

Large Eddy Simulation of Autoignition Transients in a Model Diesel Injector Configuration

Layal Hakim, Guilhem Lacaze, and Joseph Oefelein
Sandia National Laboratories

ABSTRACT

Developing an improved understanding of transient mixing and combustion processes inherent in diesel injection is an important element in the design of advanced engines. This paper provides a detailed analysis of these processes using an idealized benchmark configuration designed to facilitate precise comparisons between different models and numerical methods. The computational domain is similar to the Engine Combustion Network (www.sandia.gov/ECN) Spray-A injector with n-dodecane as the fuel. Quantified idealizations are made in the treatment of boundary conditions to eliminate ambiguities and unknowns associated with the actual injector(s) used in the experiment. These ambiguities hinder comparisons aimed at understanding the accuracy of different models and the coupled effects of potential numerical errors. Prior to understanding the impact of injector imperfections on their performance, it is first necessary to understand how models perform in a well-controlled environment with well-defined boundary conditions. Here, we focus on the latter while accurately matching the operating conditions used in the experiments. Relevant high-pressure phenomena are treated with real-fluid thermodynamics and transport for multicomponent mixtures. A highly resolved calculation is performed to study both scalar-mixing and initiation of combustion. Results are assembled into a database that can facilitate one-to-one comparisons between codes. The combined set of results is analyzed to provide physical insights related to localized broadband transient mixing and combustion processes that are typically not available from experiments.

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INTRODUCTION

Fuel injection processes in internal-combustion engines largely determine fuel-air mixture formation, which governs the detailed evolution of chemical kinetics, combustion, and emissions. Lack of accurate models is a major barrier toward the design of optimized, clean, high-efficiency engines and there is a critical need for advanced development in this area [1]. Addressing this need involves a variety of challenges, which include all of the complications associated with turbulent combustion in gas phase systems, plus significant additional complications that arise due to the presence of multiple phases. Multi-scale coupling between processes occurs over a wide range of time and length scales, many being smaller than what can be resolved in a numerically feasible manner. Further complications arise when liquid phases are present due to the introduction of dynamically evolving interface boundaries and the complex exchange processes that occur as a consequence. At the device level, high-performance, dynamic stability, low pollutant emissions, and low soot formation must be achieved simultaneously in complex geometries that generate complex flow and acoustic patterns. Flow and combustion processes are highly turbulent; i.e., integral-scale Reynolds numbers of $O(10^5)$ or greater, and the

turbulence dynamics are inherently dominated by geometry or various operating transients. In modern systems, operating pressures now approach or exceed the thermodynamic critical pressures of the working fluids. This introduces significant thermodynamic non-idealities and transport anomalies in low-temperature regions. Elevated pressures also significantly increase the system Reynolds number(s), which inherently broadens the range of spatial and temporal scales that interactions occur over.

In a Diesel engine, fuel oxidation can occur in a two stage process. A cool-flame ignition at low temperatures (typically 700-850 K) is followed by main ignition at high temperatures. This phenomenon is well known and its description must be accurately represented. To date, only detailed/skeletal mechanisms are able to account for cool-flame ignition. In this regard, it is important to note that detailed state-of-the-art chemical mechanisms for n-dodecane oxidation [2, 3, 4, 5, 6] show large variability in the prediction of the ignition delay time and their operational range is limited. Mechanisms still have to be developed and validated at temperatures below 800 K, and pressures higher than 4 MPa. This variability (shown in Fig. 1 for autoignition in homogeneous reactors at 2 MPa) raises questions

regarding how to best use detailed mechanisms at conditions they are not designed for, and what strategy should be employed to represent the critical processes associated with ignition and combustion at Diesel engine conditions. Clearly, the notion that detailed mechanisms produce the “best” accuracy is not correct, and should not be invoked to justify their use. Short of having the perfect mechanism, one must then at least construct models with a clear understanding of the potential uncertainties. Indeed, using a complex chemical mechanism for cases such as Spray-A at 6 MPa is not necessarily any better than a less expensive but optimized simple mechanism. Also, complex chemistry used in tandem with a crude turbulent combustion closure that does not account for turbulent-mixing correctly will not yield correct predictions. Applying complex chemistry under these circumstances only makes the computations more expensive without any accuracy benefits.

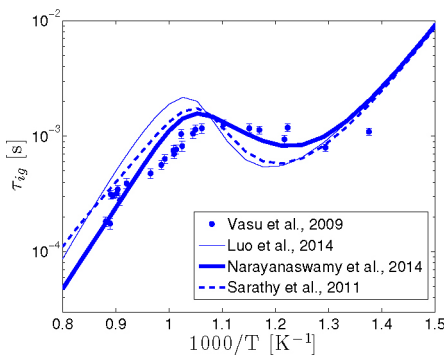


Figure 1. Comparison of the auto-ignition delay time for a stoichiometric mixture of n-dodecane/air at 2 MPa computed using the detailed mechanism by Sarathy et al. [2], the skeletal mechanism by Narayanaswamy et al. [3], and the skeletal mechanism by Luo et al. [4] compared to the experimental shock tube data by Vasu et al. [7]. The calculations are performed using a constant volume homogeneous reactor.

Currently, spray and chemistry models require calibration and it is well known that results are sensitive to the choice of parameters. Understanding the fundamental processes leading to phenomena such as autoignition and flame propagation is needed to build effective models. To do so, however, additional benchmark data beyond that available from experiments is required. Given this observation, and using results from previous works as a foundational starting point [8, 9, 10, 11, 12, 13], a high-resolution LES (2 μm spacing) of the Spray-A case described by Pickett et al. [14] has been performed. Liquid n-dodecane at 363 K is injected through a 0.09 mm diameter injector nozzle into a gaseous mixture at 900 K and 6 MPa. In the actual injector, uncertainties are caused by anomalies in the shape and symmetry of the nozzle, the nozzle angle, the machined transition between the sac and nozzle, wall surface roughness, and the injector mechanical behavior such as needle oscillation and deformation. The present simulation is performed with a simplified injector geometry, well-defined boundary conditions and models for turbulence, thermodynamics, and chemistry. This framework is combined with a real-fluid model framework and an optimized chemical mechanism for n-dodecane oxidation that efficiently captures hot flame ignition in the presence of cool-flame chemistry [15].

In the following, we first describe the LES solver and the closure models used. A brief description of the chemical scheme is also provided. A presentation of the benchmark experimental configuration then follows with details on the numerical setup and simplification assumptions. Finally, the LES results are compared to experimental data and additional data is extracted.

APPROACH

The analysis is performed using a single unified code framework called RAPTOR. Unlike conventional LES codes, RAPTOR is a Direct Numerical Simulation (DNS) solver that has been optimized to meet the strict algorithmic requirements imposed by the LES formalism. The theoretical framework solves the fully-coupled conservation equations of mass, momentum, total-energy, and species for a chemically reacting flow. It is designed to handle high Reynolds number, high-pressure, real-gas and/or liquid conditions over a wide Mach operating range. It also accounts for detailed thermodynamics and transport processes at the molecular level. A noteworthy aspect of RAPTOR is it was designed specifically for LES using non-dissipative, discretely conservative, staggered, finite-volume differencing. This eliminates numerical contamination of the sub-filter models due to artificial dissipation and provides discrete conservation of mass, momentum, energy, and species, which is an imperative requirement for high quality LES. Details related to the baseline formulation and sub-filter models are given by Oefelein [16]. Representative case studies are given by Oefelein et al. [17, 18, 19, 20, 21, 22, 23, 24, 25].

Governing Conservation Equations

For LES applications, the filtered version of Navier-Stokes equations are solved. These equations are given as:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}}) = 0, \quad (1)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{\mathbf{u}}) + \nabla \cdot \left[(\bar{\rho} \bar{\mathbf{u}} \otimes \bar{\mathbf{u}} + \frac{\bar{\rho}}{M^2} \mathbf{I}) \right] = \nabla \cdot \vec{\tau}, \quad (2)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{e}_t) + \nabla \cdot [(\bar{\rho} \bar{e}_t + \mathcal{P}) \bar{\mathbf{u}}] = \nabla \cdot \left[\left(\vec{Q}_e + M^2 (\vec{\tau} \cdot \bar{\mathbf{u}}) \right) \right] + \bar{Q}_e, \quad (3)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_i) + \nabla \cdot (\bar{\rho} \bar{Y}_i \bar{\mathbf{u}}) = \nabla \cdot \vec{S}_i + \bar{\omega}_i. \quad (4)$$

In these equations,

$$e_t = e + \frac{M^2}{2} \mathbf{u} \cdot \mathbf{u}$$

$$e = \sum_{i=1}^N h_i Y_i - \frac{p}{\rho}$$

$$h_i = h_{f,i} + \int_{T_f}^T \int_{p_f}^p C_{p,i}(T,p) dT dp$$

represent the total internal energy, internal energy and enthalpy of the i^{th} species, respectively, and $\mathbf{q}_e$ represents the energy diffusion flux.

The terms $\mathcal{P}$, $\vec{\mathcal{T}}$, $\vec{Q}_e$ and $\vec{S}_i$ represent respective composite (i.e., molecular plus sub-filter) stresses and fluxes. Quantities $\vec{Q}_e$ and $\vec{\omega}_i$ represent the filtered energy and chemical source terms, respectively.

The viscous stress tensor is assumed to follow Stokes' hypothesis, and the heat release due to chemical reaction is accounted for in the description of the specific enthalpies, h_i , as given by the enthalpy of formation, $h_{f,i}^\circ$. The heat release rate can be represented equivalently as the product of the enthalpy of formation and the local rate of production of all the species considered in the system. Using this representation, the source term and specific enthalpies are defined as

$$\vec{Q}_e = - \sum_{i=1}^N \dot{\omega}_i h_{f,i}^\circ, \text{ and} \quad (5)$$

$$h_i = \int_{p^\circ}^p \int_{T^\circ}^T C_{p,i}(T, p) dT dp. \quad (6)$$

Sub-Filter Closures

The sub-filter closure is obtained using the “mixed” dynamic Smagorinsky model by combining the models proposed by Erlebacher, Hussaini, Speziale and Zang [26], and Speziale [27] with the dynamic modeling procedure [28, 29, 30, 31, 32]. The composite stresses and fluxes in Eqs. (1), (2), (3), (4) are then given as

$$\begin{aligned} \vec{\mathcal{T}} = & (\mu_t + \mu) \frac{1}{Re} \left[-\frac{2}{3} (\nabla \cdot \tilde{\mathbf{u}}) \mathbf{I} + (\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T) \right] \\ & - \bar{\rho} (\tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}} - \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}), \end{aligned} \quad (7)$$

$$\begin{aligned} \vec{Q}_e = & \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr} \right) \frac{1}{Re} \nabla \tilde{h} + \sum_{i=1}^N \tilde{h}_i \vec{S}_i \\ & - \bar{\rho} (\tilde{h} \tilde{\mathbf{u}} - \tilde{h} \tilde{\mathbf{u}}), \text{ and} \end{aligned} \quad (8)$$

$$\vec{S}_i = \left(\frac{\mu_t}{Sc_{t,i}} + \frac{\mu}{Sc_i} \right) \frac{1}{Re} \nabla \tilde{Y}_i - \bar{\rho} (\tilde{Y}_i \tilde{\mathbf{u}} - \tilde{Y}_i \tilde{\mathbf{u}}). \quad (9)$$

The term μ_t represents the sub-filter eddy viscosity, given by

$$\mu_t = \bar{\rho} C_R \Delta^2 \Pi_\S^{\frac{1}{2}}, \quad (10)$$

where

$$\Pi_\S = \tilde{\mathbf{S}} : \tilde{\mathbf{S}}, \text{ and } \tilde{\mathbf{S}} = \frac{1}{2} (\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T). \quad (11)$$

The terms C_R , Pr_t , and $Sc_{t,i}$ represent the Smagorinsky, sub-filter Prandtl and sub-filter Schmidt numbers and are evaluated dynamically as functions of space and time. The overall model includes the Leonard and cross-term stresses and provides a Favre averaged generalization of the Smagorinsky eddy viscosity model [33] coupled with gradient diffusion models to account for sub-filter mass and energy transport processes.

The Dynamic Thickened Flame model [34] is used to close the filtered chemical source term. This approach has been successfully used in LES of piston engines and spray ignitions [35, 36] and an adapted version for autoignition in piston engines was recently described in [37].

Real-Fluid Thermodynamics and Transport

In recent work [8, 9, 10, 13], we have demonstrated that when operating pressures exceed the critical pressure of the injected fuel, interfacial diffusion layers can develop due to thickening of the gas-liquid interfaces combined with a significant reduction in the mean free molecular path and surface tension forces. These interfaces eventually enter the continuum length scale regime and disappear as interfacial fluid temperatures rise above the critical temperature of the local mixture. The lack of inter-molecular forces, coupled with broadening interfaces, promote diffusion dominated mixing processes prior to atomization. As a consequence, injected jets evolve in the presence of exceedingly large but continuous thermo-physical gradients in a manner markedly different from classical assumptions. Figure 2 illustrates the effects of the two extremes described in [8, 9] on the injected fuel. This figure shows results for n-dodecane injected at a temperature of 363 K into gaseous nitrogen at varying ambient pressures and temperatures relevant to Diesel engine operation.

From these conclusions, the property evaluation scheme is designed to account for real-fluid thermodynamic non-idealities and transport anomalies over a wide range of pressures and temperatures. The extended corresponding states model [38, 39] is employed with a cubic equation of state. Here the Peng-Robinson equation of state was used since it is more accurate for the prediction of n-dodecane density at reduced temperatures less than one. A summary of the cubic equations of state and recommended constants is given by Reid et al. [40, Chapter 3].

Having selected an analytical representation for real mixture pressure-volume-temperature (PVT) behavior, the thermodynamic properties are obtained in two steps. First, respective component properties are combined at a fixed temperature using the extended corresponding states methodology to obtain the mixture state at a given reference pressure. A pressure correction is then applied using departure functions of the form given by Reid et al. [40, Chapter 5]. These functions are exact relations derived using the Maxwell relations (see VanWylen and Sonntag [41, Chapter 10], for example) and make full use of the real mixture PVT path dependencies dictated by the equation of state. Standard state properties are obtained using

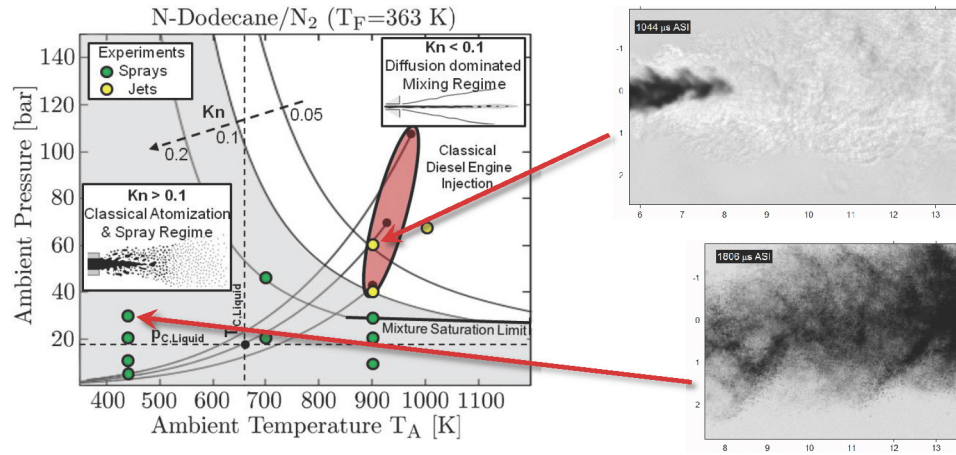


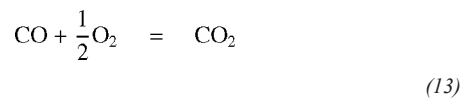
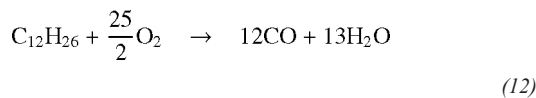
Figure 2. The regime diagram (left) describes conditions where n-dodecane injected at a temperature of 363 K into nitrogen transitions to a dense supercritical jet without drop formation [8, 9]. Corresponding high-speed imaging of a dense supercritical jet (top right) and spray (bottom right) illustrates the significant change in the thermo-physical characteristics of the injected jet as function of different ambient pressures and temperatures [10].

the databases developed by Gordon and McBride [42] and Kee et al. [43]. Chemical potentials and fugacity coefficients are obtained in a manner similar to that outlined above. Molecular transport properties are evaluated in a manner analogous to the thermodynamic properties. Viscosity and thermal conductivity are obtained using the extended corresponding states methodologies developed by Ely and Hanley [44, 45]. The mass diffusion coefficients and thermal diffusion coefficients are obtained using the methodologies outlined by Bird et al. [46] and Hirschfelder et al. [47] in conjunction with the corresponding states methodology proposed by Takahashi [48].

Chemistry Model

In this study, we use a 2-step mechanism calibrated using Bayesian inference to accurately predict autoignition in the ranges of conditions (pressure, temperature, equivalence ratio) relevant to the Spray-A case. Using Bayesian inference to calibrate the model is shown to provide not only the optimal parameter values but also their probability density functions (pdfs). These pdfs can then be propagated through the LES to quantify the resulting uncertainty on the autoignition delay time. The details of the calibration can be found in [15]. Here we give a short description of the methodology.

The present mechanism accounts for the incomplete oxidation of the n-dodecane using the following rate equations



The main idea is to allow the Arrhenius pre-exponential factor A of the first reaction to vary with the local fresh gas conditions according to the relation

$$\ln A = \lambda_0 + \lambda_1 e^{\lambda_2 \phi} + \lambda_3 \tanh((\lambda_4 + \lambda_5 \phi)T_0 + \lambda_6). \quad (14)$$

The parameters $\alpha = (E_a, \lambda_0, \dots, \lambda_6)$ are calibrated using to match the autoignition delay time given by a skeletal mechanism [3] in homogeneous reactors for temperatures, T_0 , ranging from 600K to 1200K and equivalence ratios, ϕ , between 0.5 and 4. These ranges of interest were extracted from a previous non-reacting simulation of Spray-A case [12] that characterized the mixture in the flammable region just prior to ignition. We invoke Bayes' rule to provide the posterior probability density function (pdf) of α

$$p(\alpha | \ln \tau^d) \propto p(\ln \tau^d | \alpha) p(\alpha) \quad (15)$$

Table 1. Parameters of the function given in Eq. 14.

λ_0	27.38
λ_1	-2.13
λ_2	-2.05
λ_3	1.89
λ_4	$-1.00 \cdot 10^{-2}$
λ_5	$2.87 \cdot 10^{-4}$
λ_6	8.43
E_a	31944 cal/mol

where $p(a|b)$ is the pdf of a conditioned on b , $\tau^d = (\tau_i^d)_{(1 \leq i \leq N)}$ is the vector of auto-ignition delay times given by the reference mechanism at the N data points. Assuming an unbiased additive Gaussian error model on $\ln \tau$ with standard deviation σ , the likelihood can be expressed as follows

$$p(\ln \tau^d | \alpha, \sigma) = \frac{1}{(2\pi\sigma^2)^{\frac{N}{2}}} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^N (\ln \tau_i^d - \ln \tau_i^m)^2} \quad (16)$$