



## Condensation processes in a motoring engine



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### ABSTRACT

Condensation phenomena occurring in the combustion chamber of a motoring engine were investigated using a single-fluid approach by applying the Peng–Robinson equation of state to both the vapor and liquid phases. The phase transition process is modeled through thermodynamic equilibrium calculations that are based on an entropy maximization principle. The simulations show that condensation of pure nitrogen is not possible as it can only experience condensation through an expansion process. However, condensation is possible in the compression stroke for example cases of pure n-heptane and two selected binary mixtures. This is because the compression moves the fluid into the two-phase region, and when the fluid crosses the dew point line, condensation occurs with spontaneous heat release. The amount of liquid phase is found to increase as the compression continues. In the expansion stroke, the continuous relaxation leads to evaporation of the two-phase mixture, and hence the liquid phase is continuously depleted. For pure species, condensation is first observed in the bulk flow regions and then the extend of the two-phase mixture grows. After the whole charge is two-phase, the maximum liquid volume fraction and hence minimum entropy are found in the wall regions due to heat transfer effects. Similar observations were seen for mixtures. Finally, thermodynamic analysis of binary mixtures of pure n-alkane species with nitrogen shows that condensation was only possible in the diesel engine operation range if the fuel surrogate is n-dodecane or a heavier species.

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### 1. Introduction

Numerical simulations of complex flows and combustion in diesel and gasoline engines are helpful in the development of advanced engines with low pollutant emissions and high brake thermal efficiency. One critical challenge of the modeling is that both liquid and gas phases are present in the combustion chamber. Traditionally for direct-injection diesel engine simulations, the pressurized liquid fuel injection is modeled using the “blob” injection model [1], which models the injected liquid fuel as discrete droplets with Sauter mean diameter (SMD) equal to the effective nozzle hole diameter. Formulated in this way, the evolution of the two phases is calculated separately. To track the movement of the liquid fuel parcels, the Lagrangian method is used. For the ambient gas phase, it is tracked by solving the governing equations of fluid

mechanics in Eulerian coordinates. State of the art engine spray simulations adopt the above treatments for separate tracking of the two phases (e.g., the KIVA code [2]). The common difficulty, however, is that the coupling of the phases, such as the local heat, mass and momentum transfer at fluid interfaces, requires more modeling effort. For simplicity, many correlations that were developed for the isolated droplet are used, such as the Ranz–Marshall correlation. However, the important underlying assumption is that the fuel droplet must be sufficiently small to be considered as a point source in a computational cell, which is problematic in the near nozzle region.

Many research works on engine spray simulation have focused on improving the evaporation model. This is especially true because under high-pressure engine operating conditions, the ideal mixing model for low-pressure conditions, such as the widely used Raoult’s law and gas phase non-ideality, etc., are not suitable. One major research direction is to improve transcritical evaporation modeling under supercritical ambient conditions by considering real gas effects. Earliest work was performed by Manrique and Borman [3] who investigated steady state carbon dioxide droplet vaporization in nitrogen environment using the Redlick–Kwong (RK) equation of state (EOS) [4]. Later, Jin and Borman [5] studied the evaporation of a binary component fuel composed of pentane and octane under elevated conditions. For the vapor–liquid

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equilibrium, they used a fugacity coefficient for the gas phase and the activity coefficient model for the liquid phase. Hsieh et al. [6] did a comprehensive analysis on multicomponent droplets at near critical conditions using the Soave–Redlich–Kwong (SRK) EOS applied to both the liquid and gas phases to calculate the fugacity. A binary mixture of n-pentane/nitrogen and a ternary mixture of n-pentane/n-octane/nitrogen were studied, considering gas phase solubility and thermodynamic property non-ideality. Their simulations show that droplet can reach the critical state in its early lifetime. Curtis and Farrell [7] applied the Peng–Robinson (PR) EOS [8] to study the transient evaporation of R-113, n-heptane and n-dodecane droplets in a nitrogen environment. It was found that transient effects in both the liquid and vapor phases could have great impact on the droplet heat up and vaporization processes. Recently, Harstad and Bellan [9] studied the binary mixture of n-heptane and nitrogen. They found that, at subcritical conditions, an inner layer exists and the evaporation yields convection-diffusion characteristics. But in supercritical conditions, the absence of such a layer renders only the diffusion effects. Zhu and Aggarwal [10] studied transient droplet evaporation in supercritical conditions using different EOS models. The RK EOS was found to predict a higher evaporation rate compared to the SRK and Peng–Robinson PR EOS. In addition, it was found that the PR EOS showed excellent agreement in a wide range of ambient conditions with experiments of n-heptane and nitrogen mixtures. More detailed and comprehensive reviews about the behavior of droplet evaporation under supercritical ambient conditions can be found in Refs. [11–13].

Despite all these efforts, there is no documented research investigating possible condensation, the “opposite” process of evaporation, for the conditions inside the combustion chamber of engines. In fact, experiments have shown that condensation can occur at near supercritical conditions. For instance, Roy et al. [14] investigated the injection processes of supercritical fluoroketone ( $C_6F_{12}O$ ) into a subcritical nitrogen environment using planar laser induced fluorescence (PLIF). The experimental images show that liquid droplets were formed some distance downstream of the injector. This physical process requires modeling that is completely different from cases where the liquid fuel source is anchored at the injector location, since the phase transition must be tracked. On the other hand, because an engine cycle also involves an expansion process, it is intuitive to think that not only the fuel evaporation, but also physical condensation can occur. For instance, condensation of air occurs after continuous expansion, as experimentally evidenced in the wind tunnel experiments [15,16]. In this paper, we investigate the conditions when it is possible for condensation to occur in practical engine configurations, and if it occurs, what its characteristics are. In the next section, updates to the fluid solver that considers real gas effects and the EOS model are briefly introduced. The theories and approaches to model the phase change are based on classical thermodynamics, and are described from the perspective of thermodynamic equilibrium. Simulation results of an engine filled with pure n-heptane, pure nitrogen, and two binary mixtures are then presented with discussions.

## 2. Theory and methodologies

### 2.1. The fluid solver

The fluid solver was based on the open-source computational fluid dynamics (CFD) code KIVA-3V Release 2 [17], which uses the Arbitrary Lagrangian Eulerian (ALE) approach to deal with two-phase compressible flows with the moving boundaries of piston engines. Various improved or new sub-models have been developed and incorporated to better simulate complex multiphase flows with chemical reactions [18]. The standard code solves the

conservation equations at each time step in three consecutive phases: in the Lagrangian Phase A, the source terms due to spray and combustion/chemistry are solved. In Phase B the cell is moved with the local fluid velocity, and all the physical properties (pressure, temperature, velocity, diffusion, etc.), except for convection are solved. This phase is the main part of the fluid dynamics solver. Finally, in Phase C (rezoning stage) the cell boundaries are mapped back to the position where they should be, as determined by the specified mesh motion. The partial differential equation for internal energy, but not temperature, is solved directly.

While the general governing equations for the fluid do not change, the current simulations consider real gas effects, as opposed to the ideal gas relation in the original code, for tracking phase change. Phase A is irrelevant because a non-reactive Eulerian flow is considered; real gas effects mainly show up in the SIMPLE loop iterations in Phase B, which is used for the simultaneous solution of the momentum and energy conservation equations. More details about the generalization of the thermodynamic relationship with a realistic equation of state and the modifications to the original code can be found in Refs. [19,20]. The Peng–Robinson equation of state (PR EOS) [8] is adopted here due to its relative simplicity and accuracy in calculating liquid density. In fact, it has been used by some researchers in investigating the high pressure evaporation and supercritical flows with reasonably good results. For example, it was shown in Ref. [10] that PR EOS gave better results over other cubic EOS models (e.g., RK or SRK EOS) in studying the high pressure droplet evaporation. Simulations of Kim et al. on the cryogenic liquid nitrogen jet showed that the predictions using PR EOS was slightly better over the SRK EOS in matching with experimental density profiles [21]. It should be noted that cubic EOS models still give relatively poor liquid density predictions, and one approach to reconcile this issue is to use the volume-translated EOS to correct the predictions [22]. Recently, the perturbed-chain, statistically associating fluid theory (PC-SAFT) is gaining more and more attention because of its superiority in predicting the thermodynamic properties of complex fluids by introducing extra associating effects [23,24]. However, these methods require a lot more computations so they are less practical to be used in CFD simulations.

The PR EOS has the form:

$$P = \frac{R_u T}{v - b} - \frac{a}{v(v + b) + b(v - b)} \quad (1)$$

Here,  $P$  is the pressure,  $v$  is the molar volume,  $T$  is the temperature and  $R_u$  is the universal gas constant.  $a$  and  $b$  are the two parameters determined from:

$$\begin{cases} a = 0.457235 \frac{R_u^2 T_c^2}{P_c} \cdot \xi \\ b = 0.077796 \frac{R_u T_c}{P_c} \\ \xi = [1 + \kappa(1 - \sqrt{T_r})]^2 \end{cases} \quad (2)$$

with

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad (3)$$

$T_c$ ,  $P_c$  and  $\omega$  are the critical temperature, pressure and acentric factor, respectively. When  $\omega$  is greater than 0.5, the following formula [25] is adopted:

$$\kappa = 0.3796 + 1.485\omega - 0.1644\omega^2 + 0.01667\omega^3 \quad (4)$$

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