DEVELOPMENT OF A SIMPLIFIED MODEL FOR DROPLET VAPORIZATION

by

Helin XIAO, Liangrui ZHAO, Zhongzhao LI, Mingrui WEI [*], *and Guanlun GUO*

Hubei Key Laboratory of Advanced Technology for Automotive Component,
Wuhan University of Technology, Wuhan, China

Droplet vaporization is an essential sub-process of fuel spray in diesel engines, which has important effects on combustion and emissions performance. Development of a simplified droplet vaporization model is necessary to simulate gas mixture formation in cylinder for lower computational costs, and it is also applicable in practical multi-dimension spray calculations for diesel engines. An empirical exponential equation is introduced in this paper to approximate the internal temperature profile of droplet instead of solving the partial differential equation for temperature distribution. Results indicate that the computational cost has been reduced by almost thirty percent in total. Also, the concept of effective diffusion is introduced by using an enlarged diffusivity to take account of the effect of internal circulations inside droplets. The calculated result of the simplified evaporation model has been compared with that of the infinite diffusivity model and one-dimensional model respectively. It shows that the calculation precision of the simplified model is among those two models.

Key words: *spray model, zero-dimension, droplet evaporation*

Introduction

Droplet evaporation is an essential sub-process of fuel spray in internal combustion engines. In the past few decades, the modeling of droplet vaporization has been intensively investigated [1-9]. Several kinds of models, with different accuracy and demand for computing resources, have been presented to describe the unsteady liquid phase transport inside droplet.

The computational complexity of available evaporation models for liquid phase transport ranges from zero-dimensional to 2-D. In the most detailed model (vortex model), 2-D axisymmetric equations for mass, momentum and energy conservations are used to describe transient evolutions of temperature and mass fractions within droplets. The vortex motion inside the droplet is described by vorticity and stream function equations or analytical solutions [10, 11]. However, the computing cost is too expensive and prevents the model from being applied in practical multi-dimensional spray simulations for tracing thousands of liquid parcels with each parcel representing a collection of droplets that have the same properties. At the opposite extreme, the infinite diffusion (zero-dimensional) model assumes diffusive coefficients of mass and heat are large enough to ensure that physical properties and chemical components inside

---

[*] Corresponding author; e-mail: hlxiao_qcxy@whut.edu.cn

droplets are always uniform. Due to the lower computing cost, the zero-dimensional model is preferred in multi-dimensional spray simulations. However, zero-dimensional models always bring large errors since temperature distributions and vortex motions inside droplets are all neglected. Between these two extremes, both pure diffusion model and simplified vortex model use 1-D governing equations to describe the transport process of mass and heat flux within droplet [12-14]. The simplified vortex model includes more physics than the pure diffusion model. Pure diffusion models ignore the internal circulation effect, which is represented by artificially enlarged diffusivities or by using the similarity transformation in simplified vortex models. Both above approaches are found to be effective and yield similar results to detailed vortex models.

Some zero-dimensional models were also formulated. Tong and Sirignano [15] simplified partial differential equations to a set of ordinary differential equations by using similar transformation and an integral approach based on the Green function and eigenvalue methods, which captured transient variations of droplet surface temperature and mass fractions. Renksizbulut *et al.* [16] related the difference between the surface and average values (*e. g.*, temperature or mass fractions) to the mass or flux at the droplet surface by using Sherwood and Nusselt numbers. These zero-dimensional models are preferred in multi-dimensional spray simulations because of low computing expenses. In this paper, a modified zero-dimensional model based on 1-D models is proposed by using an empirical exponential equation instead of using an 1-D partial differential equation to approximate the temperature distribution within droplets. This will further reduce the computing cost, while maintaining sufficient precisions as similar to 1-D simplified vortex models. The following of the paper particularly describes this modified zero-dimensional model, and the basic framework will be firstly given to determine the droplet vaporization rate and the heat flux to the droplet. Then results and computing performance will be discussed for the proposed model.

Physics and mathematical model

In order to simplify the droplet vaporization model, some assumptions should be presented. Firstly, the coupling effect of heat and mass transformation within droplet can be neglected because of the very sm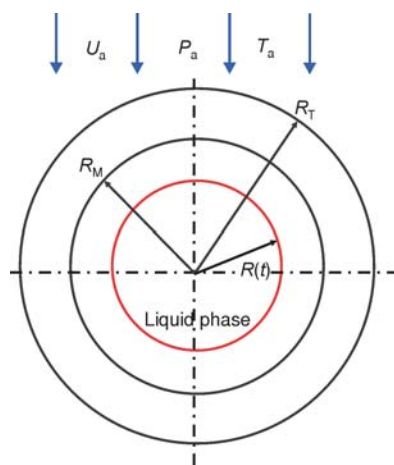all phenomenological coefficient of the coupling effect. Secondly, the energy radiation band of the gas does not coincide with most of the liquid energy absorbing band, so the heat radiation can be neglected comparing with the thermal conduction and convection. Finally, the droplet is constantly a sphere and the evaporation is spherically symmetric.

Modeling of mass and heat transfers for gas phase ($r > R(t)$)

A film method is introduced to calculate heat and mass transfers for gas phase, which considers heat and mass transfers in a practical droplet similar to molecule conductions and diffusions in a spherical-symmetric film. The physical scheme of the film method is shown as fig.1, in which $R(t)$, R_T and R_M denote the radius of droplet, temperature film, and concentration film, respectively.

Figure 1. Physical scheme of film method

Sirignano model is used here and governing equations are:

$$\dot{m} = 2\pi \rho_g D_g R(t) \text{Sh} \ln(1 + B_M)$$

(1)

$$\dot{m} = 2\pi \left(\frac{k_g}{C_{p,v}} \right) R(t) \text{Nu} \ln(1 + B_T)$$

(2)

In above two equations, $\dot{m}, \rho, k$ and C_P account for mass evaporating rate, density, conductivity, and constant-pressure specific capacity respectively. Sh, Nu, B_M, and B_T, respectively, denote Sherwood number, Nusselt number, Spalding mass transfer number, and thermal conduction number and are given by:

$$B_M = \frac{Y_{v,s} - Y_{v,a}}{1 - Y_{v,s}}$$

(3)

$$B_T = C_{p,v} \frac{T_a - T_s}{\dfrac{L + Q_l}{\dot{m}}}$$

(4)

$$\text{Nu} = 2 + 0.6 \, \text{Re}^{0.5} \, \text{Pr}^{1/3}$$

(5)

$$\text{Sh} = 2 + 0.6 \, \text{Re}^{0.5} \, \text{Sc}^{1/3}$$

(6)

Here Y, T, L, and Q_l, respectively, represent mass fraction, temperature, phase change enthalpy, and quantity of heat transferring rate into droplet. Re, Pr, and Sc are gas phase Reynolds number, Prandtl number, and Schmidt number, respectively. The subscript g, v, s, and a, respectively, denote gas phase, fuel vapor, droplet surface, and environment condition.

In this work, Stefan flow effects on film radius are considered by using modified Nu^* and Sh^* to replace Nu and Sh in eqs. (1) and (2), as equations:

$$\text{Nu}^* = 2 + \frac{\text{Nu} - 2}{F_T}$$

(7)

$$\text{Sh}^* = 2 + \frac{\text{Sh} - 2}{F_M}$$

(8)

Here, F_T and F_M are radius modified factors of the film and given by eqs. (9) and (10):

$$F_T = \frac{(1 + B_T) \ln(1 + B_T)}{B_T}$$

(9)

$$F_M = \frac{(1 + B_M) \ln(1 + B_M)}{B_{TM}}$$

(10)

The temperature and the concentration mentioned in above equations are given by the one-third principle:

$$T_g = \frac{T_s + (T_a - T_s)}{3}$$

(11)

$$Y_g = \frac{Y_{v,x} + (Y_{v,a} - Y_{v,s})}{3}$$

(12)

340

Xiao, H., *et al.*: Development of a Simplified Model for Droplet Vaporization
THERMAL SCIENCE: Year 2016, Vol. 20, No. 1, pp. 337-345

Modeling of thermal conductions for liquid phase

The governing equation of 1-D thermal conduction model is:

$$\rho_l C_{p,l} \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(k_l r^2 \frac{\partial T}{\partial r} \right) \tag{13}$$

In eq. (13), r stands for spatial co-ordinate and subscript l denotes liquid phase. When the liquid phase thermal conductivity, k_l, tends toward infinity, the 1-D model can be transformed into a zero-dimensional model. In 1-D evaporation models, the vortex circulation effect inside the droplet is considered by using a modified thermal conductivity, which is given by the following equation:

$$k_{\text{eff}} = x k_l \tag{14}$$

Here, x is given by the equation:

$$x = 1.86 + 0.86 \tanh \left[2.225 \log \frac{\text{Pe}}{30} \right] \tag{15}$$

where Pe is the Peclet number of the liquid phase. Although the 1-D model describes the temperature distribution inside the droplet not as accurately as the multidimensional model, obtained results of droplet surface temperature and radius are similar to those of vortex models, so 1-D models have been widely applied with promotion of computer performance.

The variation rate of the droplet radius can be given by following droplet mass conservation equation:

$$-\rho_l [R(t), t] \dot{R}(t) = \frac{\dot{m}}{4 \pi R^2(t)} + \int_0^{R(t)} \left(\frac{r}{R(t)} \right)^2 \frac{\partial \rho_l(r,t)}{\partial t} \mathrm{d}r \tag{16}$$

Boundary conditions for liquid phase are:

$$r = 0: \ \frac{\partial T}{\partial r} = 0 \tag{17}$$

$$r = R(t): \ 4 \pi r^2 k_l \frac{\partial T}{\partial r} = Q_l \tag{18}$$

In this paper, a temperature distribution function inside droplet is presented instead of solving eq. (13):

$$T(t,r) = T_c + (T_s - T_c) \left(\frac{r}{R(t)} \right)^n \tag{19}$$

Subscripts c in eq. (19) denotes the droplet center, s – the droplet surface, and n – the exponential number of droplet temperature distribution function, which changes with boundary conditions. Based on the calculation result of temperature distribution inside a droplet using 1-D models, an empirical equation is presented to determine the exponential number n:

$$n = \left(1 + \frac{T_a - T_w}{T_w - 300} \right) \left(\frac{1 + P_a}{P_{cr}} \right) \tag{20}$$

where

$$T_w = 137 \left(\frac{T_b}{373.15} \right)^{0.68} \ln(T_a) - 45 \tag{21}$$

Subscripts a, w, cr, and b denote environmental conditions, equilibrium state of droplet evaporation, critical state of droplet, and boiling state, respectively. Equation (21) is an em-

pirical formula for temperature of droplet evaporation equilibrium state [17]. Combining eqs. (18) and (19) following equation can be derived:

$$T_s - T_c = \frac{Q_l}{4\pi n k_l R(t)} \tag{22}$$

According to the droplet energy conservation equation, the following equation can be written:

$$\int_0^{R(t)} 4\pi r^2 \rho_l(r,t) C_{p,l} \frac{\partial T}{\partial t} dr = Q_l \tag{23}$$

Combining eqs.(19), (22) and (23), the following equation can be derived:

$$\int_0^{R(t)} r^2 \rho_l(r,t) C_{p,l} \frac{\partial T}{\partial t} dr = \frac{n k_l R(t)(T_s - T)}{1 - \left(\dfrac{r}{R(t)}\right)^n} \tag{24}$$

The variation rate of droplet surface temperature, dT_s/dt, can be solved by eq. (24). The temperature used to evaluate physical parameters is defined by:

$$\overline{T} = 3 \int_0^{R(t)} \frac{4\pi r^2 T(t,r) dr}{4\pi R(t)^3} \tag{25}$$

Through the coordinate system transformation, the problem of the boundary movement caused by droplet interface regression can be dealt with constructing the governing equation in a moving coordinate system.

Results and discussions

Comparisons with other models

As shown in fig. 2, the radius of decanted droplet when evaporating in air, is calculated by the proposed model in comparison with those of zero and 1-D models. It shows that the accuracy of the proposed model is between zero and 1-D models. In fig. 2(a), it is shown that curves from three models do not agree with each other very well at the beginning of droplet evaporation, but at the end of droplet lifetime, the curve of the modified model agrees very well with that of the 1-D model. However in fig. 2(b), curves of three models are very similar along the droplet lifetime. At high temperature environment, the temperature gradient inside droplet is
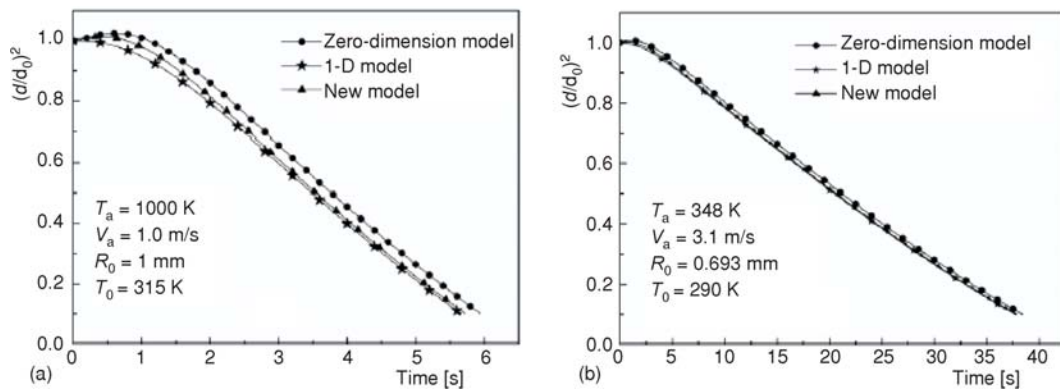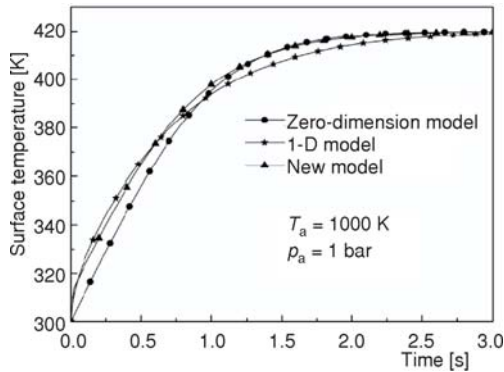

Figure 2. Comparison of computational results for three models at different calculation conditions
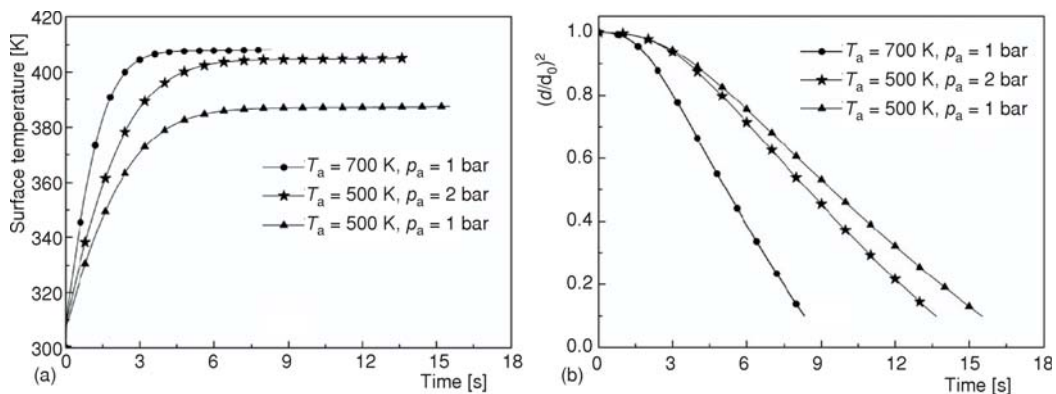
Figure 3. Comparison of droplet surface temperature for three models

so large that the zero-dimensional model can not describe the temperature distribution, while the modified model can approximate the temperature profile, which results in the proposed model agreeing quite well with the 1-D model. At low temperature environment, the temperature gradient inside the droplet is small and the temperature is almost uniform, so curves of three models are almost the same.

Figure 3 describes the calculated surface temperature of a droplet during evaporation process. At the beginning of droplet evaporation at high temperature environment, the temperature gradient inside the droplet is so large that the heat can not be transferred quickly into the droplet center which leads to heat accumulation on the surface. So the surface temperature calculated by the modified model with consideration of temperature gradient agrees well with that of the 1-D model and increases faster than that of the zero-dimensional model. This can be seen in fig. 3. At the end of evaporation process, the temperature inside the droplet is almost uniform which leads to the results of the zero-dimensional model meeting with the 1-D model better than the modified model. In a word, above three models coincide with each other well in all droplet lifetime.

Droplet evaporation characteristics

Figures 4 to 8, show the calculated results of the modified model with the characteristics of droplet evaporation. Heat is always transferred into droplets by collisions from high temperature gaseous molecules. At high temperature environment, droplets absorb lots of heat through touching higher-temperature gaseous molecules and their surface temperature increases rapidly. In the same way, droplet surface temperature can also increases rapidly by touching more gaseous molecules under higher-pressure. It may be the reason, as shown in fig. 4 (a), that the increment of environmental temperature or pressure can increase the droplet surface temper-

Figure 4. Influences of ambient temperature and pressure on droplet surface temperature and vaporization characteristics

Xiao, H., *et al.*: Development of a Simplified Model for Droplet Vaporization
THERMAL SCIENCE: Year 2016, Vol. 20, No. 1, pp. 337-345

343

ature rapidly. In fig. 4 (b), the lifetime of droplet becomes shorter with increasing environmental temperature or pressure. This indicates that the higher droplet surface temperature can make droplets evaporate quicker at higher environmental temperature or pressure. However, higher environmental pressure also makes the gas denser, which will reduce the vapor diffusivity and extend the droplet lifetime especially at low temperature, as shown in fig. 5(b).
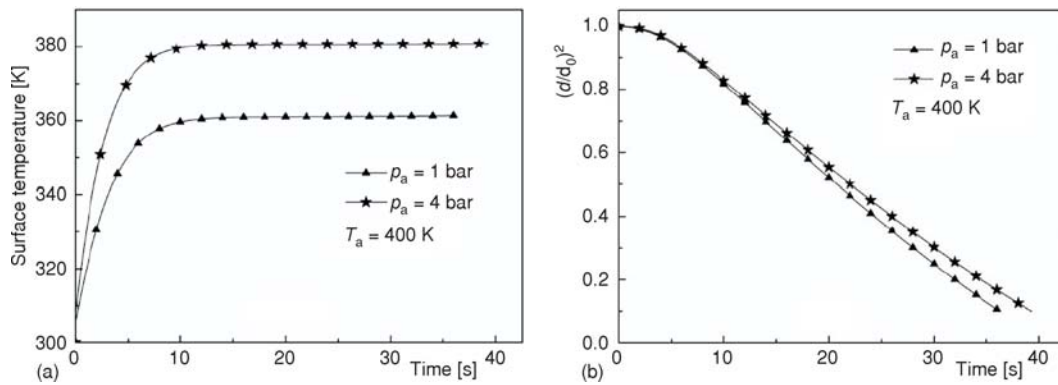

Figure 5. Influences of ambient pressure on droplet surface temperature and vaporization characteristics

In figs. 4(b) and 5(b), the droplet radius decreases very slowly and the evaporation rate is very small at the beginning of droplet evaporation, but the droplet temperature increases quickly which leads to bigger droplet radius because of low density. The combined effect of above two factors makes the droplet radius change slowly at the beginning of evaporation.

In fig. 6, droplet lifetime declines rapidly with increment of environment temperature especially below 400 K. As shown in figure, higher environment pressure leads to longer droplet lifetime at the temperature below 420 K. However, when the temperature is higher than 420 K, the low pressure will extend the droplet lifetime. The main reason may be that the heat

Figure 6. Influences of ambient temperature and pressure on droplet lifetime

absorption rate of the droplet is proportional to the temperature at low temperature environment and the droplet lifetime changes rapidly with the environment temperature, but at high environment temperature the droplet can always absorb heat sufficiently and evaporate rapidly, so the lifetime is affected less by the temperature.
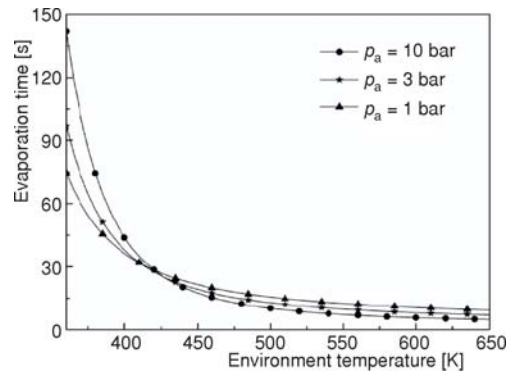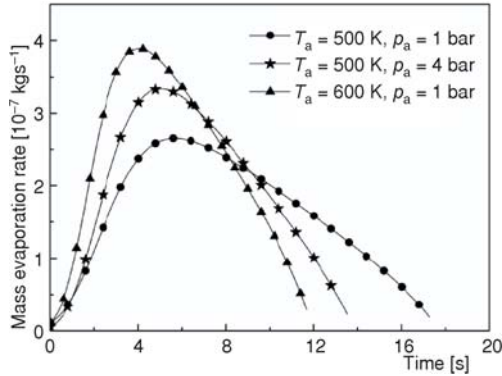
Figure 7 reflects the relationship between mass evaporation rate and time. In the first period of droplet evaporation, the mass evaporation rate rises rapidly with time until reaching the highest value, after that the rate declines rapidly until the lifetime of droplet is over. It can also be found that the increase of the environment temperature or pressure can narrow the evaporation curve, but the total mass under curves is constantly equal to the droplet mass. At the be-

344

Xiao, H., *et al*.: Development of a Simplified Model for Droplet Vaporization
THERMAL SCIENCE: Year 2016, Vol. 20, No. 1, pp. 337-345

Figure 7. Influences of ambient temperature and pressure on droplet mass evaporation rate

ginning of evaporation, the rare vapor surrounding the droplet leads to rapid evaporation, but at the last period, the vapor is saturated which makes the evaporation slow.

Conclusions

By using an empirical exponential equation to approximate the temperature profile inside the droplet, this paper has developed a preferential model for droplets evaporation and sprays simulations with the complexity of zero-dimensional model. The proposed model is validated by comparing with the simplified vortex model (1-D) and zero-dimensional model. It can reduce the computing cost by almost thirty percent of the simplified vortex model in total while maintaining the same accuracy as the 1-D model. This indicates that this new model is applicable in practical multi-dimensional spray simulations.

Acknowledgments

Nomenclature

C_D – drag coefficient, [–]
C_P – heat capacity, [Jkg^{-1}K^{-1}])
$C_{p,v}$ – specific heat capacity, [Jkg^{-1}K^{-1}]
D – diffusion coefficient, [m^{2}s^{-1}]
d – diameter of droplet, [m]
F – radius modified factor, [–]
g – gravity acceleration, [ms^{-2}]
h – convective heat transfer coefficient
k – thermal conductivity coefficient, [Wm^{-1}K^{-1}]
k' – thermal conductivity coefficient
L – latent heat of vaporization, [Jkg^{-1}]
m – mass, [kg]
$\dot{m}$ – mass evaporating rate
p – pressure, [Pa]
Q_l – quantity of heat transfer rate, [Js^{-1}]
r – co-ordinate in radial direction, [m]
T – temperature, [K]
t – time, [s]
U – relative velocity of droplet
V – volume, [m^3]
v – velocity, [ms^{-1}]
Y – mass fraction
$Y_{v,a}$ – environment mass fraction
$Y_{v,s}$ – droplet surface mass fraction

Greek symbols

μ – dynamic viscosity
ρ – density, [kgm^{-3}]

Non-dimensional numbers

Nu – Nusselt number (= hd/k)
Pe – Peclet number (= Ud/D)
Pr – Prandtl number (= $C_p\mu/k$)
Re – Reynolds number (= $\rho Ud/\mu$)
Sc – Schmidt number (= $\mu/\rho D$)
Sh – denoted Sherwood number (= $k'd/D$)

Subscripts, superscript

a – environment condition
b – boiling state respectively
c – droplet center
cr – critical state of droplet
eff – efficacious
g – gas phase
l – liquid phase
n – droplet temperature distribution function
s – droplet surface
v – fuel vapor
w – equilibrium state of droplet evaporation

Xiao, H., *et al.*: Development of a Simplified Model for Droplet Vaporization
THERMAL SCIENCE: Year 2016, Vol. 20, No. 1, pp. 337-345

345

References

[1] George, S., *et al.*, Numerical Investigation of the Evaporation of Two-Component Droplets, *Fuel, 90* (2011), 4, pp. 1492-1507

[2] Xu, W., *et al*., Numerical Investigation of Droplet Evaporation and Transport in a Turbulent Spray with LES/VSJFDF Model, *Chemical Engineering Science, 119* (2014), 8, pp. 251-260

[3] Sazhin, S. S., *et al.*, A Quasi-Discrete Model for Heating and Evaporation of Complex Multi-Component Hydrocarbon Fuel Droplets, *International Journal of Heat and Mass Transfer, 54* (2011), 19-20, pp. 4325-4332

[4] Nakoryakov, V. E., *et al*., Non-Iso Thermal Desorption of Droplets of Complex Compositions, *Thermal Science, 16* (2012), 4, pp. 997-1004

[5] Ebrahimian, V., Gorji-Bandpy, M., Two-Dimensional Modeling of Water Spray Cooling Superheated Steam, *Thermal Science, 12* (2008), 2, pp.79-88

[6] Jafarmadar, S., *et al*., Numerical Investigation of the Effect of Injection Mode on Spray/Wall Interaction and Emission Formation in a Direct Injection Diesel Engine at Full Load State, *Thermal Science, 14* (2010), 14, pp.1039-1049

[7] Michael, S., *et al.*, One-Dimensional Models of Nanoliter Droplet Evaporation from a Hot Surface in the Transition Regime, *International Journal of Heat and Mass Transfer, 57* (2013), 2, pp. 473-483

[8] Raghuram, V., R., *et al.*, Two-Phase Modeling of Evaporation Characteristics of Blend Methanol-Ethanol Droplets, *International Journal of Multiphase Flow, 52* (2013), June, pp. 46-59

[9] Zeng, Y., Lee, C, F., A Model for Multi-Component Spray Vaporization in a High-Pressure and High-Temperature Environment, *Journal of Engineering for Gas Turbines and Power, 124* (2002), 3, pp. 717-724

[10] Megaridis, C. M., Sirignano, W. A., Numerical Modeling of a Vaporizing Multicomponent Droplet, Proceedings, 23rd Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, Penn., USA, 1990, pp. 1413-1421

[11] Abramzon, B., Sirignano, W. A., Droplet Vaporization Model for Spray Combustion Calculations, *International Journal of Heat and Mass Transfer, 32* (1989), 9, pp. 1605-1618

[12] Law, C. K., Internal Boiling and Superheating in Vaporizing Multicomponents Droplets, *AIChE J, 24* (1987), 4, pp. 626-632

[13] Jin, J. D., Borman, G. L., A Model for Multicomponent Droplet Vaporization at High Ambient Pressures, SAE Technical paper, 850264, 1985

[14] Tong, A. Y., Sirignano, W. A., Multicomponent Transient Droplet Vaporization with Internal Circulation: Integral Equation Formulation And Approximate Solution, *Heat Transfer, 10* (1986), 3, pp. 253-278

[15] Tong, A. Y., Sirignano, W. A., Multicomponent Droplet Vaporization in a High Temperature Gas, *Combust. Flame, 66* (1986), Dec., pp. 221-235

[16] Renksizbulut, M., *et al*., A Droplet Vaporization Model for Spray Calculations, *Part. Syst. Charact, 9* (1992), 1-4, pp. 59-65

[17] Miller, R. S., *et al*., Evaluation of Equilibrium and Non-Equilibrium Evaporation Models for Many-Droplet Gas-Liquid Flow Simulations, *International Journal of Multiphase Flow, 24* (1998), 6, pp.1025-1055