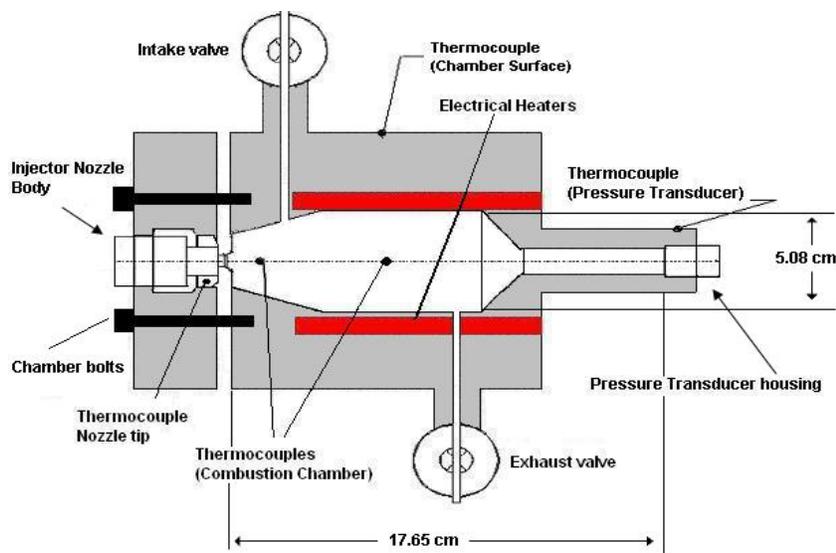
**Figure 1. The Ignition Quality Tester (IQT)**

*(Note: All photos were taken by the authors.)*



**Figure 2. Typical combustion pressure and needle-lift traces used to determine ignition delay; n-heptane,  $m \approx 73$  mg/inj., ignition delay = 3.78 ms**

Several electric rod heaters are inserted into the outer wall of the stainless steel combustion chamber [11]; they maintain a constant charge temperature of approximately 550°C (in the vicinity of the nozzle tip). There is approximately a 40°C temperature gradient (increase) to the second thermocouple (7 cm down range) along the axial direction of the combustion chamber. The lower injection end temperature is due to the heat transfer to the coolant around the injection nozzle body and surface exposure to ambient air (Figure 3). The chamber (volume  $\approx 0.21$  L) is pressurized to approximately 21 bar prior to injection of the fuel [10,14].

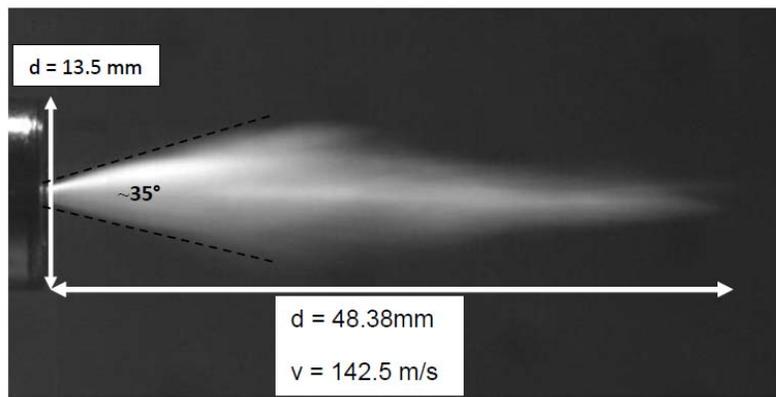


**Figure 3. Schematic of the IQT combustion chamber**

## 2.2 Spray characterization of the IQT fuel injection system

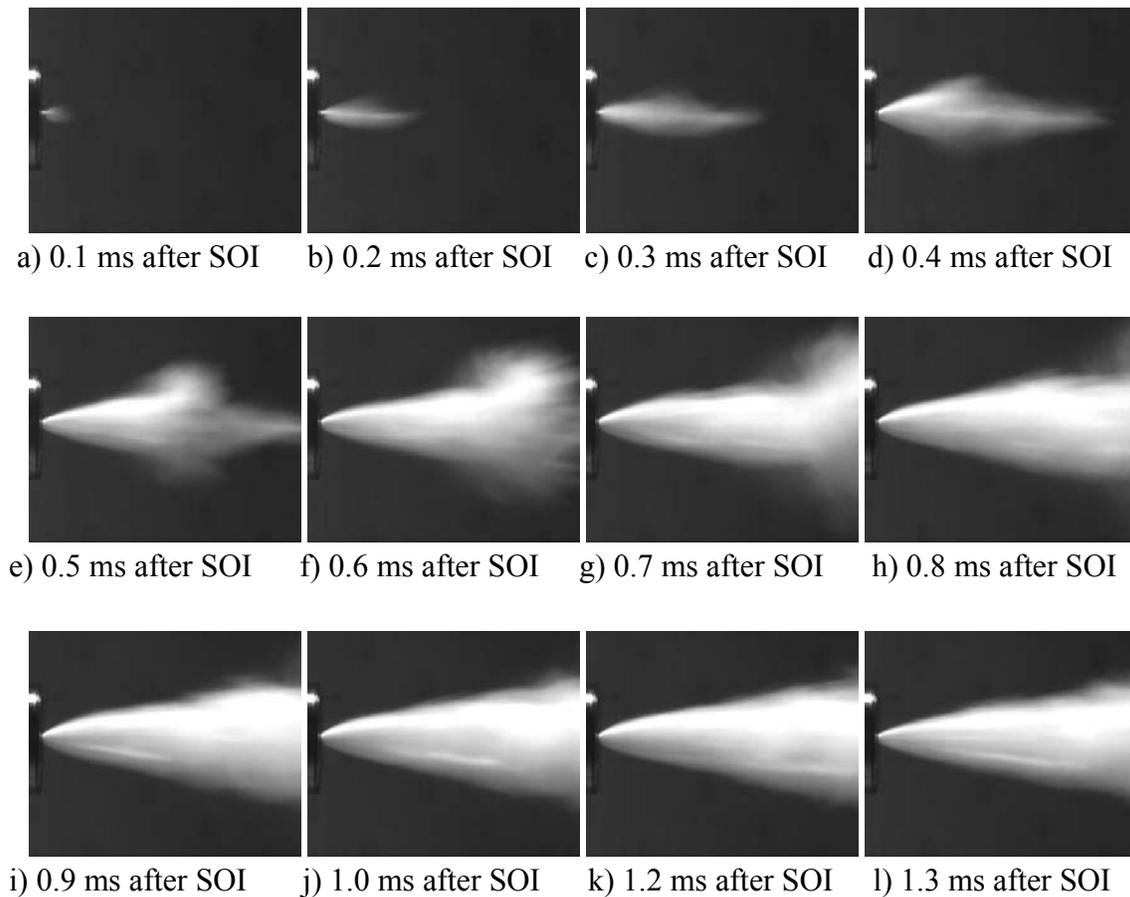
The goal of validating ignition kinetic models using the IQT requires a thorough understanding of the combustion and injection processes within the IQT, as the measured ignition delay is a combination of the physical dynamics of the spray and combustion chemistry. A three-dimensional model was developed and utilized to gain a better understanding of the injection and combustion processes. Compared with a reciprocating engine, the well-controlled experimental parameters of the IQT—such as charge pressure, chamber wall temperature, air temperature, oxygen concentration, and mass of fuel injected—facilitate accurate implementation of these parameters into the model. This improves the model’s ability to predict realistic and representative combustion events. To ensure the accuracy of the modeled spray, experimental tests capture IQT injection system spray events at ambient conditions using high-speed charge-coupled device (CCD) imaging.

**2.2.1 High-speed imaging.** The IQT injection system is placed in a fume hood and controlled using the system’s software to study fuel spray under ambient conditions ( $T_a = 22^\circ\text{-}25^\circ\text{C}$ ,  $P_a = 0.87$  bar). The injection pressures ( $\sim 225$  bar at 0.027-in. needle-lift) are the same ones used during normal operation of the IQT. The needle-lift sensor is attached to the injector body during imaging to correlate the position of the injector needle with the fuel spray. The fuel spray images are captured using a Photron SA3 (120k-M2) high-speed digital camera capable of capturing images at 250,000 frames per second (fps). For this study, images are captured at 10,000 fps, resulting in a 0.1 ms time-step and 512x256 resolution for a main injection period of approximately 2 ms. However, high-speed imaging continued over a period of 4–6 ms to capture secondary fuel spray injections (see the needle-lift traces in Figure 2). High-speed imaging of the fuel spray provides injection velocity, cone angle, and penetration depth as a function of the injection period (Figure 4).



**Figure 4. Spray imaging (0.4 ms after SOI) (cone angle:  $\sim 35^\circ$ , penetration depth: 48.38 mm, spray tip velocity: 142.5 m/s); n-heptane**

Photron FASTCAM Viewer software is used to determine the penetration depth of the fuel spray by using the diameter of the nozzle tip as a scale (see Figure 4). The spray tip velocity is calculated based on the penetration depth for each time step of 0.1 ms along with the cone angle. The CCD imaging also provides insight into the nonuniformity of the fuel spray and captures the highly complex spray patterns that develop during the injection process (Figure 5). The nonuniformity of the spray pattern is due to the use of an inward opening pintle nozzle. The geometry of the injector needle and pintle tip allows a small fraction of the fuel to exit during the beginning of the injection process before allowing the bulk of the fuel to exit the nozzle at a higher velocity and wider angle. The nonuniformity of the spray patterns can have a significant effect on the outcome of the predicted combustion event; therefore, it is currently under investigation and will be implemented in the numerical model.



**Figure 5. High-speed images of the fuel spray during typical injection process; n-heptane,  $P_f \approx 225$  bar**

*2.2.2 Fuel injection parameters.* The discharge coefficient is defined as the ratio of the experimentally determined mass injection rate to the theoretical mass injection rate [19]. As a result of the complex geometry of the S-type pintle nozzle and injector needle movement, the mass injection rate changes as functions of needle displacement (injection pressure) and nozzle orifice. Because the bulk of the fuel is injected from 2.5 to 3.5 ms (Figure 2), the injection process is simplified here by considering only the steady-state fuel flow during the main injection period, in which the injection pressure and nozzle orifice are constant. Thus, the discharge coefficient calculated from the mass flow rate during this period is considered the input parameter for the numerical model. Further work is required to determine the discharge coefficient during the entire injection process, which will lead to a detailed look-up table that accounts for the change in needle-lift position (injection pressure) and orifice area. The measured fuel spray tip velocities, along with needle-lift position as a function of the injection period, are in the current look-up table. The fuel spray parameters from both experiments and imaging (Table 1) are utilized in the numerical model. Initial droplet size is not measured; thus, maximum droplet size is estimated based on the spacing of the orifice of the injector nozzle as a function of time; details are presented later in this paper. The mass of fuel injected is an average of three test collections of the fuel (each composing 10 injections) as directed by the IQT manual [20].

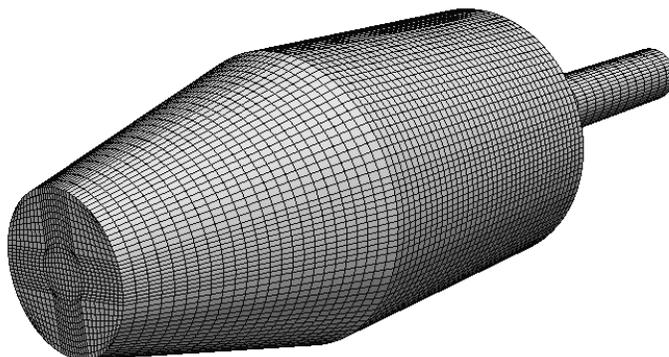
**Table 1. Fuel spray parameters for numerical model**

Fuel	n-heptane
Fuel temperature (°C)	~56
Air temperature (°C)	~590
Mass of fuel injected (mg/inj.)	73–76
Injection duration (ms)	1.8–2
Discharge coefficient ( $C_D$ )	~0.8 (steady-state)
Cone angle	7°–35° (over range of injection period)
Initial droplet size	estimated based on nozzle orifice
Injection velocity (m/s)	0–182 (over range of injection period)

### *2.3 Numerical model*

Reacting fuel spray is simulated using a modified version of KIVA-3V software [21]. The code couples Lagrangian particle tracking of liquid spray droplets with Eulerian simulation of three-dimensional fluid flow as governed by the Navier-Stokes equations. These equations are solved on a structured grid domain of 59,868 cells generated using ANSYS ICEM computational fluid dynamics (CFD) commercial software (Figure 6). The Reitz Kelvin-Helmholtz Raleigh-Taylor (KHRT) spray breakup model [22] governs droplet breakup, as implemented in KIVA-3V by Professor Tsai [23]. A custom look-up table coded for this analysis specifies the time-varying

liquid injection velocity, mass flow rate, initial droplet size, and spray cone angle. Single step and reduced/skeletal chemical mechanisms simulate n-heptane combustion. Mechanisms include a 33-species mechanism from Nissan [24], a 42-species mechanism created by adding  $\text{NO}_x$  reactions and removing iso-octane reactions from a 41-species mechanism developed at the University of Wisconsin [25], and a 60-species mechanism developed at the University of California-Berkeley [26].



**Figure 6. Isometric view shows the block structure of the ~60,000 cell IQT grid**

### **3. Results**

To create a functional numerical model of the IQT, the modeled spray physics and combustion chemistry are tuned to match experimental conditions. This is accomplished by first developing a valid model for the flow physics of a nonreacting spray and then adding chemical reactions. Once the model accurately reproduces experimental IQT behavior, the relative effects of physical and chemical phenomena are compared.

#### *3.1 Tuning the spray parameters*

The spray model is tuned at ambient conditions, in which high-speed imaging provides a visible time history of flow structure without the confounding effects of chemical reactions. Defining the spray requires setting the initial droplet diameter, injected velocity, instantaneous mass flow rate, spray cone angle and thickness, and fuel temperature. The characteristic Kelvin-Helmholtz breakup time directly scales with the input coefficient,  $B1$ , which accounts for the internal effects of the injector [22]; thus,  $B1$  must be empirically specified, though it is expected to fall within the range of 1.73 to 60.

Instantaneous injected mass flow rate is assumed to be proportional to measured instantaneous injector valve needle lift, with the flow rate normalized such that the integral of the mass flow rate gives a total injected mass of 73 mg. The time history of injector valve needle lift also leads

to a specification of initial droplet diameter, with the initial Sauter Mean Diameter set equal to the nozzle opening ( $\sim 120 \mu\text{m}$ ).

With all other injection parameters specified, B1 can be tuned in KIVA until the time history of spray penetration depth matches the spray penetration depth measurements at ambient conditions (Figure 7). A visual comparison of the time history of the spray penetration depth comparing the high-speed imaging and KIVA is in Figure 8.

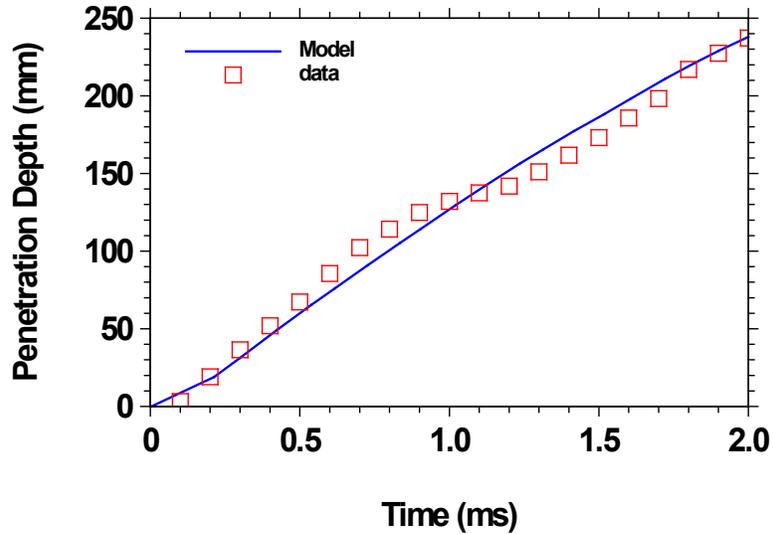
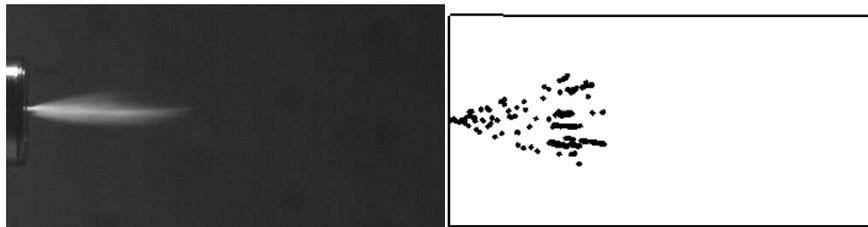


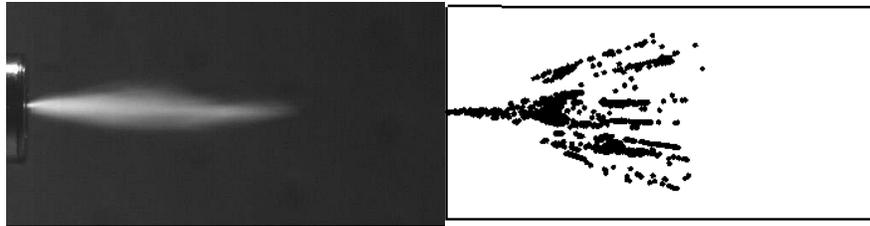
Figure 7. Spray penetration depth comparisons of experiments and model



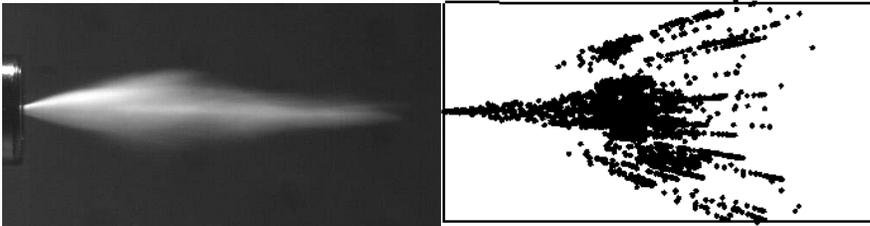
a) 0.1 ms after SOI



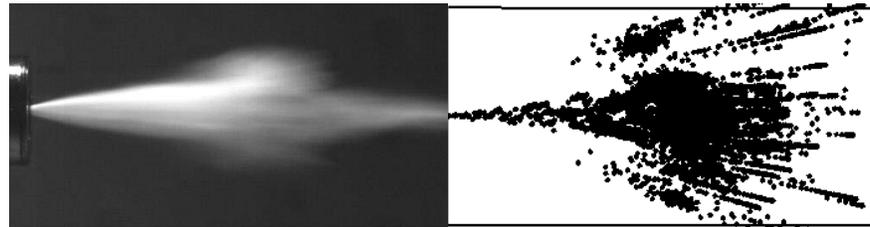
b) 0.2 ms after SOI



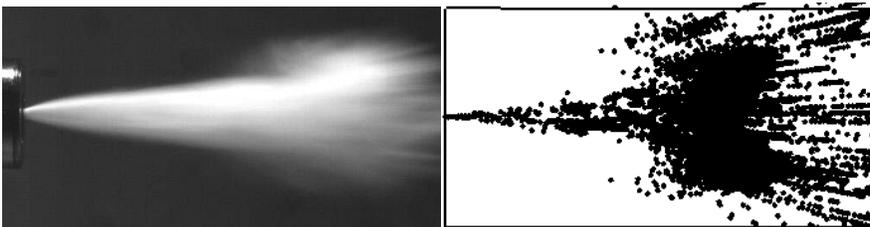
c) 0.3 ms after SOI



d) 0.4 ms after SOI



e) 0.5 ms after SOI



f) 0.6 ms after SOI

**Figure 8. Visual comparison of the spray penetration depth; n-heptane,  $P_f = 225$  bar,  $P_a = 0.87$  bar,  $T_f \approx 30^\circ\text{C}$ ,  $T_a \approx 25^\circ\text{-}30^\circ\text{C}$**

Transitioning from ambient conditions to the IQT combustion chamber environment ( $P_a = 21$  bar and  $T_a = 550^\circ\text{C}$ – $590^\circ\text{C}$ ) requires an adjustment of spray velocity in the model, as the pressure drop across the injector will be smaller and produce a slower initial injection velocity in comparison to ambient conditions. Bernoulli's equation accomplishes this scaling by relating fuel injection pressure, air pressure within the chamber, and the density of the fuel injected

(Equation 1). The cone angle of the spray at ambient conditions is assumed to be relatively unchanged with higher back pressures in the combustion chamber [27].

$$v(m/s) = \sqrt{\frac{2 \cdot [P_f - P_a]}{\rho_f}} \cdot C_D, \quad \text{Equation (1)}$$

where  $P_f$  = fuel pressure,  $P_a$  = pressure of air in the chamber,  $\rho_f$  = density of the fuel, and  $C_D$  = the discharge coefficient.

### 3.2 Chemical mechanism comparison for high-pressure IQT system

With valid spray physics implemented, reacting behavior is modeled through the inclusion of an n-heptane chemical mechanism in the three-dimensional KIVA model. Single-step, 33-species, 42-species, and 60-species mechanisms vary in their simulated overall ignition delay behavior, as shown by the pressure histories of Figure 9.

The 42-species n-heptane mechanism predicts the ignition delay times closest to the experimental ignition delay times, which is explained by the conditions under which the mechanism was validated when developed. Designed for internal engine applications, the 42-species n-heptane mechanism was validated under direct injection diesel conditions and was specifically tuned to capture the rich onset of autoignition in regions where fuel evaporation has locally cooled the mixture [25]. This contrasts with the 33-species mechanism, which was tuned primarily for lean homogeneous charge compression ignition (HCCI) combustion. Using the 33-species mechanism under the predicted fuel-rich IQT combustion conditions results in an overall ignition delay of  $\sim 1.7$  ms longer than the experimental value. The 33 species mechanism's overprediction of ignition delay at this rich equivalence ratio,  $\Phi \approx 2.0$ , possibly stems from model's exclusion of H, H<sub>2</sub>, CH<sub>3</sub>, and CH<sub>4</sub> reactions [24].

The 60-species mechanism, which was validated for lean HCCI combustion environments [26], predicts ignition delays  $\sim 0.9$  ms shorter than those in the experimental data. The variation in performance of these validated chemical mechanisms in the IQT environment indicates the IQT's suitability as a validation tool for direct-injection autoignition engines, because of the IQT's similarities to such an environment.

Differences in modeled ignition delay time between the chemical mechanisms likely result from the variance in chemical reactions and reaction rates related to autoignition chemistry. Chemical autoignition delay times for each mechanism, calculated using a Senkin zero-dimensional well-mixed reactor (WMR) model [28] initially at 590°C and 21 bar, are in Figure 10. In addition to the reduced mechanisms, the full detailed n-heptane mechanism from Lawrence Livermore National Laboratory was employed as a reference [29]. These simulations show that the

differences in chemical autoignition delay times within the range of equivalence ratios at which autoignition initiates ( $1 < \Phi < 3$ ) are comparable to the differences in overall delay in the 3-D models. For example, the 60-species mechanism has a zero-dimensional chemical delay time 1.3 ms shorter than that of the 42-species mechanism, while the KIVA modeled ignition delay time, using the 60-species mechanism, is about 1.5 ms shorter when flow physics are included. The 42-species n-heptane mechanism predicts ignition delay times closest to the experimental ignition delay times; thus, the 42-species n-heptane mechanism is utilized for further investigation of the combustion event inside the chamber.

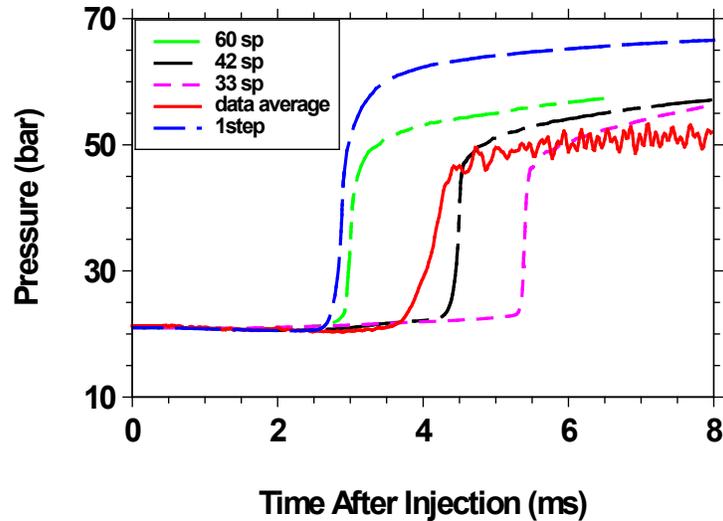


Figure 9. Varying chemical mechanism affects the predicted ignition delay

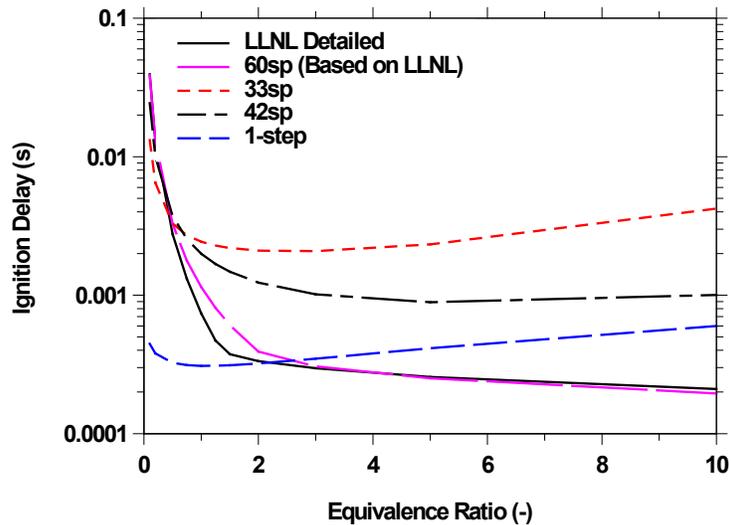
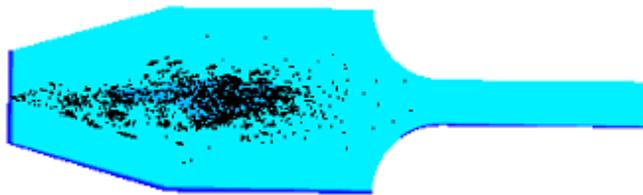
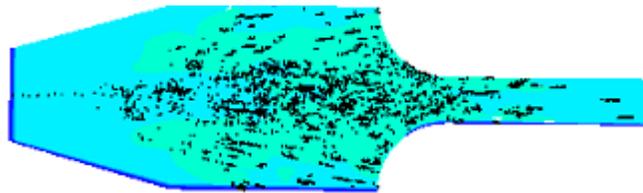


Figure 10. Chemical mechanism ignition delay time dependence on  $\Phi$  explains differences in behavior; autoignition occurs where  $\Phi$  is slightly rich, as seen with the 33-species mechanism, with the longest delay time, and with the 1-step mechanism, with the shortest delay time

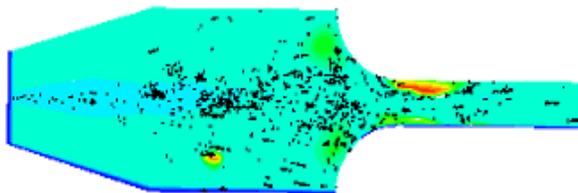
Further evidence of the governing effects of autoignition on the predicted combustion event can be seen in an evolution of the KIVA model at the onset of ignition. Dispersed locations within the chamber ignite as favorable conditions for autoignition are met, and no single propagating diffusion flame front dominates the process (Figure 11). The observed rich onset of autoignition near  $\Phi = 2$  for n-heptane mixtures that have been cooled by evaporative cooling is well documented in the literature [30,25].



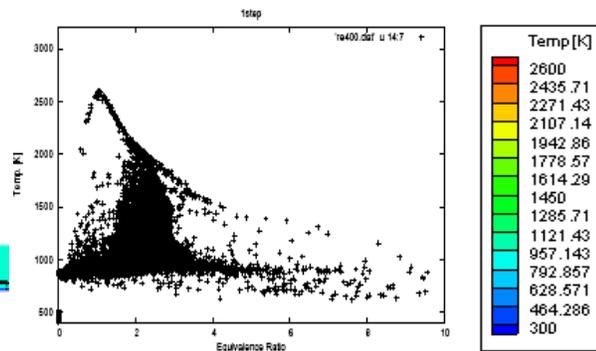
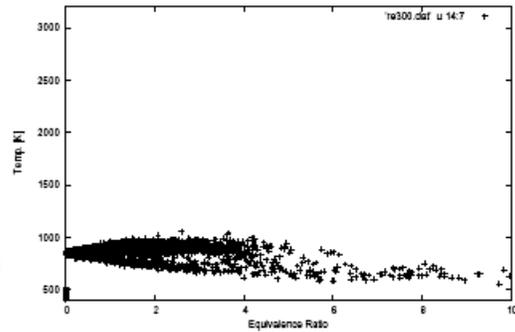
t = 1.41 ms

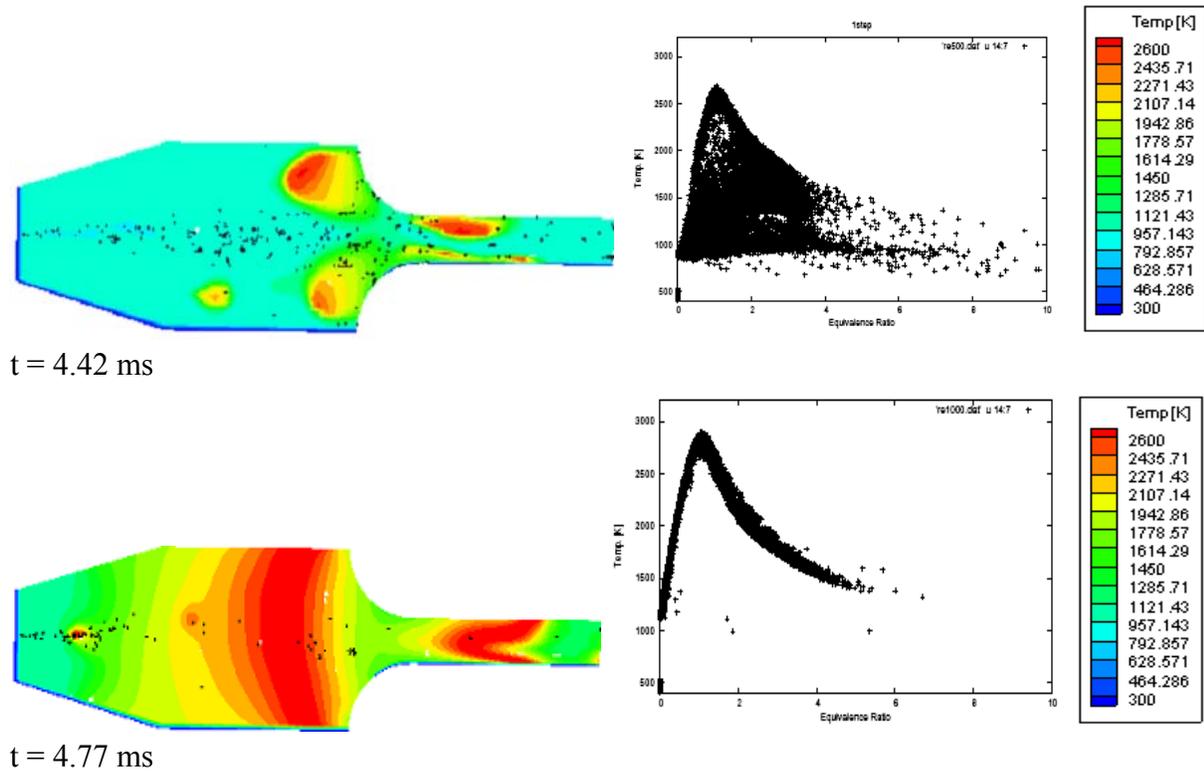


t = 3.69 ms



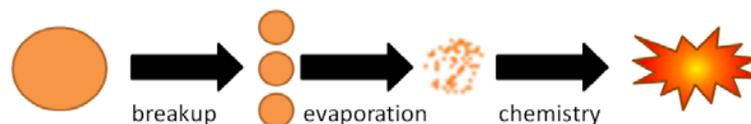
t = 4.29 ms





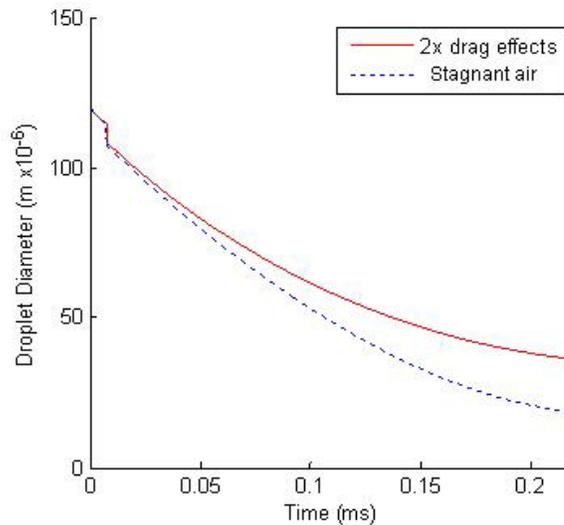
**Figure 11. The role of autoignition is shown by the time evolution of the temperature contour plots (left) and the corresponding plots of temperature vs. equivalence ratio (right), which demonstrate that the onset of combustion occurs primarily in the rich regions around  $\Phi = 2$**

*3.3 Comparing the relative effects of physics, chemistry, and thermodynamics on ignition delay*  
 For the IQT to become a useful tool for chemical mechanism validation, the relative influence of chemical interactions must be higher than the uncertainties in spray fluid mechanics. A series of physical processes precede chemical autoignition; the overall ignition delay time from start of injection is thus roughly approximated by a combination of breakup time, evaporation time, and chemical reaction time (Figure 12). The following analysis examines the characteristic times of these processes for comparison purposes. These processes operate continuously on the spray; therefore, initial sites of chemical autoignition may influence remaining unburned fuel spray.



**Figure 12. Droplet breakup and evaporation processes precede chemical autoignition**

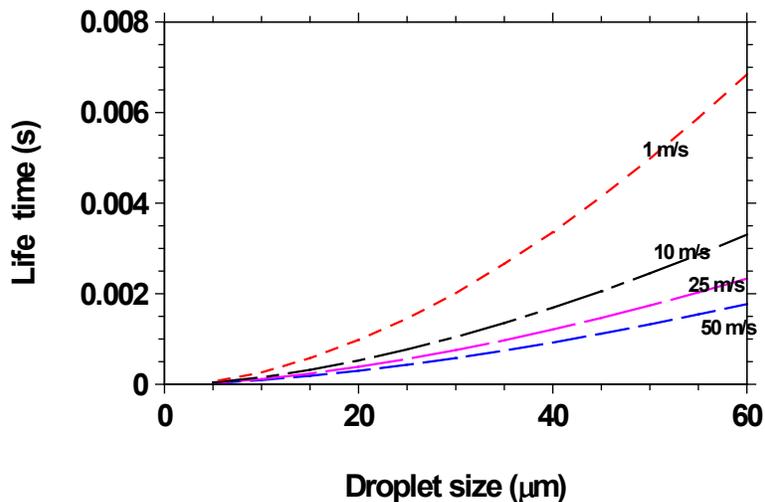
*3.3.1 Droplet breakup time.* Droplets leaving the injector nozzle that are on the order of the pintle opening in size would take a long time to evaporate and combust if not for the aerodynamic forces that lead to their breakup into smaller droplets. In this model, the droplet breakup is modeled considering both Kelvin-Helmholtz and Raleigh-Taylor instabilities [22]. The KHRT breakup algorithm [31] was coded into MATLAB® and applied to a single droplet 120  $\mu\text{m}$  in diameter traveling at an initial velocity of 120 m/s, which is typical of a droplet injected into the KIVA-3V model. Correct quantification of momentum transfer from the droplet to the surrounding air complicates the analysis, as the relative droplet velocity in the surrounding air governs breakup events. For this reason, two analyses were run: one in which the surrounding air stays stagnant and one in which the air gains velocity as the droplet loses velocity, implemented by doubling the rate at which drag forces decrease the relative velocity. Breakup rates in both cases slow after 0.2 ms (Figure 13), so 0.2 ms is chosen as the characteristic breakup time. Though the breakup times are coincidentally similar, the stagnant air model ends with a 21  $\mu\text{m}$  droplet traveling at 43.4 m/s and the drag-doubled model ends with a 38  $\mu\text{m}$  droplet traveling at 32.7 m/s. The effects of these differences in final droplet velocity and diameter are described in the following section, in the discussion of the evaporation time calculation.



**Figure 13. Drag model treatment affects the KHRT breakup model predictions**

*3.3.2 Droplet evaporation time.* Droplet vaporization is a critical step in spray combustion, as it generates the vapor necessary for gas-phase combustion. Droplet diameter decreases as heat transfer from the surrounding gases evaporate the liquid fuel. The lifetime of a droplet is governed by the rate of heat transfer to the droplet and its initial size. Convective effects increase

the heat transfer rate such that droplets moving faster have shorter lifetimes. In Figure 14, results are charted of numerical simulations of droplet lifetimes at varying initial diameters and velocities, demonstrating these important relations. In the previous section, a 21  $\mu\text{m}$  diameter droplet traveling at 43 m/s and a 38  $\mu\text{m}$  diameter droplet traveling at 32.7 m/s were presented as the results of 0.2 ms of breakup processes under varying momentum transfer rates. Supposing now that this droplet evaporates, the numerical model suggests that it will turn completely into vapor in 0.5 ms, given the initial conditions resulting from the stagnant air case, or in 1 ms, given the initial conditions resulting from the double-drag case. At this point, the fuel is in gas phase, and assuming well-mixed conditions, combustion chemistry begins.



**Figure 14. Projected lifetime for a single droplet decreases as droplet velocity increases and as droplet initial diameter decreases**

**3.3.3 Chemical reaction time.** Chemical oxidation mechanisms have associated induction periods (i.e., chemical ignition delay) during which initial hydrogen abstraction by oxygen produces alkyl, hydroperoxyl, and hydroxyl radicals, leading to the chain reactions that consume the hydrocarbon and release heat. The KIVA model results described showed that the 42-species mechanism most accurately reproduces IQT behavior. For this mechanism, the zero-dimensional, well-mixed reactor simulation (see Figure 10) demonstrates that the chemical ignition delay times in the relevant equivalence ratio range vary from 1.8 ms at  $\Phi = 1$  to 1.0 ms at  $\Phi = 3$ .

**3.3.4 Discussion.** A compilation of the ranges of characteristic times from the preceding analyses is presented in Table 2. Uncertainties in these values come from treatment of momentum transfer to the surrounding fluid. Additional discrepancy from actual behavior comes from the serial nature of the calculations, the lack of calculation of a characteristic mixing time for the turbulent flow, and the assumption of constant temperature in the ambient air.

**Table 2. Delay time breakdown comparison**

<b>Phenomenon</b>	<b>Zero-Dimensional Parametric Study</b>	<b>Three-Dimensional KIVA-3V Model</b>	<b>IQT Experiment</b>
Breakup time (KHRT model)	0.2 ms	Processes modeled simultaneously	Processes occur simultaneously
Evaporation time (single droplet model)	0.5 ms–1 ms		
Chemical ignition delay (zero-dimensional WMR, 42 species mechanism)	1.0 ms–1.8 ms		
<b><i>Total Delay Time</i></b>	<b><i>1.7 ms–3 ms</i></b>	<b><i>4.2 ms</i></b>	<b><i>3.78 ms</i></b>

#### 4. Conclusions

In this study, a KIVA-3V model is developed for the IQT spray combustion system and tested with n-heptane. The model predicts that the combustion event is governed by autoignition, and that dispersed ignition events occur throughout the combustion chamber. KIVA predicts an ignition delay time of approximately 4.2 ms in comparison to the experimental ignition delay time of 3.78 ms; further investigation into the overprediction of ignition delay time is required. Modeled differences show that overall ignition delay changes significantly when chemical mechanisms vary in their chemical ignition delay time; thus, performing a sensitivity analysis of the various chemical reactions and reaction rates in each mechanism may provide insight into the cause of the varying prediction of chemical ignition delay times.

The efficacy of validating fuel combustion kinetic mechanisms during spray combustion using the IQT depends on the relative importance of the chemical reaction time to the overall ignition delay. An accurate understanding of the physics of the fuel spray is thus vital for capturing and isolating physical effects on the overall ignition delay time. The physics of the fuel spray implemented in the model are based on a detailed experimental characterization of the fuel spray and an analytical estimation when necessary. The KIVA-3V model of the IQT combustion chamber allows a comparison of the overall ignition delay times through sensitivity analyses of various experimental parameters and the use of different reduced chemical mechanisms.

Simplified models of droplet breakup, evaporation, and chemical ignition solved serially provide insight into the relative impact of chemical mechanism, initial droplet size, and initial droplet velocity on the overall ignition delay time. This leads to a better understanding of the predicted overall ignition delay times from the KIVA model, in which physics and chemistry are coupled. The chemical ignition delay time (42 species) accounts for approximately half (at  $\Phi = 1$ ) of the overall ignition delay time using a zero-dimensional, well-mixed reactor model. The physical ignition delay time (droplet breakup and evaporation) accounts for the other half of the overall ignition delay time, and the time necessary for droplet evaporation is dominant. Thus, reducing the initial droplet size and increasing its initial velocity will reduce the overall impact of the spray physics on the overall ignition delay time, permitting a more direct study of the chemical ignition delay times between various fuels. Future analyses will show if the relative impact of chemical ignition delay can be improved by using a higher temperature spray with smaller and/or faster droplets to improve breakup and evaporation.

The KIVA-3V model provides detailed insight into the coupling of the fuel spray and combustion chemistry, providing valuable information about the processes governing combustion within the IQT chamber. Zero-dimensional modeling, in contrast, allows the physics of the fuel spray and combustion chemistry to be decoupled, so that parametric effects can be compared. The greater understanding of spray physics and combustion chemistry gained from these models will ultimately permit optimization of the experimental system, leading to a robust system with engine-like conditions in which chemical kinetics studies can be performed. The model most accurately predicts ignition delay using a 42-species chemical mechanism for n-heptane, which was originally validated under spray combustion conditions in a diesel engine. Thus, for direct-injection, autoignition applications, the well-controlled conditions of the IQT make it a potentially attractive chemical mechanism validation platform.

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