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Simulation of supercritical fuel injection with condensation

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ABSTRACT

Supercritical injection and the accompanying potential condensation processes were numerically investigated with a consistent treatment for both the fluid dynamics and thermodynamics with a realistic equation of state model. Qualitative and quantitative improvement was seen on the predicted injectant density with real gas simulations when compared to available experimental data, emphasizing the importance of thermodynamic property non-ideality at supercritical conditions. Recently developed phase stability and equilibrium solvers utilizing fundamental thermodynamics principles were also applied to capture phase transitions. To our knowledge, this is the first comprehensive simulation against experimental data of supercritical injection with phase separation. Furthermore, the simulation results were found to agree with the experimental results in three aspects related to the phase change. The first observation is that condensation is predicted to occur if and only if the temperature difference between the injectant and ambient is large enough to promote strong heat transfer interactions. The simulations also show that condensation becomes intensified when the chamber temperature is further reduced. Second, such condensation is only possible for supercritical-to-subcritical but not for supercritical-to-supercritical injections. Third, a condensed liquid phase is found to form at the jet boundary where the energy and mixing interactions between the “hot” injectant and the “cold” surrounding gas are strong. The intensive local heat exchange finally sends the mixture into the two-phase region by crossing the dew point line with condensation.

1. Introduction

Liquid fuel injection is a common process that occurs in a number of energy conversion devices, such as gas turbines, diesel engines and gasoline direct-injection (GDI) engines. Understanding the complex physical processes (e.g., liquid jet breakup, atomization, turbulent mixing, evaporation, etc.) is critical to better utilize the fossil fuels because the fuel–air mixing plays a critical role in the subsequent gas phase combustion processes. A number of classical physical breakup and atomization models have been widely accepted and used in spray simulations. For instance, the Kelvin–Helmholtz Rayleigh–Taylor breakup model [1–3], which identifies the fastest growing wave (with highest surface instability) on a droplet surface and considers it to be responsible for the subsequent breakup, has been widely used in state-of-the-art multidimensional diesel spray simulations [4–10]. Current diesel engines are generally equipped with high pressure injectors, and to enhance the fuel/air mixing processes, the injection pressure has been increased from around 1000 bar to as high as 2000–3000 bar in recent years. Under such high pressure conditions, the injected fuel is far above its thermodynamic critical pressure so it is in a highly compressed liquid state.

Recent large eddy simulation (LES) modeling shows that, under high injection pressure conditions, an *n*-heptane fuel jet may be approximated as a dense fluid, for which the traditional atomization and breakup processes do not exist [11]. Dahms and Oefelein [12] applied a linear gradient theory to quantify at what operating pressures the phase transition processes can be analyzed using classical two-phase atomization theories, or quite differently, based on diffusion-dominated mixing. Some potential benefits of injecting supercritical diesel fuels in engines have also been experimentally proved. Anitescu et al. [13] found that the jet spreading angle was enlarged and the observable jet core length was reduced, which is direct evidence that fuel/air mixing was significantly enhanced when dieseline (a mixture of diesel and gasoline) was injected in a supercritical state. It was also argued that such distinctive behavior could further reduce the fuel impingement and wall film formation in direct injection engines [13]. This is especially beneficial to advanced low temperature combustion (LTC) strategies for which early fuel injection is generally a prerequisite to improve the homogeneity of the fuel air mixture. For instance, in

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Nomenclature

a	energy parameter in Eq. (A1)
a_i	energy parameter for component i in Eq. (A5)
a_{ij}	energy parameter between component i and j in Eq. (A5)
b_i	volume parameter for component i in Eq. (A5)
b	volume parameter in Eq. (A1)
C_1	constant used in Eq. (B2)
C_2	constant used in Eq. (B2)
C_P	isobaric heat capacity
C_S	isentropic sound speed
C_V	isochoric heat capacity
f	fugacity
f_{obj}	the objective function in Eq. (4)
F	heat flux term
h	specific enthalpy
J	viscous stress tensor
k	turbulent kinetic energy
k_B	Boltzmann constant used in Eq. (B1)
K	heat conduction coefficient
m	molecular mass used in Eq. (B1)
Ma	the Mach number
n_i	mole number of component i
n_{ij}	mole number of component i in phase j
n	mole number
N_c	number of components
N_P	number of phases
P	pressure
Re	the Reynolds number
R_u	universal gas constant, 8.314 J/mol-K
S	entropy
T	temperature
u	specific internal energy
U	internal energy
v	specific molar volume
v^{liq}	molecular volume of the liquid phase
$\vec{V}$	velocity vector
x^{liq}	mole fraction of the liquid phase
x_i	mole fraction of component i
Z	compressibility factor

Greek letters

α	parameter in Eq. (A2)
$\mathcal{D}$	mass diffusion coefficient
ε	turbulent dissipation rate
γ	specific heat ratio
$\delta_{i,j}$	binary interaction parameter between component i and j
κ	parameter in Eq. (A3)
λ	vapor phase volume fraction
τ	characteristic time scale to reach equilibrium
μ	dynamic viscosity coefficient
ξ	constant used in Eq. (B1)
ρ	density
σ	surface tension
φ	fugacity coefficient
ω	acentric factor

Subscripts

c	critical property
L	liquid phase
V	vapor phase

Superscripts

0	ideal gas
d	departure value
liq	liquid phase
$spec$	specified value
s	saturation state of a pure species
T	transpose

Abbreviations

ASI	after start of injection
C_6F_{14}	perfluorohexane
$C_6F_{12}O$	fluoroketone
CO_2	carbon dioxide
CFD	computational fluid dynamics
DNS	direct numerical simulation
EOS	equation of state
GDI	gasoline direct-injection
H_2O	water
LES	large eddy simulation
LTC	low temperature combustion
MW	molar weight
N_2	nitrogen
PLIF	planar laser induced fluorescence
PR	Peng–Robinson
RANS	Reynolds-average Navier–Stokes
RCCI	reactivity controlled compression ignition
TKE	turbulent kinetic energy
UVn	isoenergetic–isochoric flash
VLE	vapor–liquid equilibrium

dual-fuel reactivity controlled compression ignition (RCCI) combustion, the first injection is as early as 67 crank angles before top dead center [14], which can introduce a significant amount of fuel impingement on the cylinder walls and in the piston-liner region.

Fluid behavior under supercritical conditions has been widely investigated and has been shown to be drastically different from that under subcritical conditions. Newman and Brzustowski [15] reported the first experimental work on supercritical carbon dioxide (CO_2) as the injectant and nitrogen (N_2) as the ambient, for which the pressure was above the critical pressure of CO_2. Experiments show that the higher the ambient gas density at high temperature, the finer the spray (e.g., reduced droplet size and number density), similar to the situation for subcritical environments. In the following, otherwise specified, supercritical or subcritical is used with reference to the critical properties of the injectant. In a supercritical temperature environment, liquid droplets can reach their critical temperature during the heating process, resulting in a significant reduction of surface tension.

Analysis at supercritical temperatures using turbulent submerged single-phase jet theory (e.g., velocity and temperature similarities) in Ref. [15] showed that the predicted jet flow behavior (e.g., variation of the axial mean velocity, location of jet boundaries) resembled jets at supercritical chamber temperatures. When the local evaporating rate was low due to high concentrations of the injectant, and when the injection velocity was high, the authors concluded that the “spray” could be characterized as “single-phase” turbulent gas jet. A thorough review is beyond the scope of the present paper, but can be found in a recent review article by Chehroudi [16], which includes many well-illustrating experimental images. The major conclusion regarding a single jet issuing into a quiescent chamber is that: when the chamber pressure exceeds the critical pressure of the injectant, classical liquid jet breakup and droplet formation are suppressed or not observed.