

Detailed Modeling and Simulation of High-Pressure Fuel Injection Processes in Diesel Engines

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ABSTRACT

This paper provides an analysis of high-pressure phenomena and its potential effects on the fundamental physics of fuel injection in Diesel engines. In particular, we focus on conditions when cylinder pressures exceed the thermodynamic critical pressure of the injected fuel and describe the major differences that occur in the jet dynamics compared to that described by classical spray theory. To facilitate the analysis, we present a detailed model framework based on the Large Eddy Simulation (LES) technique that is designed to account for key high-pressure phenomena. This framework is then used to perform a thermodynamic analysis of the flow. We focus on the experiments being conducted in the high-pressure combustion vessel at Sandia National Laboratories using n-heptane as a reference fuel. The calculations are performed by rigorously treating the experimental geometry and operating conditions, with detailed treatment of relevant thermophysical mixture properties. Results demonstrate that n-heptane enters the chamber as a compressed liquid, not a spray, and is heated at supercritical pressure. Further analysis suggests the classical view of spray atomization as an appropriate model at these particular conditions is questionable. Instead, nonideal real-fluid behavior must be taken into account using a multicomponent formulation that applies to arbitrary hydrocarbon mixtures at high-pressure supercritical conditions.

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INTRODUCTION

Turbulent multiphase combustion processes are prevalent in a wide variety of propulsion and power systems including internal-combustion (IC) engines, gas-turbines, and liquid-rockets. As such, development of predictive models that reliably treat these processes is recognized as an important priority in research and there are a variety of challenges. Turbulent flows involving heterogeneous chemically reacting and/or multiphase mixtures (as is the case for all propulsion and power devices) have a variety of complicating factors including highly nonlinear chemical kinetics, small-scale velocity and scalar-mixing, turbulence-chemistry interactions, compressibility effects (volumetric changes induced by changes in pressure), and variable inertia effects (volumetric changes induced by variable composition or heat addition). 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 multiple 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 highly confined geometries that generate extremely 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 turbulence dynamics are dominated by geometry and various operating transients. In many cases operating pressures approach or exceed the thermodynamic critical pressure of the fuel or oxidizer. Operation at elevated pressures significantly increases system Reynolds numbers and inherently broadens the range of spatial and temporal scales over which interactions occur. It also has been shown to have a dramatic effect on the structure and dynamics associated with liquid jet breakup.

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]. Most of this research has been done in the context of liquid-rocket propulsion, which involves direct injection of both liquid fuel and oxidizer into the combustion chamber. However, the observed trends are equally valid for other liquid fueled devices. Here we focus on Diesel engines. Figure 1 illustrates the two distinctly different sets of processes liquid jets exhibit as a function of pressure. At subcritical cylinder pressures,

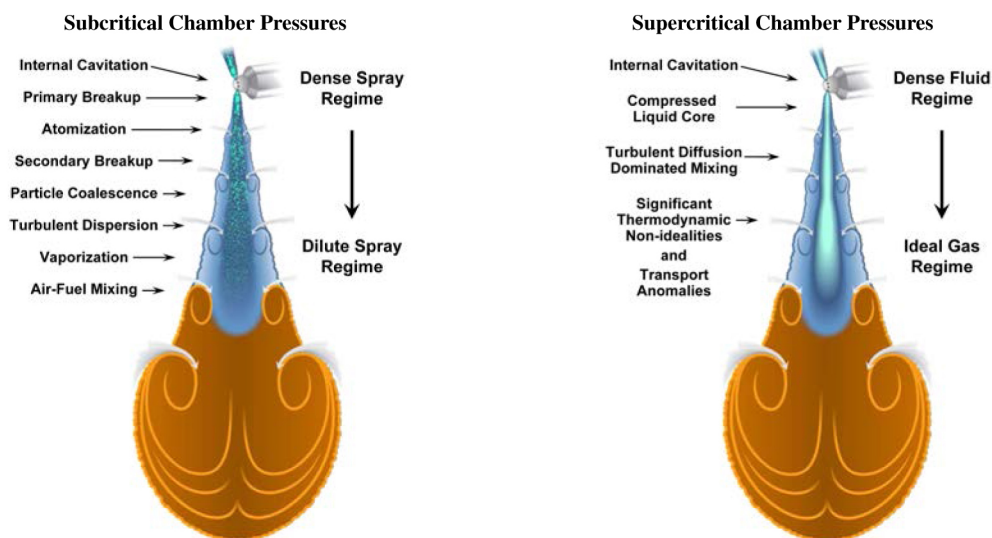


Figure 1. Schematic diagram illustrating the two distinctly different sets of processes liquid jets exhibit as a function of pressure.

the classical situation exists where a well defined interface separates the injected liquid from ambient gases due to the presence of surface tension. Dynamic shear forces and surface tension promote primary atomization and secondary breakup processes that evolve from a very dense state, where the liquid exists as sheets filaments or lattices intermixed with sparse pockets of gas; to a very dilute state, where drop-drop interactions are negligible and the theory associated with isolated drops can be used. As chamber pressures exceed the critical pressure of the fuel, however, the situation becomes quite different. Under these conditions, a distinct gas-liquid interface does not exist. Instead, injected liquid jets undergo a transcritical change of state as interfacial fluid temperatures rise above the critical temperature of the local mixture. Effects of surface tension become diminished, and the lack of these inter-molecular forces promote diffusion dominated mixing processes prior to atomization. The injected jets evolve in the presence of exceedingly large (but continuous) thermophysical gradients in a manner that is markedly different from the classical picture typically assumed.

Modeling either of the two extremes described above poses a variety of challenges. While issues related to the treatment of classical spray phenomena are well known, those related to the treatment of transcritical injection dynamics are not as well understood. Thus, this paper focuses on the latter. To enhance our understanding of these processes in the context of Diesel engines, we have performed a series of high-fidelity calculations using the Large Eddy Simulation (LES) technique. The LES calculations are performed using a single unified theoretical-numerical framework developed by Oefelein [13]. The theoretical framework solves the fully coupled conservation equations of mass, momentum, total-energy and species for a chemically reacting multiphase 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 real-fluid (gas/liquid) thermodynamics and transport processes at the molecular level, and is sophisticated in its ability to handle a generalized subgrid-scale (SGS) model framework. Using this framework, we have performed detailed validation and analysis using the experimental data provided by Pickett *et al.* as part of the Engine Combustion Network (see www.ca.sandia.gov/ECN [14]). Namely, the “Baseline n-Heptane” case. This experiment is designed to emulate conditions typically observed in a Diesel engine with injection conditions of approximately 900 K and 60 bar. Significant attention is focused on corroborating measured and modeled results as a function of distinctly different phenomenological processes that occur as a function of pressure. This is accomplished by rigorously treating the experimental geometry (injector and vessel) and operating conditions.

APPROACH

The analysis is performed using a single unified code framework called RAPTOR [13]. Unlike conventional solvers, RAPTOR is a Direct Numerical Simulation (DNS) solver that has been optimized to meet the strict algorithmic requirements imposed by the LES formalism. The numerical formulation treats the compressible form of the conservation equations, but can be evaluated efficiently in the incompressible limit. A noteworthy aspect of RAPTOR is that it is designed specifically for LES using non-dissipative, discretely-conservative, staggered, finite-volume differencing stencils. This eliminates numerical contamination of the SGS models due to artificial dissipation and provides discrete conservation of mass, momentum, energy and species, which is an imperative requirement for LES.

For LES applications the instantaneous conservation equations are filtered yielding:



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• Mass:

$$\frac{\partial}{\partial t}(\theta \bar{\rho}) + \nabla \cdot (\theta \bar{\rho} \tilde{\mathbf{u}}) = \bar{\dot{\rho}}_s. \quad (1)$$

• Momentum:

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

• Total Energy:

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

• Species:

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

The terms θ , $\bar{\rho}_s$, $\bar{\mathbf{F}}_s$, $\bar{\vec{Q}}_s$ and $\bar{\vec{\omega}}_{s_i}$ represent the filtered void fraction and spray source terms which account for exchange of mass, momentum, total energy and species, respectively. The terms $\mathcal{P}$, $\bar{\vec{T}}$, $\bar{\vec{Q}}_e$ and $\bar{\vec{S}}_i$ represent respective composite (i.e., molecular plus SGS) stresses and fluxes. The terms $\bar{\vec{Q}}_e$ and $\bar{\vec{\omega}}_i$ represent the filtered energy and chemical source terms.

The baseline SGS closure is obtained using the “mixed” dynamic Smagorinsky model by combining the models proposed by Erlebacher, Hussaini, Speziale and Zang [15] and Speziale [16] with the dynamic modeling procedure [17, 18, 19, 20, 21]. The composite stresses and fluxes in Eqs. (1), (2), (3), (4) are given as

$$\bar{\vec{T}} = (\mu_t + \mu) \frac{1}{Re} \left[-\frac{2}{3} (\nabla \cdot \tilde{\mathbf{u}}) \mathbf{I} + (\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T) \right] - \bar{\rho} (\tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}} - \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}), \quad (5)$$

$$\bar{\vec{Q}}_e = \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr} \right) \frac{1}{Re} \nabla \tilde{h} + \sum_{i=1}^N \tilde{h}_i \bar{\vec{S}}_i - \bar{\rho} (\tilde{h} \tilde{\mathbf{u}} - \tilde{\tilde{h}} \tilde{\mathbf{u}}), \text{ and} \quad (6)$$

$$\bar{\vec{S}}_i = \left(\frac{\mu_t}{Sc_{t_i}} + \frac{\mu}{Sc_i} \right) \frac{1}{Re} \nabla \tilde{Y}_i - \bar{\rho} (\tilde{Y}_i \tilde{\mathbf{u}} - \tilde{\tilde{Y}}_i \tilde{\mathbf{u}}). \quad (7)$$

Here, the term μ_t represents the SGS eddy viscosity given by the relation

$$\mu_t = \bar{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}}, \quad (8)$$

where

$$\Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}}, \text{ and } \tilde{\mathbf{S}} = \frac{1}{2} (\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T). \quad (9)$$

The terms C_R , Pr_t , and Sc_{t_i} represent the Smagorinsky, SGS-Prandtl and SGS-Schmidt numbers and are evaluated dynamically as functions of space and time. Thus, there are no tuned constants employed anywhere in the closure. The overall model includes the Leonard and cross-term stresses and provides a Favre averaged generalization of the Smagorinsky eddy viscosity model [22] coupled with gradient diffusion models to account for SGS mass and energy transport processes.

The property evaluation scheme is designed to account for thermodynamic nonidealities 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 (see [23] for details). The extended corresponding states model [24, 25] is employed with a cubic equation of state. In past studies [6, 26] modified versions of 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 dense multicomponent multiphase 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 computationally expensive.

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 a wide range of pressures, temperatures and mixture states of typical interest in a variety of devices. SRK coefficients are fit to vapor pressure data and are thus more suitable for conditions when the reduced temperature is less than one. PR coefficients, on the other hand, are more suitable for conditions when the reduced temperature is greater than one. A summary of the cubic equations of state and recommended constants is given by Reid *et al.* [27, Chapter 3].

Having established an analytical representation for real mixture 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 outlined above 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.* [27, Chapter 5]. These functions are exact relations derived using the Maxwell relations (see VanWylen and Sonntag [28, Chapter 10] for example) and