

Effects of Real-Fluid Thermodynamics on High-Pressure Fuel Injection Processes

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ABSTRACT

This paper first summarizes a new theoretical description that quantifies the effects of real-fluid thermodynamics on liquid fuel injection processes as a function of pressure at typical engine operating conditions. It then focuses on the implications this has on modeling such flows with emphasis on application of the Large Eddy Simulation (LES) technique. The theory explains and quantifies the major differences that occur in the jet dynamics compared to that described by classical spray theory in a manner consistent with experimental observations. In particular, the classical view of spray atomization as an appropriate model at some engine operating conditions is questionable. Instead, non-ideal real-fluid behavior must be taken into account using a multicomponent formulation that applies to hydrocarbon mixtures at high-pressure supercritical conditions. To highlight the implications and needs related to modeling, we present a series of studies using LES that focus on experiments being conducted in the high-pressure combustion vessel at Sandia National Laboratories. We extend LES studies performed previously to the Engine Combustion Network (www.sandia.gov/ECN) Spray-H and Spray-A injectors using n-heptane and n-dodecane as the respective fuels. The accompanying analysis reveals the structural characteristics associated with the inherent scalar mixing processes at conditions directly relevant to advanced Diesel engines.

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INTRODUCTION

Multiphase combustion processes are prevalent in a wide variety of advanced combustion systems; e.g., internal combustion engines and gas turbines for propulsion and power. Treating these processes involves a variety of challenges that 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 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. Operation at elevated pressures 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.

Research over the past decade has provided significant insights into the structure and dynamics of multiphase flows at high pressures [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. There are two extremes that must be considered in modern devices. At subcritical, or certain supercritical operating pressures, the classical situation exists where a well-defined molecular interface separates the injected liquid from ambient gases due to the presence of surface tension. Interactions between dynamic shear forces and surface tension promote primary atomization and secondary breakup processes that evolve from a dense state, where the liquid exists as sheets filaments or lattices intermixed with sparse pockets of gas; to a dilute state, where drop-drop interactions are negligible and dilute spray theory can be used. When operating pressures exceed the critical pressure of the injected liquid, however, the situation can become quite different. Under these conditions, interfacial

diffusion layers can develop as a consequence of vanishing surface tension forces, broadening gas-liquid interfaces, and reduced mean free molecular path. These interfaces eventually enter the continuum length scale regime and disappear as interfacial fluid temperatures rise above the critical temperature of the local mixture. 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.

Recent research has shown that the transitional change described above is controlled by the multicomponent nature of the liquid-gas interface [13, 14]. Detailed analysis of the interfacial structure shows how it disintegrates as a function of pressure, temperature, and the local multicomponent mixture properties. A key output are regime diagrams for liquid injection such as the example shown in Fig. 1. 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. The classical spray regime (highlighted in white) and diffusion-dominated mixing regime (gray) are found using the Knudsen number (i.e., molecular-mean-free-path divided by the interfacial-thickness) criterion explained in Reference [14]. To illustrate the relevance of this diagram, ambient gas pressure-temperature lines, which span a range of conditions during different Diesel engine compression cycles, are shown for three representative initial conditions; a) turbo-charged (2.5 bar, 363 K), b) medium-load (1.6 bar, 343 K), and c) light-load (1 bar, 335 K) operation. Fuel injection occurs at full compression conditions, as indicated by the three respective points in the diagram. Interestingly, the

cylinder pressures at full compression exceed the supercritical mixture pressure for all of the cases considered. Only at light-load operation does there appear to be a chance that classical fuel spray atomization takes place. Thus, contrary to conventional wisdom, the theory indicates that classical spray phenomena does not occur at the particular set of Diesel injection conditions considered here. Instead, the injected fuel jet exhibits diminished interfacial structure and surface tension, which leads to diffusion-dominated mixing. Predictions have been corroborated using microscopic imaging to visualize the features of dense-fluid jets (top right image in Fig. 1) and classical spray atomization (bottom right image).

Applying the analysis to a variety of system specific operating conditions suggests that almost all modern high-performance combustion devices operate over ranges of pressures and temperatures in the vicinity of, or across, the transitional regime. Figure 2 shows the typical operating envelopes associated with advanced Diesel, gas turbine, and gasoline direct-injection systems using n-dodecane, n-decane, and iso-octane as respective fuel surrogates. The diagram is constructed for liquid injection temperatures from 300 to 363 K in a general manner by normalizing the ambient gas pressure and temperature by the corresponding critical properties of the liquid phase. The Classical Spray Regime is highlighted in green, the Supercritical Fluid Regime is highlighted in blue, and the Transitional Regime is highlighted in red. Respective operating envelopes are then indicated by the oval white areas. In each case the operational envelope crosses into the transitional regime, which exemplifies the need to understand both classical spray and supercritical fluid phenomena simultaneously over relevant ranges of conditions.

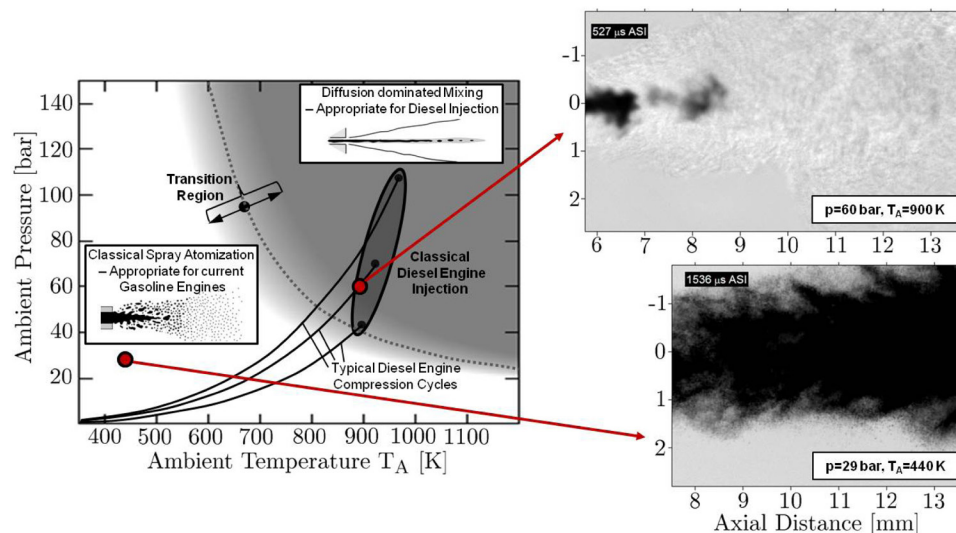


Figure 1. The regime diagram (left) describes conditions where n-dodecane injected at a temperature of 363 K into nitrogen transitions to a dense supercritical jet without drop formation. Corresponding high-speed imaging of a dense supercritical jet (top right) and spray (bottom right) illustrates the significant change induced as a function of different ambient pressures and temperatures [13, 14] (Images on right courtesy of L. M. Pickett, Sandia National Laboratories).

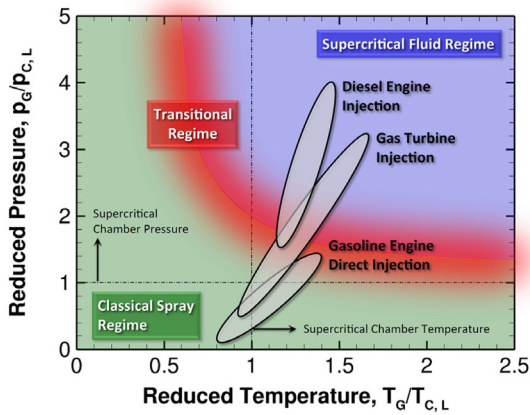


Figure 2. Typical operating envelopes associated with advanced Diesel, gas turbine, and gasoline direct-injection systems using n-dodecane, n-decane, and iso-octane as respective fuel surrogates. The diagram is constructed for liquid injection temperatures from 300 to 363 K. The ambient gas pressure and temperature are normalized by the corresponding critical properties of respective liquid phases.

APPROACH

To enhance our understanding of the processes described above in the context of Diesel engines, we have combined the new theoretical findings and high-fidelity Large Eddy Simulation (LES) to gain a more detailed view into direct-injection processes at high-pressures. We use the experimental data provided by Pickett *et al.* as part of the Engine Combustion Network cases (i.e., the ECN workshop, see www.ca.sandia.gov/ECN [15]) as key targets. The analysis is performed using a single unified code framework called RAPTOR. Unlike conventional LES codes, RAPTOR is a 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, and is sophisticated in its ability to handle a generalized model framework in both the Eulerian and Lagrangian frames. 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 subgrid-scale 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 subgrid-scale models are given by Oefelein [16]. Representative case studies are given by Oefelein *et al.* [6, 17, 18, 19, 20, 21, 22, 23, 24].

The baseline system of equations are cast in dimensionless form using a reference length-scale δ_{ref} , flow speed U_{ref} , and fluid state characterized by a reference density ρ_{ref} , sound speed c_{ref} , constant pressure specific heat C_{pref} , and dynamic viscosity μ_{ref} . Using these quantities, a reference Mach and Reynolds number are defined as $M = U_{ref}/c_{ref}$ and $Re = \rho_{ref}U_{ref}\delta_{ref}/\mu_{ref}$. With these definitions, the instantaneous conservation equations of mass, momentum, total-energy and chemical species can be written in conservative form as follows:

- Mass:

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

- Momentum:

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

where

$$\tau = \frac{\mu}{Re} \left[-\frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I} + (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right]$$

represents the viscous stress tensor.

- Total Energy:

$$\frac{\partial}{\partial t}(\rho e_t) + \nabla \cdot [(\rho e_t + p)\mathbf{u}] = \nabla \cdot [\mathbf{q}_e + M^2(\tau \cdot \mathbf{u})], \quad (3)$$

where

$$\begin{aligned} e_t &= e + \frac{M^2}{2} \mathbf{u} \cdot \mathbf{u} \\ e &= \sum_{i=1}^N h_i Y_i - \frac{p}{\rho} \\ h_i &= h_{f,i}^\circ + \int_{p^\circ}^p \int_{T^\circ}^T C_{p,i}(T, p) dT dp \end{aligned}$$

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

- Species:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{u}) = \nabla \cdot \mathbf{q}_i + \dot{\omega}_i \quad i = 1, \dots, N-1, \quad (4)$$

where $\mathbf{q}_i$ and $\dot{\omega}_i$ represent the mass diffusion fluxes and the rate of production of the i^{th} species, respectively.

Equations (1), (2), (3), (4), coupled with 1) an appropriate equation of state, 2) appropriate treatments of thermodynamic and transport properties, and 3) validated mixing and combining rules for the mixtures of interest accommodate the most general system of interest including cases when multicomponent and/or preferential diffusion processes are present. The viscous stress tensor is assumed to follow Stokes hypothesis, and the heat release due to chemical reaction in

Eq. (3) is accounted for in the description of the specific enthalpies, h_p , as given by the enthalpy of formation, $h_{f,i}^\circ$. The heat release rate can be represented equivalently, as a source term on the right hand side of Eq. (3), 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

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

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

For LES applications, the filtered version of Eqs. (1), (2), (3), (4) are solved. These equations are given respectively as:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}}) = 0, \quad (7)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{\mathbf{u}}) + \nabla \cdot \left[\left(\bar{\rho} \bar{\mathbf{u}} \otimes \bar{\mathbf{u}} + \frac{\mathcal{P}}{M^2} \mathbf{I} \right) \right] = \nabla \cdot \vec{\mathcal{T}}, \quad (8)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{e}_t) + \nabla \cdot [(\bar{\rho} \bar{e}_t + \mathcal{P}) \bar{\mathbf{u}}] = \nabla \cdot \left[\left(\bar{\mathcal{Q}}_e + M^2 (\vec{\mathcal{T}} \cdot \bar{\mathbf{u}}) \right) \right] + \bar{\mathcal{Q}}_e, \quad (9)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_i) + \nabla \cdot (\bar{\rho} \bar{Y}_i \bar{\mathbf{u}}) = \nabla \cdot \vec{\mathcal{S}}_i + \bar{\omega}_i. \quad (10)$$

The terms $\mathcal{P}$, $\vec{\mathcal{T}}$, $\vec{\mathcal{Q}}_e$ and $\vec{\mathcal{S}}_i$ represent respective composite (i.e., molecular plus subgrid-scale) stresses and fluxes.

Quantities $\bar{\mathcal{Q}}_e$ and $\bar{\omega}_i$ represent the filtered energy and species source terms, respectively.

The subgrid-scale closure is obtained using the “mixed” dynamic Smagorinsky model by combining the models proposed by Erlebacher, Hussaini, Speziale and Zang [25], and Speziale [26] with the dynamic modeling procedure [27, 28, 29, 30, 31]. The composite stresses and fluxes in Eqs. (7), (8), (9), (10) are then given as

$$\vec{\mathcal{T}} = (\mu_t + \mu) \frac{1}{Re} \left[-\frac{2}{3} (\nabla \cdot \bar{\mathbf{u}}) \mathbf{I} + (\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T) \right] - \bar{\rho} (\bar{\mathbf{u}} \otimes \bar{\mathbf{u}} - \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}), \quad (11)$$

$$\vec{\mathcal{Q}}_e = \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr} \right) \frac{1}{Re} \nabla \bar{h} + \sum_{i=1}^N \tilde{h}_i \vec{\mathcal{S}}_i - \bar{\rho} (\bar{\mathbf{u}} \tilde{h} - \tilde{\mathbf{u}} \bar{h}), \text{ and} \quad (12)$$

$$\vec{\mathcal{S}}_i = \left(\frac{\mu_t}{Sc_{t,i}} + \frac{\mu}{Sc_i} \right) \frac{1}{Re} \nabla \bar{Y}_i - \bar{\rho} (\bar{\mathbf{u}} \tilde{Y}_i - \tilde{\mathbf{u}} \bar{Y}_i). \quad (13)$$

The term μ_t represents the subgrid-scale eddy viscosity, given by

$$\mu_t = \bar{\rho} C_R \Delta^2 \Pi_s^{\frac{1}{2}}, \quad (14)$$

where

$$\Pi_s = \tilde{\mathbf{S}} : \tilde{\mathbf{S}}, \text{ and } \tilde{\mathbf{S}} = \frac{1}{2} (\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T). \quad (15)$$

The terms C_R , Pr_t and $Sc_{t,i}$ represent the Smagorinsky, subgrid-scale Prandtl and subgrid-scale 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 [32] coupled with gradient diffusion models to account for subgrid-scale mass and energy transport processes.

The property evaluation scheme is designed to account for thermodynamic non-idealities and transport anomalies over a wide range of pressures and temperatures. The scheme is comprehensive and intricate, thus only a skeletal description can be given here. The extended corresponding states model [33, 34] is employed with a cubic equation of state. In past studies, both the Benedict-Webb-Rubin (BWR) equation of state and cubic equations of state have been used to evaluate the pressure-volume-temperature (PVT) behavior of the inherent dense multicomponent mixtures. Use of modified BWR equations of state in conjunction with the extended corresponding states principle has been shown to provide consistently accurate results over the widest range of pressures, temperatures, and mixture states, especially at near-critical conditions. A major disadvantage of BWR equations, however, is that they are not computationally efficient. Cubic equations of state can be less accurate, especially for mixtures at near-critical or saturated conditions, but are computationally efficient. Experience has shown that both the Soave-Redlich-Kwong (SRK) and Peng-Robinson (PR) equations, when used in conjunction with the corresponding states principle, can give accurate results over the range of pressures, temperatures, and mixture states of