

Modeling the Ignitability of a Pilot Injection for a Diesel Primary Reference Fuel: Impact of Injection Pressure, Ambient Temperature and Injected Mass

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ABSTRACT

In this paper, we studied the accuracy of computational modeling of the ignition of a pilot injection in the Sandia National Laboratories (SNL) light-duty optical engine facility, using the physical properties of a cetane/iso-cetane Diesel Primary Reference Fuel (DPRF) mixture and the reaction kinetics of a well-validated mechanism for primary reference fuels. Local fuel-air equivalence ratio measurements from fuel tracer based planar laser-induced fluorescence (PLIF) experiments were used to compare the mixture formation predictions with KIVA-ERC-based simulations. The effects of variations in injection mass from 1 mg to 4 mg, in-cylinder swirl ratio, and near-TDC temperatures on non-combusting mixture preparation were analyzed, to assess the accuracy of the model in capturing average jet behavior, despite its inability to model the non-negligible jet-by-jet variations seen in the experiments. Fired simulations were able to capture well the measured ignitability trends at the different injection conditions tested, but showed some deviations in the minimum temperature needed for robust ignition, pointing out the need for further work to focus on achieving fully comprehensive modeling with detailed chemical kinetics of the DPRF58 mixture and a full engine geometry representation.

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INTRODUCTION

Usage of pilot injection strategies in diesel engines operated with conventional diesel combustion (CDC) modes is widely adopted in order to reduce the delay of the main ignition event, smoothen the premixed combustion phase and consequently reduce noise and pollutant emissions at partial loads [1, 2, 3, 4]. However, more advanced and low-temperature compression ignition combustion strategies typically feature early injections and high charge dilution levels achieved by means of high exhaust gas recirculation (EGR) rates. Here, the benefits of adding pilot injection stages before the main injection can be difficult to achieve and are still not well understood. In fact, small pilot quantities may fail to ignite when the local charge conditions are too dilute or temperatures are too low, and robust ignition may be re-established by increasing the pilot injected mass, at the price of compromising the emissions performance of the low-temperature combustion (LTC) strategy, especially as far as soot and NO_x are

concerned [5, 6, 7, 8]. However, if properly optimized, the adoption of pilot injections in combination with low-temperature combustion strategies may help compensate for their drawbacks, including reducing overall HC and CO emissions that are among the major challenges of low-temperature combustion modes.

Computational modeling of pilot injection phenomena may aid experimental investigations by providing more insight into how mixture preparation develops and what are the sources of ignition and pollutant formation. As a matter of fact, the reliability of detailed engine computer models is crucial to the development and assessment of new combustion concepts for internal combustion engines, such as homogeneous-charge compression ignition (HCCI), partially-premixed combustion (PPC), and reactivity-controlled compression ignition (RCCI). However, typical computational model validations are carried out against simplified, reference benchmarks that are not always able to represent the full range of conditions at which

models are requested to perform. This is particularly true when looking at light-duty diesel engines, where the fuel spray is injected in highly swirling environments, and typical injection strategies feature massive jet impingement and flow separation at the piston bowl rim. A number of previous studies have shown how engine computational fluid dynamics (CFD) models can be used effectively to capture mixture preparation and ignition in low-temperature, partially premixed combustion strategies, and aid in the understanding of the main sources of pollutant emissions arising from overly lean mixtures forming below the ignition limits. However, there is lack of validation studies considering the transient conditions typical of pilot injections, which feature small injected masses, low injection pressures and non-steady injector needle behavior. The aim of this study was thus to assess and validate a CFD engine model for simulating pilot injection phenomena in the Sandia light-duty optical diesel engine, operated with a Diesel Primary Reference Fuel mixture. Extensive experimental campaigns have been conducted on this engine to measure and understand the mixture preparation and pilot ignition limits for a wide range of operating conditions relevant to low-temperature combustion strategies [9,10].

The study is structured as follows. First, the major details of the experimental campaigns are given. Then, the computational methodology is described, and the sub-models chosen to describe the spray physical processes and the ignition kinetics are studied for some simple, fundamental test-cases. Finally, the model's reliability with varying operating parameters is assessed against local equivalence ratio measurements of [9], and the ignitability limits of a pilot injection over a range of charge dilutions and pilot injection parameters are modeled and compared to the experiments of [10].

EXPERIMENTAL SETUP

All of the experimental measurements were carried out using the Sandia National Laboratories light-duty optical engine facility [9,10]. The engine used in the studies is a modified version of the GM light-duty 1.9L engine, provided with an optical piston that retains the full geometric details of the production piston. Optical access to the combustion chamber allows extensive measurements of local quantities in the squish region and in the piston bowl, as schematically represented in Figure 1. The engine is also provided with a variable swirl generation device placed upstream of the intake valves, which features adjustable throttle plates. Different throttling strategies can be used to generate swirl ratios from about 1.5 up to about 5.5. A summary of the main engine characteristics, along with the injector parameters and composition of the fuel used in the experiments, is reported in Table 1.

All of the pilot injection experiments considered in this study were run at a fixed engine speed of 1500 rev/min, and with variable intake conditions, but keeping an approximately constant average near-TDC ambient density of 19.6 kg/m³. The timing of the single pilot injection was held fixed at 15°

before top dead center (TDC), so as to limit the impact of spray targeting, variable in-cylinder flows, and transients in the in-cylinder density and temperature on the ignition and mixture formation process. The primary independent variables were thus near-TDC temperature, ambient O₂ concentration, pilot mass, injection pressure, and swirl ratio.

Although ignition studies were carried out in environments with different O₂ concentrations, measurements of the mixture formation process (local equivalence ratio distributions) were taken in a non-reacting environment of pure nitrogen using a fuel tracer-based planar laser-induced fluorescence technique (PLIF).

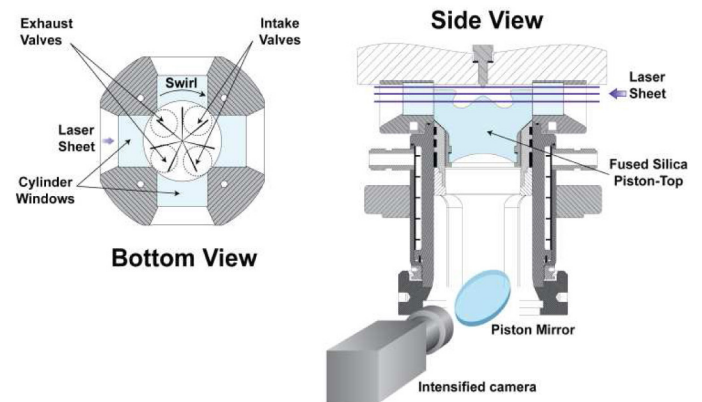


Figure 1. Schematic representing the optical access engine setup, including the three laser sheet locations and camera viewing direction (from [9]).

Table 1. Main engine and experimental setup specifications for the experimental pilot injection campaigns.

Engine specifications

Bore x stroke [mm]	82.0 x 90.4
Unit displacement [cm ³]	477.2
Compression ratio	16.4 : 1
Squish height at TDC [mm]	0.88

Injector parameters

Sac volume [mm ³]	0.23
Number of holes	7
Included angle [deg]	149
Nozzle diameter [mm]	0.14
Hole protrusion [mm]	0.3

Fuel properties for PLIF studies

Composition [mole fractions]	42% nC ₁₆ H ₃₄
	58% iso-C ₁₆ H ₃₄
Fluorescent tracer [mass fraction]	0.5% 1-C ₁₁ H ₁₀
Equivalent Cetane Number [-]	50.7

Fuel properties for ignition studies

US #2 diesel fuel	CN=47
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Table 2. Operating conditions details for both the reacting (ignition studies) and non-reacting (mixture formation studies) cases.

Non-reacting intake charge composition [mole fractions]	100% N ₂
Non-reacting intake temperatures [K]	300, 381
Reacting intake charge composition [mole fractions]	10% O ₂ , 81% N ₂ , 9% CO ₂ 12% O ₂ , 80% N ₂ , 8% CO ₂ 14% O ₂ , 80% N ₂ , 6% CO ₂ 16% O ₂ , 80% N ₂ , 4% CO ₂ 18% O ₂ , 79% N ₂ , 3% CO ₂
Intake temperatures [K]	303, 323, 363, 403
Engine speed [rpm]	1500
Injected fuel mass [mg]	1.0, 2.0, 3.0, 4.0
Start of Injection [deg]	-15.0 ± 0.1

An absence of O₂ was required to avoid excessive fluorescence quenching of the 1-methylnaphtalene tracer that was added to the diesel primary reference fuel (DPRF) mixture. Use of the DPRF fuels was required to minimize fluorescence from species other than the 1-methylnaphtalene. Two different intake temperatures were employed to investigate the impact of temperature on the mixture formation process. The PLIF measurements were made in three moving planes to track the mixture preparation process, as reported in Figure 2. One plane bisected the squish region, one was located at the bowl rim height and one was deeper within the piston bowl, at its maximum radius.

Experiments with ignitable intake charges were made for a matrix of charge compositions, corresponding to in-cylinder oxygen concentrations from 18% down to 10%, as well as near-TDC temperatures ranging from approximately 800K up to more than 950K. A summary of the experimental conditions for both the non-reacting and the reacting cases is reported in Table 2.

Finally, as noted above, a DPRF mixture was used for the PLIF imaging. The blend featured two cetane isomers, 42% n-hexadecane and 58% 2,2,4,4,6,8,8-heptamethylnonane (or iso-cetane) by volume. These proportions were selected to mimic well the ignition properties of the US #2 diesel fuel used in the ignitability experiments, with a cetane number of CN = 47 measured using ASTM D613. Note that the fuel mixture has a higher cetane number, CN = 50.7, than the #2 diesel fuel - despite the well-matched ignition behavior. The DPRF58 surrogate more closely matches the representative physical properties of the diesel fuel than a previously used, lighter and significantly more volatile PRF25 mixture [11,12], made up of 25% iso-octane and 75% n-heptane by volume, that had similar ignition characteristics as diesel fuel [39] but different physical properties relevant to spray injection, atomization and vaporization.

MODEL DEVELOPMENT

The experimental campaigns of [9,10] provide a unique opportunity for the validation of spray models for internal combustion engine simulations, since the exact fuel components can be modeled for the physical processes occurring in the engine: injection, atomization, vaporization, and mixing and ignition. Although the ignitability studies were conducted with the #2 diesel fuel, the careful matching of the ignition behavior to the DPRF blend, and to the PRF25 blends used in earlier work [11,12] allows the chemical modeling to be pursued with confidence.

Furthermore, modeling of pilot injection phenomena is a challenging task for computational modeling as the fuel injection process is fully transient and the injector needle never reaches its maximum lift (cf. Figure 16). This also affects the experimental campaigns, where the effects of stochastic phenomena are amplified, including interferences due to presence of residual liquid-phase fuel, or non-consistent nozzle-by-nozzle behavior due to internal injector dynamics and surface in-homogeneities [9]. For these reasons, in order to define an accurate computational model setup for the engine simulations, the choice of appropriate sub-models was based on validations against more fundamental test cases.

Numerical Setup and Improvements to KIVA

The study was carried out using a modified version of the KIVA-ERC code, a custom build of the KIVA3V CFD code [13] that features improved sub-models for fuel spray, turbulence, heat transfer and combustion modeling. Fast, detailed chemical kinetics capability was added to the code by using the SpeedCHEM sparse analytical Jacobian chemistry solver [14], and a High-Dimensional Clustering (HDC) algorithm [15,16,40] for chemistry cell grouping. Furthermore, a piston compressibility model, previously developed and validated for the current engine facility, was used. This model noticeably improved the prediction of the cylinder compression ratio without needing to artificially modify the in-cylinder volume to match the measured pressure trace [17]. Details of the commonly used turbulence, spray and heat transfer sub-models activated for the present study are reported in Table 3.

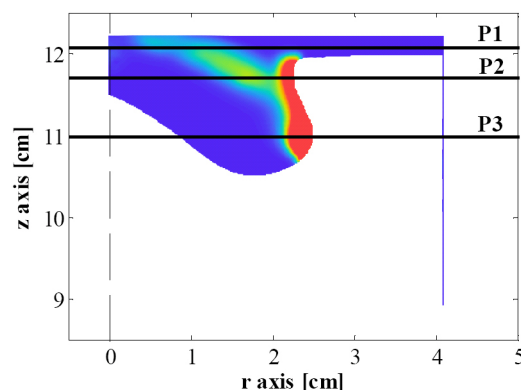


Figure 2. View of the measurement planes on the combustion chamber cut-plane of the combustion chamber geometry.

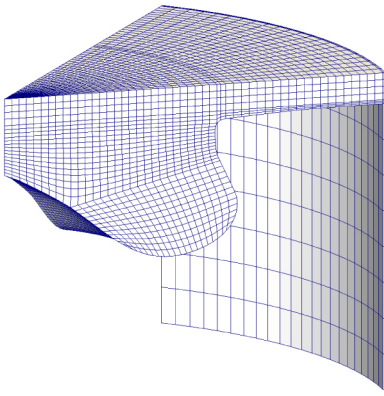


Figure 3. View of the computational grid used for this study near TDC.

Previous studies [17,18] have pointed out the need for using an appropriate grid resolution in order to correctly capture fuel vapor penetration for low-load, partially premixed compression ignition cases. This led to a converged grid resolution slightly smaller than 1 mm, with about 105k cells at bottom dead center (BDC), as represented in Figure 3. As the original KIVA3 code structure was not developed for such large domains, the simulations were extremely inefficient, leading to large computational times even for simple, motoring or non-reacting operating conditions. Thus, significant modifications in the code's architecture were introduced to make it more suitable for extensive computations with refined geometries, while maintaining the underlying numerical algorithms. The major modifications can be divided into three major classes:

1. Removal of all static common-block structures and their replacement with modern, fully encapsulated and dynamically allocated Fortran modules;
2. Refactoring of the code's time-step restart capability, with selective storage/retrieval of the relevant simulation parameters based on the instantaneous simulation status (presence of spray drop parcels, activation of select sub-models, etc.);
3. Replacement of computationally expensive temperature-dependent functions, including thermo-chemistry and physical property functions of the gas-phase and liquid mixtures with SpeedCHEM's optimal-degree interpolation approach [14].

The updated code was found to provide identical results as the previous build, while achieving noticeable computational speed-ups for both small and large grids. As an example, a comparison between the previous and the current release of the code in terms of fluid flow solver CPU times is reported in Figure 4. Here, two extreme cases are compared: motored engine operation with a refined 2D mesh having only about 3000 cells at BDC and the same resolution as the mesh used in this study, and non-reacting pilot injection simulation using the grid with about 105000 cells at BDC of Figure 3. For the simple 2D simulation, requested CPU time was reduced by about 3.2 times to less than two minutes on a single core, while for the sector mesh setup relevant to this study the

computational time was reduced from 29.9 hours down to less than 13 hours, corresponding to an overall speed-up by a factor of about 2.3.

Table 3. Main sub-models activated in the KIVA-ERC+ code for modeling pilot injections in the Sandia-GM optical engine.

Phenomenon	Sub-model
Spray breakup	KH-RT instability, Beale and Reitz [19]
Near-nozzle flow	Gas-jet theory, Abani et al. [20]
Spray angle	Reitz and Bracco [21]
Droplet collision	O'Rourke model [22] with ROI (radius-of-influence), [20]
Wall film	O'Rourke and Amsden [22]
Evaporation	Discrete multi-component, Ra and Reitz [23]
Turbulence	RNG k- ϵ , Han and Reitz [24]
Combustion	SpeedCHEM, Perini et al. [14,16]
Chemistry grouping	High-Dimensional Clustering, Perini et al. [15,16, 40], with $\epsilon_T = 10$ K, $\epsilon_V = 10^{-4}$
Optical piston compressibility	Perini et al. [17]

Diesel Primary Reference Fuel Modeling

As described earlier, the present 42%/58% mass distribution of the DPRF58 surrogate was found in the experiments to yield the same ignition timings as a US #2 Diesel fuel [11,12]. Since the overall ignition event is the result of a chain of physical and chemical processes involving fuel spray atomization and evaporation, mixture formation and charge ignition kinetics, it was chosen to model the fuel liquid and gas phases in the engine model as close as possible to the real fuel used in the experiments, in terms of both physical and thermo-chemical properties. Thus, liquid and gas-phase fuel component properties were obtained from the pure hydrocarbons' database of Daubert and Danner [25], while the JANAF thermo-chemistry cards in the reaction mechanism for Diesel Primary Reference Fuels by Westbrook et al. [26] were used for gas-phase modeling. It should be noted that, even if the ideal gas formulation in KIVA was used, at the operating conditions tested in this study, a real-gas equation of state could have a non-negligible effect on predicted local charge vaporization cooling.

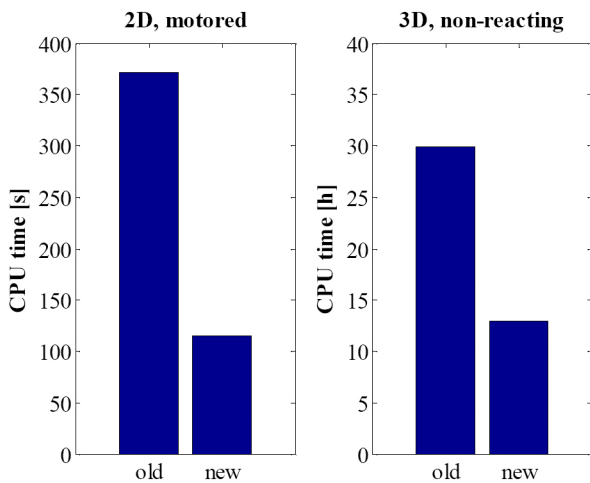


Figure 4. CPU time comparison between the standard and current build of KIVA-ERC. (left) 2D motored case, (right) 3D sector non-reacting pilot injection case.

Unlike the modeling of the physical spray dynamics and vaporization processes, it was not possible to model the ignition processes using only exact multi-component models for the diesel primary reference fuel used in the experiments, due to the fact that a sufficiently reduced chemical kinetics model for ignition of DPRF surrogates is not available. The detailed model by Westbrook et al. [26] features 2837 species and 10719 reactions, and, even with sparse chemistry capabilities, its incorporation was made impossible by the excessive computational burden required to advect this huge number of species.

Thus, the widely used approach that separates the physical spray behavior from the ignition kinetics was adopted. Since the ignition of the PRF25 of [17,18] was found to be similar to the DPRF58 fuel of the current study, the ERC PRF reaction mechanism was used [27]. The spray modeling used the physical properties of DPRF58.

Fuel Property Determination

Mixture-averaged physical properties for DPRF58 were determined and single-component-equivalent fitting coefficients were computed over the temperature range of the liquid phase and introduced in the fuel library. The coefficients and the formulations used are reported in [Appendix A](#).

The predictive capabilities of the model were assessed for three test cases: adiabatic evaporative cooling of liquid fuel; vaporization of a single droplet in a steady environment; ignition of a PRF or DPRF mixture in a homogeneous, constant-volume adiabatic reactor.

Mixture Evaporative Cooling

In order to test if the local temperature of a DPRF mixture after vaporization would be appropriate for modeling with PRF25 reaction kinetics, a mixture evaporative cooling test case was developed and its equivalence ratio sensitivity was studied. In

order to find the final mixture properties, the program computes the final mixture thermal properties through three discrete states:

- A) Initial state:
 Liquid fuel (f) at temperature T_L
 Gas-phase air (a) at temperature T_A
- B) Vaporized state:
 Fuel vapor (f) at temperature T_L
 Gas-phase air (a) at temperature T_B

where:

$$f(T_B) = \frac{A}{F} (h_a(T_A) - h_a(T_B)) - h_{f,lv}(T_L) = 0;$$

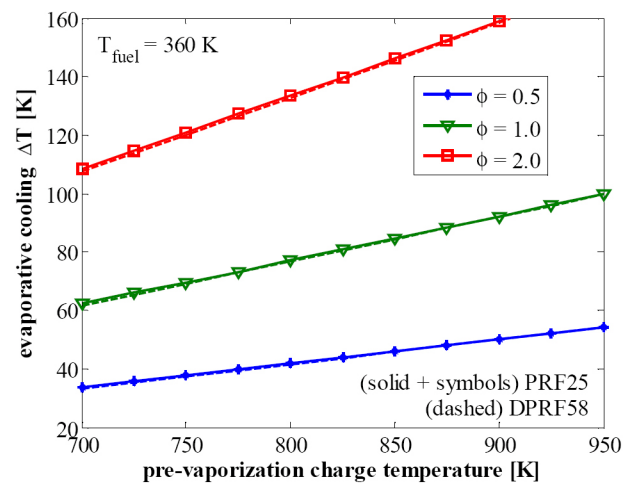


Figure 5. Evaporative cooling effects of PRF25 and DPRF58 fuels: amount of cooling after fuel vaporization and mixing versus the initial charge temperature, at a liquid fuel temperature $T_{fuel} = 360$ K, and different final mixture equivalence ratios.

- C) Fully mixed state:
 Gas-phase air+fuel mixture (m) at temperature T_M

where:

$$Y_m = \left[\frac{A}{F} Y_a + Y_f \right] / \left[\frac{A}{F} + 1 \right],$$

$$f(T_M) = \left(\frac{A}{F} h_a(T_B) + h_f(T_L) \right) - h_m(T_M) = 0.$$

As shown in [Figure 5](#) for an initial liquid fuel temperature of 360K and different initial charge temperatures close to the near-TDC conditions tested in the current study, PRF25 and DPRF58 have similar cooling effects. The same analysis carried out for different PRF numbers and DPRF numbers, as reported in [Figure 6](#), did not show noticeable changes in these results, confirming that, provided the final equivalence ratio is the same, both fuel representations lead to similar adiabatic mixture temperatures, thus leaving ignition timing to rely on the suitability of the kinetics modeling.

Droplet Vaporization Process

Both atomization and vaporization have a crucial effect on the predicted spray structure and mixture preparation. It was found that calibration of the Kelvin-Helmholtz Rayleigh-Taylor (KHRT) model constants had little effect on predicted liquid fuel penetration and gas-phase mixture preparation when simulating short, pilot injections. The KH time scale constant B_1 of [19] was varied from $B_1 = 10$ to 80, and the previously established value of $B_1 = 40$ [17] was eventually chosen. To validate and to examine the impact of the fuel vaporization modeling, in this section the vaporization behavior of the discrete multi-component fuel model used was assessed for both single- and multi-component fuel compositions.

The evaporation of a single n-heptane droplet in a steady environment under micro-gravity conditions was modeled and validated against the experiments by Nomura et al. [28] - see Figure 7.

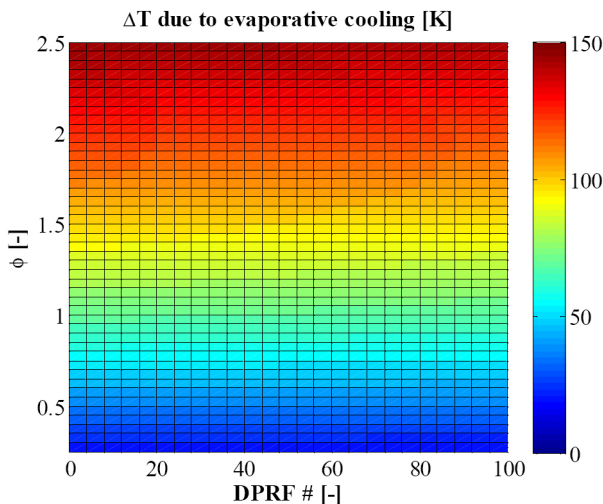


Figure 6. Evaporative cooling effects of DPRF number liquid fuels at different final equivalence ratio. Liquid fuel temperature $T_{\text{fuel}} = 360\text{K}$, initial charge temperature $T_{\text{air}} = 800\text{K}$.

The simulation matched the experiment; however, the initial liquid drop temperature was not known, and was assumed to be $T = 330\text{K}$. The initial and transient droplet temperature behavior is a primary source of uncertainty in single droplet evaporation experiments, where the droplet itself is suspended from one or more threads, and thermal conductivity effects cannot be avoided [28]. However, the model showed good agreement with the measured vaporization histories.

The same setup was used to compare the vaporization histories of the DPRF58 mixture, when modeled 1) as a single component with the mixture-averaged physical properties described earlier, or 2) as a binary liquid mixture. In Figure 8, the vaporization history using the two approaches is compared in a high-pressure environment and at temperatures relevant to near-TDC engine conditions, with an initial drop diameter $d = 0.7\text{mm}$ and temperature $T = 330\text{K}$. In either case, the model clearly captures the initial thermal expansion effects due to heating of the droplet in the high-temperature environment. As

far as the vaporization diameter slope is concerned, the single-component model cannot represent the different volatilities of the two fuel components, and the mixture-averaged behavior leads to a slightly faster vaporization at low temperatures. However, the difference between the two approaches narrows as temperature increases and the overall vaporization process is very well captured at high temperatures. It is expected that these differences become negligible in the engine, where the vaporization process is ruled by significant convective heat transfer. Thus, the single-component approach is an effective way to model the vaporization of the DPRF mixture, the ignition of which is modeled using PRF kinetics.

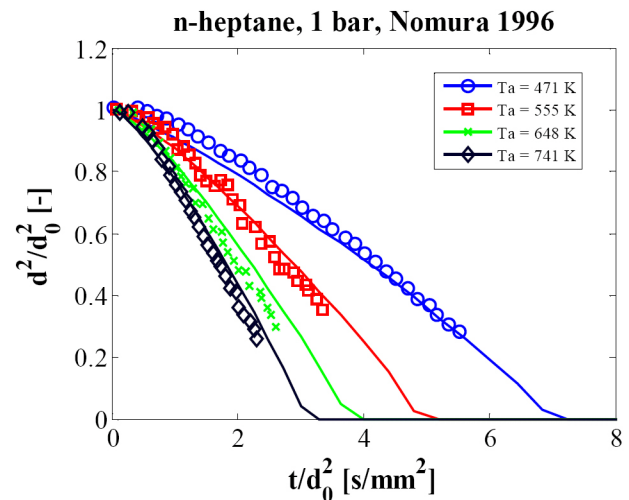


Figure 7. Predicted (DMC model of Ra and Reitz [23]) vs. measured (Nomura 1996, [28]) vaporization histories of a single n-heptane droplet in a steady high-temperature environment under micro-gravity conditions.

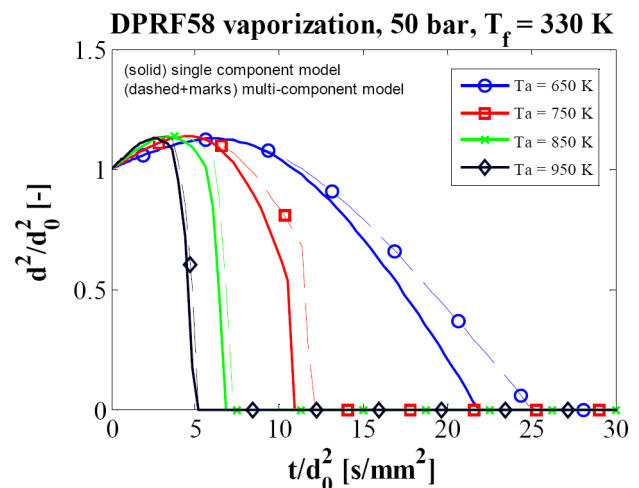


Figure 8. Predicted vaporization history of a single DPRF58 droplet, with initial radius of 0.7 mm, in a steady, high-temperature and high-pressure environment. (solid lines) single-component averaged fuel properties; (dashed lines) full multi-component model.

Finally, single drop vaporization was used to compare predicted vaporization histories of the two fuel surrogates with the multi-component model. In Figure 9 the predicted PRF25