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Numerical Model Progress of Liquid Fuel Micro-droplets Evaporation

Yang Yu[1] and Xiao Zhang*, [2]

[1]School of Mechanical Engineering and Automation, Northeastern University, 110819, Shenyang
[2]School of Ocean, Yantai University, 264005, Yantai
zxzn2004@163.com

Abstract. The evaporation of spray injected in material and mechanical engineering has significant effect on mixture formation, emissions and power output. In fact, for only micro-droplets in regular arrangement, fluid motion, supercritical and various shapes changed with time and so on, these common phenomena are quite complex and difficult to be understood and simulated. Especially, the studies of latest decade can show the development level of the relevant models, which will be reviewed in this paper. Some typical traditional quasi- and multi-dimensional models predicting various evaporation characteristics are reviewed for the newest developments to understand much more complex species, momentum and heat transport phenomena through the gas-liquid interface in industrial sprays with real operating conditions. Some experiments used to compare with these models developed are analyzed to reveal some aspect to be improved both for experiment and model. As can be seen from the comparison of the multidimensional results with the quasi-dimensional ones, the more comprehensive models are apparently in favor of understanding the micro-droplet evaporation better. Furthermore, the micro-droplet group shows more complex evaporation process than that of isolate micro-droplet.

1. Introduction

The conventional spray combustion is still the most effective way to provide energy in internal combustion engine. The conceptual model with relative experiments has been revealed the mechanism of soot emission due to dense premixed mixture produced by the conventional spray. So the production of the dense mixture has significant effect on soot, which is influenced by evaporation of spray injected. Especially, the exhaust gas recirculation (EGR) can lowing soot emission due to high proportion of premixed mixture which is confirmed by the conceptual model with relative experiments. The species of EGR inevitably affect the evaporation of the fuel. And if the evaporation can be controlled by some technique, the mixing of fuel and oxygen can be improved so that the dense mixture and soot are lowered. So the evaporation of spray needs to be studied further [1-11].

2. Model of Micro-droplet Evaporation

Ragab R and Wang T [1] develop a three-zone model to simulate the evaporation: (a) the droplet zone with water liquid mass fraction of 1, (b) the shell zone around the droplet with mass source for water vapor and energy sink to simulate liquid evaporation, and (c) the outer domain represents the rest of the flow field. So interface boundary conditions are used between the droplet, the shell, and the domain. And these three distinct cell zones are connected via non-conformal grid interfaces to allow the transport equations to be solved in the whole domain. The fluid and temperature fields are given more detail, though in fact the internal flow of droplet must be influenced by outer domain. Especially,

they thought Biot number should be studied further which can help provide an idea of how thermal resistance ratio would affect heat flow distribution.

To be capable of considering the integral computation region, Strotos et al [2] modeled the evaporation of droplet in using volume of fluid method to track the interface of fuel and air. They found that the velocity streamline is regular under convention flow, but the velocity streamline are not very regular relatively which has two different parts. It's known that the internal circulation has important effect on the evaporation. And the three-dimensional simulation can consider this effect, which should further be studied such as velocity, direction, location and area. For both conditions, the high concentration regions of vapor occur at the downstream of the flow direction. It means that the vapor also flow radically and downwardly. Also, it's interesting that below the droplet there is backflow. That's quite different from the other simulation and the phenomenon of the spray. The backflow may be due to the suspender existing redundantly. However, the results were still close to the experiments in fig 1.

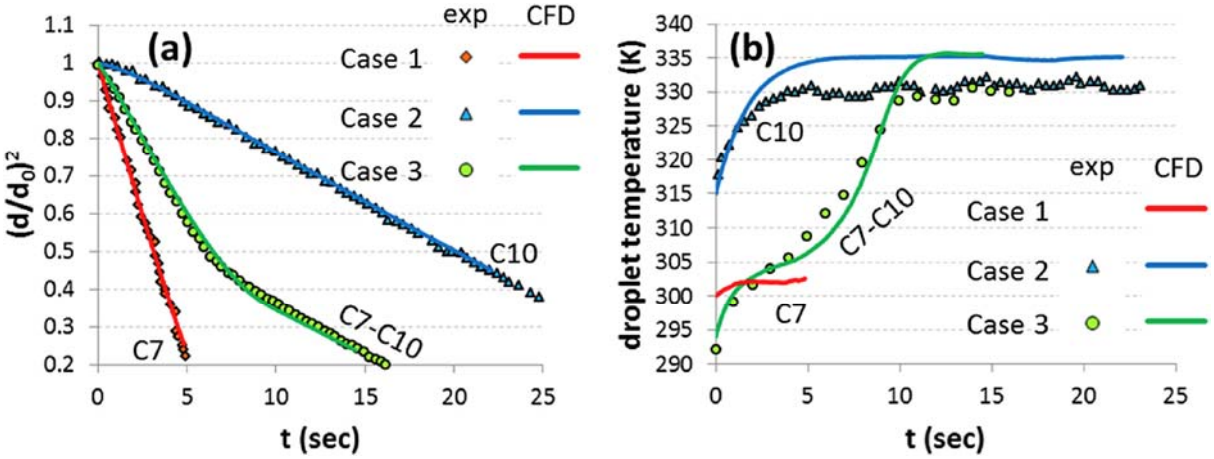

Figure 1. Model predictions for the experimental data[2]

Saufi A E et al [3] designed a camber with different thermocouple to realize the experiments in a wide range of operating conditions, controlling the heating rate (up to 1000 K/s), the pressure (from 0.1 kPa to 10 MPa) and the atmosphere composition (usually nitrogen or air). The suspender using one thermocouple for droplet was hanged on the top face. The temperature field showed the temperature was very hard to be controlled though using three thermocouples. From the other new study, Naito Y et al [4] established a vessel only with one thermocouple and adiabatic material wall. So the current equipments are hard to keep constant temperature for several seconds. Rehman H L et al [5] studied the outcome of varying support size, support material, ambient temperature, ambient velocity and droplet size on the droplet evaporation process. The average over estimation of mean droplet evaporation rates in the absence of heat conduction for linear extrapolation are found to be 30% and 8% for thermocouples and glass fibers respectively. This non-linearity behavior in droplet evaporation rate curves was more profound for thermocouple than glass fiber due to higher thermal conductivity as shown in fig 2. So the equipment should be organized carefully to compare with the mathematical model.

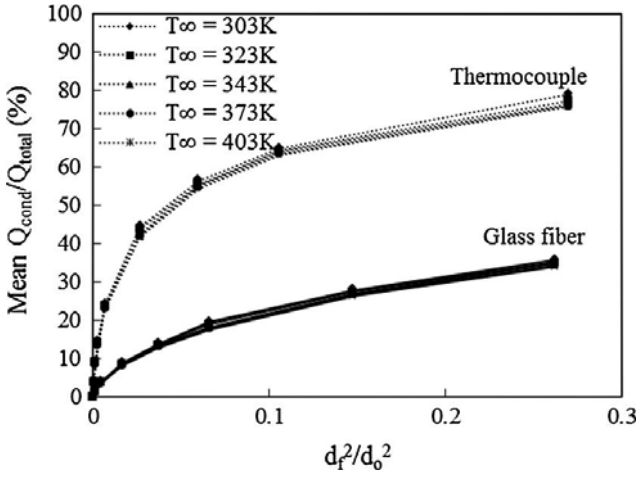

Figure 2. Variation of heat transfer through conduction[5]

Saufi A E et al [3] also adopted VOF to simulate the droplet evaporation, considering non-ideal mixtures evaluated with the UNIFAC approach. The results of the acetic acid mass fraction in the mixture shows the vapor distributed uniformly around the droplet that is quite different from the pure matter. In Naito Y et al' study [4], they only use quasi-dimensional vaporization model for the multi-component. And for temperature distributions inside the droplet, a quadratic polynomial distribution was introduced which is common in three-dimensional simulation. The different types of enthalpy diffusion term in heat flux were discussed. Muthuramalingam V P and Karlsson A [6] considered the non-ideal gas-liquid equilibrium utilizing the NRTL method in quasi-dimensional vaporization model which was incorporated into CFD code. The results showed that the vapor mass fractions were higher in non-ideal cases than in ideal cases.

Recently, differing from the traditional way with several common methods above, the sphere of droplet is queried and become another way to improve the vaporization model [7]. Though the shapes of droplets in spray are complex and change frequently, special droplet shapes approximating to prolate and oblate spheroids were still studied to find some way for first step. They use ellipsoidal coordinates to solve the equations system of original vaporization model. So the shape of droplet was controlled by eccentricity. were integrated using the finite-element-based PDE modules of COMSOL Multiphysics including Moving Mesh The temperature fields also presented ellipsoidal distribution. Note that the temperature is lower around the short axis, which should be given the explain.

The microcosmic methods for kinetic and molecular dynamics appear for a long time. Sazhin S S et al [8] brought forward the method combined kinetic model with traditional quasi-dimensional vaporization model in fig 3. It is shown that in all cases the kinetic effects lead to a decrease in droplet surface temperature and an increase in the evaporation time. The kinetic effects on the droplet evaporation time are shown to increase with increasing gas temperatures. There usually existed a series of assumptions at molecule level and the simulating results have not shown more advantages than the traditional ones. Especially, the quantum-chemical effects on the evaporation coefficient for realistic multi-component fuel droplets have not been investigated.

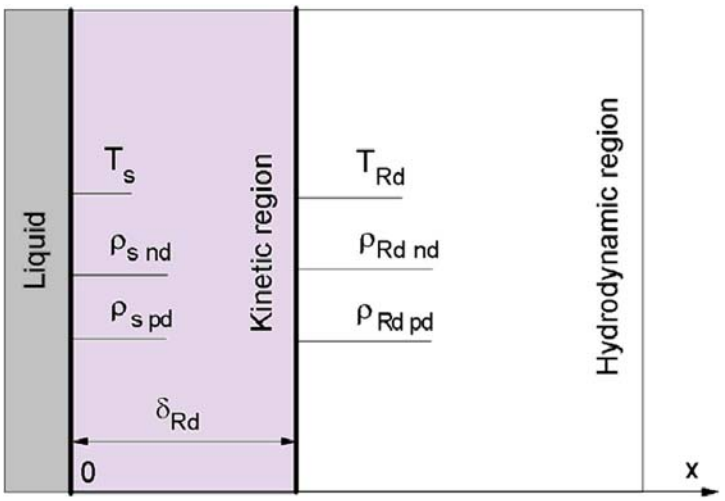

Figure 3. Variation of heat transfer through conduction[8]

The lattice Boltzmann method (LBM) is the no tracking methods without the need for generating an interface which is tried to compute the thermal multiphase fluid with evaporation [9]. A multiple relaxation time and exact difference method scheme was considered to simulate the heating and vaporization of a droplet under forced convection. The density near the gas-liquid interface is treated with one function of some given thick value, and the computations adopted two dimensional planar coordinate with 300×300 lattice to simulate the circle in the central section of droplet. However it is found that the method shows good agreement with the well-known D^2 law that prescribes the evaporation rate.

Zoby M R G [10] suggested examining the effects of the complex interactions of droplet arrays and turbulence on evaporation rates in inert and reactive turbulent environments using Direct Numerical Simulations (DNS). In particular the local temperature affects the evaporation rates of droplets are hard to be studied in previous works. Other than the above studies, the Level Set method has been combined with the Ghost Fluid method, which is not inherently mass conserving but can obtain smoother gas-liquid surface. They found that when combustion occurs as a group phenomenon, a reduction in the evaporation rates is observed. Evaporation processes of some droplets are quite different from that of isolate droplet. And turbulence does not seem to have significant effects on evaporation rates under any of the conditions.

Except for the above methods, the phase-field also can be used to handle multiphase fluid problem. Safari H et al [11] combined the phase-field with the level set to compute the evaporation. The modified convective Cahn-Hilliard equation is employed to reconstruct the dynamics of the interface topology, which was added a source term considering the phase change within the interface. They set the initial droplet temperature and the inflow air temperature to the range near the room temperature. For the laminar forced convective case, especially, the minimum temperature point pushes to the aft section of the droplet and eventually the cooled liquid is drawn into the droplet interior due to the internal circulation.

3. Conclusions

In fact, though providing enough description of evaporation process, the above results of these present models should be still compared with more detailed experimental data to validate various hypotheses simplifying reality. Shadowgraphs of the evaporating micro-droplets have been acquired, though temporally and spatially resolved composition profiles were measured along a line through the micro-droplets using one-dimensional Raman spectroscopy. It was quite clear that the surface regression rate is not a constant but a non-linear decrease. And if further considering the solubility of gas into liquid under not only supercritical condition but also the wider one and multicomponent' evaporation, the study of evaporation still need noticeable progress.

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