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Title	Modeling wall film formation and vaporization of a gasoline surrogate fuel			
Author(s)	Kobashi, Yoshimitsu; Zama, Yoshio; Kuboyama, Tatsuya			
Citation	nternational journal of heat and mass transfer, 147, 119035 https://doi.org/10.1016/j.ijheatmasstransfer.2019.119035			
Issue Date	2020-02			
Doc URL	http://hdl.handle.net/2115/83975			
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Rights(URL)	http://creativecommons.org/licenses/by-nc-nd/4.0/			
Туре	article (author version)			
File Information	Manuscript_w_Figure_Table.pdf			



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Modeling Wall Film Formation and Vaporization of a Gasoline Surrogate
 Fuel
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### 7 Abstract

To simulate the wall film formation and vaporization processes in gasoline direct-8 injection spark-ignition engines including considerations of the physical properties and 9 10 vapor-liquid equilibrium of multi-component fuels, spray-wall interaction sub-models were implemented with the 3D-CFD software HINOCA which has been developed for 11 automotive engine cylinder simulations. The models used were the Senda model for 12spray-wall impingement including splash, deposition, droplet-droplet interactions, and 13droplet-film interactions; the O'Rourke model for heat transfer and film vaporization; a 1415simple film flow model considering momentum conservation; and Raoult's law for vaporliquid equilibrium. First, the model validated the calculated results for a single-16component fuel (iso-octane) through comparisons with experimental data in terms of wall 17film area and heat flux between the wall and film. Second, numerical simulations were 1819conducted with a 5-component gasoline surrogate fuel which was designed taking into 20account the average octane number, aromatic content, and distillation characteristic. The results showed clear differences in the contributions of the 5 components to the wall film, 21and the possibility that the aromatic content with higher carbon atoms could be a source 22of soot formation. 23

- Keywords: Gasoline Direct Injection Engine, Wall Film, Spray, Gasoline Surrogate Fuel
   25
- 26 Nomenclature:
- 27 A Area [m<sup>2</sup>]
- 28 *d* Diameter of droplet [m]
- 29 E Kinetic energy of droplet or wall film [J]

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30	Ecrit	Energy needed to break up droplet [J]			
31	Κ	Critical parameter which correlates deposition and splash [-] (= $Z$ · $Re^{1.25}$ )			
32	La	Laplace number [-]			
33	т	Mass of droplet or wall film [kg]			
34	M	Total mass [kg]			
35	Oh	Ohnesorge number [-] (= $\sqrt{We}/Re$ )			
36	р	Pressure [Pa]			
37	Ż	Heat flux [W/m <sup>2</sup> ]			
38	Re	Reynolds number [-]			
39	t	Time [s]			
40	tr	Time interval parameter [-] (= $\Delta t / \tau_{res}$ )			
41	Т	Temperature			
42	V	Velocity of droplet or wall film [m/s]			
43	We	Weber number of droplet [-]			
44	У	Mass fraction [-]			
45	Subscrip	ots:			
46	1	Before impingement on wall			
47	2	After impingement on wall			
48	crit	Critical			
49	f	Wall film			
50	g	Gas			
51	i	Component			
52	inj	Injection			
<b>53</b>	l	Liquid			
54	n	Normal to wall			
55	S	Surface of wall film			
56	t	Tangential to wall			
57	W	Wall			
58	Greek sy	mbols:			
<b>59</b>	$\delta$	Film thickness [m]			
60	$\delta_N$	Non-dimensional film thickness (= $\delta/d_p$ ) [-]			
61	$\Delta t$	Time interval between two continuous droplets reaching a wall [s]			
62	$\varphi$	Equivalence ratio [-]			
63	λ	Thermal conductivity [W/(m·K)]			
64	μ	Viscosity [Pa·s]			
65	ρ	Density [kg/m <sup>3</sup> ]			
66	$\sigma_l$	Surface tension of liquid [N/m]			
67	$ au_{air}$	Shear force between airflow and wall film [Pa]			

68	$ au_{res}$	Droplet residence time on wall [s]
69	$ au_{W}$	Friction stress between wall film and wall [Pa]

## 70 1. Introduction

71Due to the improvements in thermal efficiency and engine power output, modern 72gasoline engines have employed direct-injection spark-ignition (DISI) systems. In this strategy, however, soot may be produced as the result of the formation of a liquid film 73(wall film) on the piston surface and from pool fires fed by the wall film [1][2]. To develop 74DISI engines which avoid the wall film formation and reduce the mass and number of 7576soot particulate, it is crucial to develop numerical analysis schemes that treat the spraywall interaction, film flow, and film vaporization processes in more detail, as well as to 77develop an understanding of the source of the soot particles. 78

Over the past decades, a number of spray-wall impingement models have been 7980 developed. Naber and Reitz [3] proposed one of the first impingement models, which 81 considers three regimes including stick, rebound, and slide of the impinged droplets. Bai and Gosman [4] proposed a more detailed model which includes wider impingement 82 regimes; adhesion (stick and spread) and splash for dry walls; rebound, spread, and splash 83 for wetted walls, while employing Wecrit as the critical Weber number for regime transition 84 85 criterion. Stanton and Rutland [5], assuming wetted walls, also derived a model in which 86 Wecrit was used as the critical criterion of the regime transition. A single-droplet experiment by Mundo et al. showed that the limit of adhesion and splash can be correlated 87 in terms of the Reynolds number Re and the Ohnesorge number Oh, and an additional 88 critical parameter K (=  $Oh \cdot Re^{1.25}$ ) was also introduced [6]. The recent study [7] has 89 demonstrated that using Kuhnke's spray-wall interaction model [8], in which the effects 90 of the critical parameter K and a thermal parameter defined as the ratio of the wall 91temperature and the droplet boiling temperature are considered, a good agreement of wall 92

93 film height distributions between the measurements and calculations. Zhang et al. 94proposed a model considering the droplet/film interaction on the film dynamics, and the 95 dissipative energy loss during the expansion of the lamella formed by the deformation of 96 the deposited droplet [9]. Senda et al. [10-11] proposed a more comprehensive model which considers the effects of the Weber number We and liquid film thickness on spray-97 wall interaction behaviors as well as a Wecrit parameter as the regime transition criterion. 98 For wall film vaporization, the model developed by O'Rourke and Amsden [12] is 99 100 reliable and often used in the literature, as it consists of physical processes like the wall 101 film energy balance, heat transfer from the wall to the film and to the impinging droplets, and the temperature profile in the film normal to the surface. Recently, Jiao and Reitz 102 103 employed the model to simulate the soot formation from the wall film in a DISI engine [13]. Another important aspect in the wall film vaporization is the distillation 104 105characteristics of fuels as gasoline is multicomponent fuel, and the component remaining 106 in the wall film has a significant impact on the soot formation, like for example, many of 107 high boiling point gasoline components are aromatics [14] which tend to increase soot 108 emissions. A number of vaporization models have been developed for multicomponent 109fuels [15-21]. However, there have been few studies that conducted extensive validation 110 of the models including the film evaporation process and heat flux between the wall and wall film, although the heat flux modeling was studied well for single component liquid 111 [9, 22]. In addition, little has been reported on the correlation between the vaporization 112process of wall films and the distillation characteristics of fuels. Köpple et al. proposed a 113gasoline surrogate fuel consisting of n-hexane, iso-octane and n-decane [23]. Using this 114surrogate fuel, Köpple et al. validated the heat transfer between the piston wall and wall 115116 film [7], and showed a good correlation between the calculated mixture formation and the measured particulate emissions [23]. Schulz and Beyrau demonstrated that this gasoline 117surrogate fuel represents the wall film vaporization of real gasoline [24]. 118

The purpose of the present study is to develop a simulation scheme that predicts the 119120wall film formation and vaporization of multicomponent fuel sprays with a high degree 121of accuracy, and to investigate the potential source of soot in DISI gasoline engines. Submodels accommodating this were incorporated into the platform software HINOCA [25]. 122The calculated wall film area and heat flux between the wall and wall film in this study 123were validated via comparisons with data obtained by measurements developed specially 124for this study, followed by modifications to the sub-models. A gasoline surrogate fuel was 125126designed to meet the average octane number, aromatic contents, and distillation 127characteristic of real gasoline fuel. Finally, the correlation between the formation and vaporization processes of wall films and the components of the gasoline surrogate fuel 128129was examined.

## 130 **2. Model description**

The platform software employed in this study is HINOCA [25] which is an automotive engine cylinder simulation software, based on fully compressible Navier-Stokes equations which are filtered for Large Eddy Simulation (LES), and employs Cartesian grid and immersed boundary (IB) methods. The grid is set to be equally spaced for simplicity of the code. The wall adapting the local eddy viscosity (WALE) model which is capable of predicting wall limiting behaviors without the calculation of the wall distance [26] is also adopted.

Spray models are based on a DDM (Discrete Droplet Model) which describes spray droplets by stochastic particles that are termed parcels, and spherical parcels having a diameter equal to the nozzle hole are injected. The KH-RT model [27] was used to simulate the primary and secondary breakup processes. When a spray parcel impinges on a wall, it is converted into a wall film parcel. This process was modeled, and here in this 143 following section, where wall film models implemented in HINOCA are introduced.

144 2.1 Spray-wall impingement model

145A number of spray-wall impingement models have been proposed [3-11]. The authors selected a model developed by Senda et al. [10-11] as the base model since it is 146comprehensive with consideration of the effects of the liquid film (wall film) thickness, 147148and the diameter and Weber number of the impinging droplets  $We_{1,n} (= \rho_l d_1 v_{1,n}^2 / \sigma_l, \rho_l$ : liquid density,  $d_1$ : diameter of droplets impinging on a wall, and,  $v_{1,n}$ : velocity component 149150of droplets, normal to a wall, with,  $\sigma_l$ : the surface tension). Further, the present study focuses on the wall film formation, and agreement of the wall film shape between the 151measurements and numerical simulation was demonstrated with the Senda model [28]. 152Note that the Senda model developed in the literatures [10-11] is only applicable to a 153limited range of temperatures of droplets and walls, where the boiling-induced breakup 154155is negligible.

Figure 1 (a) summarizes the classification of impinging droplet characteristics in the Senda model, where the non-dimensional film thickness  $\delta_N$  is defined as the film thickness  $\delta$  divided by droplet diameter  $d_1$  [10-11]. The model is divided into two regimes based on the Weber number,  $We_{1,n}$  of an impinging droplet as shown in Fig.1 (b).

160 (1) Low Weber number model ( $We_{1,n} \leq 300$ )

161 (1-1) Wet wall

162 Three types of breakup: rim type; cluster type; and column type are considered when 163 a droplet impinges on a wet wall, and the droplet diameter after the breakup  $d_2$  is given 164 as a function of the non-dimensional film thickness  $\delta_N$  to fit experimental results as 165 follows [29]:

166  $d_2/d_1 = 0.6478 - 0.5480 \,\delta_N + 1.9825 \,\delta_N^2 - 2.1082 \,\delta_N^3 + 0.6894 \,\delta_N^4$  (1) 167 The droplet velocity after the breakup is determined with the Weber number of the 168 bouncing droplet. The relation between the Weber number and non-dimensional film

 $\mathbf{6}$ 

169 thickness  $\delta_N$  is determined to fit experimental results as follows [29]:

170 
$$We_{2,t} = 0.3818 - 0.00537 \,\delta_N - 0.8937 \,\delta_N^2 + 0.8644 \,\delta_N^3 - 0.2301 \,\delta_N^4$$
 (2-1)

171 
$$We_{2,n} = -2.1518 + 1.1493 \,\delta_N + 26.238 \,\delta_N^2 - 24.480 \,\delta_N^3 - 5.5650 \,\delta_N^4$$
 (2-2)

where  $We_{2,t}$  is the Weber number, tangential to a wall, of the bouncing droplet, and  $We_{2,n}$ is that normal to a wall.

174 (1-2) Dry wall

175 Almost all droplets stick when impinging on a dry wall, but some bounce after the 176 impingement. A subsequent droplet likely collides with the foregoing one, causing 177 breakup of the droplets. The probability of the breakup can be estimated with a time 178 interval parameter,  $t_r$  which is defined as follows:

$$179 t_r = \Delta t / \tau_{res} (3)$$

180 where  $\Delta t$  is the time interval between the two continuous droplets reaching a wall, and  $\tau_{res}$ 181 is the droplet residence time on the wall, expressed as follows [30]:

182 
$$\tau_{res} = \pi \sqrt{\rho_l d_1^3 / (16\sigma_l)}$$
 (4)

The model defines that the breakup occurs at the *t*<sup>*r*</sup> from 0.4 to 0.6, where high breakup probabilities were determined in experiments [29]. In the present study, the diameter and velocity of the droplet after the breakup was calculated assigning  $\delta_N = 0$  in Equations (1), (2-1) and (2-2).

187 (2) High Weber number model (
$$We_{1,n} > 300$$
)

At  $We_{1,n}$  numbers above 300, the model assumes that the droplet impinging on a dry wall causes the breakup while that impinging on a wet wall leads to splashing or deposition in the wall film. The critical Weber number,  $We_{crit}$  is used as a criterion that distinguishes splashing from deposition, according to the experimental work of Cossali et al. [31] as follows:

193 
$$We_{crit} = (2100 + 5880 \,\delta_N^{1.44})La^{-0.2}$$
 (5)

- 194 where *La* is the Laplace number (=  $\sigma_l \rho_l d_1 / \mu_l^2$ ,  $\mu_l$  : liquid viscosity).
- 195 The droplet diameter after the breakup and splash is determined according to the 196 experimental data of Mundo et al. as follows [32]:

197 
$$d_2/d_1 = 3.932 \times 10^2 \times K^{-1.416}$$
 (for rough surfaces) (6)

198 
$$d_2/d_1 = 3.903 \times 10^{10} \times K^{-5.116}$$
 (for smooth surfaces) (7)

199 where *K* is a non-dimensional parameter defined as:

$$200 K = Oh \cdot Re^{1.25} (8)$$

with  $Oh = \mu_l / \sqrt{\rho_l \sigma_l d_1}$  the Ohnesorge number and  $Re = \rho_l d_1 v_{1,n} / \mu_l$  the Reynolds number. This study applied Equation (6) to wet walls, and Equation (7) to dry walls, in analogy with the original model.

The droplet velocity after the wall impingement is critical to determine the velocity of growth of a wall film as will be explained in Equation (12). The original model calculates the velocity while solving the balance between the energy needed to break up the droplet,  $E_{crit}$  and the kinetic energies of the droplets before the impingement,  $E_1$  and after the impingement (including droplets becoming part of the liquid film,  $E_f$  and being airborne,  $E_2$ ) as:

210 
$$E_1 - E_{crit} = E_f + E_2$$
 (9)

The film flow calculated with Equation (9), however, was inconsistent with the experimental results in this study. This study then employed the film flow model proposed by Kalantari and Tropea [33] which expresses the droplet velocity after the wall impingement as:

215 
$$v_{2,n}/v_{1,n} = -1.1 \cdot W e_{1,n}^{-0.36}$$
 (10)

216 
$$v_{2,t} = 0.862 \cdot v_{1,t} - 0.094$$
 (11)

with  $v_{2,n}$  the velocity component, normal to a wall, and  $v_{2,t}$  that tangential to a wall.

218 2.2 Film flow model

To calculate the flow characteristics of the wall film, a momentum balance equation

was solved. In the model, parcels of injected fuel are deposited on one IB cell which isassumed to form a rigid wall film, and the equation is expressed as:

222 
$$\Delta(M_f \vec{v}_f) = \sum (m_1 \vec{v}_1 - m_2 \vec{v}_2) + \vec{\tau}_{air} A dt - \vec{\tau}_w A dt$$
(12)

where  $M_f$  and  $\vec{v}_f$  are the total mass and velocity vectors of the wall film in a cell. The first term on the right side is the momentum provided from impinging droplets to the wall film, with  $m_1$  and  $m_2$  the mass of the droplets before and after impingement. The *A* is the area of the wall film and is identical with the cross-sectional area of the IB cell. The  $\tau_{air}$ is the shear force between the airflow and wall film, and the  $\tau_w$  is the frictional stress between the wall film and wall.

#### 229 2.3 Film vaporization model

The model proposed by O'Rourke and Amsden [12] was used to calculate the film 230vaporization and heat transfer to the wall film. This model considers the change in the 231232structure of the turbulent boundary layers above the wall films because of the gas velocity normal to the wall induced by vaporization and consequent convective transport. Two 233assumptions are made: (1) the total transport is independent of the coordinate normal to 234the wall and is the sum of the transport due to turbulent diffusion and due to convection 235236by the vaporization velocities; (2) there is a linear increase in the turbulent diffusivity 237with the distance from the wall.

The temperature profile in the wall film normal to the wall is approximated as linear, 238varying from the temperature at the wall  $T_w$  to the mean temperature  $T_f$  in the lower half 239(the half nearest the wall) of the film, and from  $T_f$  to the film surface temperature  $T_s$  in 240the upper half of the film, as schematically suggested in Fig.2, where  $\dot{Q}_s$  and  $\dot{Q}_w$  are 241the heat fluxes between the gas and liquid film, and between the liquid film and wall, and 242 $\lambda_l$  is the thermal conductivity of the liquid. The energy balance is solved considering the 243heat transfer between the gas and film and the wall and film, and the changes in the 244temperature resulting from the film movement and droplet impingement. 245

246 The mass vaporization rate,  $\dot{M}_{vap}$  is given by

247 
$$\dot{M}_{vap} = H_y \ln\left(\frac{1-y_v}{1-y_s}\right)$$
(13)

where  $y_v$  is the fuel vapor mass fraction, and  $y_s$  is the equilibrium vapor mass fraction at the surface temperature. One of the authors (Kobashi) has developed a method for estimating the vapor-liquid equilibrium of vaporizing multicomponent sprays with the Soave-Redlich-Kwong equation of state combined with the UNIFAC method [34], but Raoult's law for an ideal multicomponent mixture was employed for simplicity in this study since the fuels used were with non-polar molecules, and all numerical simulations were implemented at atmospheric pressure.

## $255 H_y$ is expressed as:

256 
$$H_{y} = \frac{\rho_{g} u_{\tau}}{y_{c}^{+} sc_{L} + \frac{Sc_{T}}{\kappa} ln\left(\frac{y^{+}}{y_{c}^{+}}\right)} \qquad \text{if } y^{+} > y_{c}^{+}$$
257 
$$H_{y} = \frac{\rho_{g} u_{\tau}}{y^{+} sc_{L}} \qquad \text{if } y^{+} < y_{c}^{+} \qquad (14)$$

where  $Sc_L$  and  $Sc_T$  are the laminar and turbulent Schmidt numbers,  $u_\tau$  is the frictional velocity defined as  $u_\tau = (\tau_w/\rho_g)^{0.5}$ ,  $y^+ = y \, u_\tau/v_L$ , y is the distance normal to the wall,  $\tau_w$  is the wall shear stress, and  $v_L$  is the kinematic viscosity. The transition between the laminar and fully turbulent region,  $y_c^+$  is 11.05, and Karmann's constant,  $\kappa$  is 0.433, according to the literature [12].

263 The wall film thickness,  $\delta$  was calculated as follows:

$$\delta = \frac{\Sigma V_p}{A} \tag{15}$$

where  $\sum V_p$  is the sum of the volume of parcels adhering to a wall defined by a Cut-Cell method, and *A* is the cross-sectional area of the wall.

## 267 **3. Experimental Setup and Procedures**

269In a constant volume vessel, the temporal development of the wall film area was 270measured with the refractive index matching (RIM) method which allows photography 271of the wall films based on the principle that the light transmission decreases when liquid is deposited on a frosted glass wall [2]. A schematic of the experimental system is shown 272in Fig.3. The fuel was pressurized by the high pressure pump and injected into the vessel 273in which the frosted glass wall was placed. Use of continuous light emitted from the metal 274halide lamp (Photron: HVC-UL) and a high speed digital camera (Vision Research: 275276Phantom-MIRO) allowed sequential imaging of deposition and flow of the wall film from the rear of the wall. Electrical signals sent from the pulse generator were utilized to 277determine the fuel injection period as well as the triggers for the injection and image 278279recording.

The arrangement of the sprays and the wall are shown in Fig.4. The injector was 280281equipped with a 6-hole nozzle. Spray from the No.6 nozzle impinged on the wall at an angle of 23° from a distance of 22 mm, while sprays of the No.2, 3, and 4 nozzles which 282were in the same plane and impinged at the angle of 45°. As the sprays of the No.1 and 5 283nozzles geometrically do not result in wall impingement, the numerical simulations were 284implemented only for the sprays No.2, 3, 4, and 6. The rear view image in Fig.4 (c) is an 285286example of the RIM image with the numbers of the sprays superimposed near the positions where impingement takes place. The dark areas represent regions where the wall 287film has formed, while the thicker film is located near the position of spray impingement 288and appears white as the wall film here became thicker than the surface roughness of the 289290frosted glass.

291 3.2 Measurement of the wall heat flux

The experimental setup for the measurements of the wall heat flux is shown in Fig.5. As shown in Fig.5 (a), the wall was placed below the injector, and a Loex-bodied thinfilm thermocouple developed by Enomoto [35] was embedded in the wall. The body 295material of the Loex has a density, heat capacity, and heat conductivity closely equivalent to the wall material. The diameter of the body of the thermocouple was 3.0 mm, and the 296297 diameter of the electrically-insulated center wire made of constantan was 0.15 mm. A thin copper film, about 10  $\mu$ m thick, was formed to establish a hot junction of the Loex – 298constantan with a very low heat capacity on the top surface of the thermocouple, while a 299cold junction was made inside the body of the thermocouple at the distance of 3.5 mm 300 from the top surface. Another thermocouple, of iron - constantan, was embedded near the 301 302cold junction and with the cold junction immersed in ice water. Overall, it was possible 303 to measure the temperature differences between the hot and cold junctions of the Loex constantan thermocouple and to calculate the wall heat flux as the absolute temperature 304 305 of the cold junction was measured with the iron – constantan thermocouple. The accuracy of the measurement system has been investigated by Enomoto who reported that the wall 306 307 heat flux measured was about 5 % higher than the true value [35].

The thermoelectrical power from the thermocouple was amplified and recorded with 308 the data logger. The temperature of the wall surface was controlled with a heater, based 309 on the temperature measured by the iron - constantan thermocouple. The fuel was 310 311pressurized with nitrogen gas and introduced to the injector. Electrical signals sent from 312the pulse generator were used to determine the fuel injection period as well as the triggers for the injection, data logging, and image recording. The wall film images were recorded 313with the high speed digital camera (NAC: HX-3) and the wall film was illuminated with 314 the metal halide lamp (Photron: HVC-UL), and recorded from a position diagonally 315316 above the wall.

Figure 5 (b) shows the layout of the fuel sprays and thermocouple for the measurement of the wall heat flux. The fuel injector equipped with a 6-hole nozzle was different from the one used in the film area measurements. The fuel spray injected from one nozzle hole orthogonally above the wall impinged on the thermocouple embedded in the piston while

the other sprays were masked with the metallic plate. The gap between the target spray and metallic plate is large enough, and it was confirmed that the other sprays have a limited impact on the target spray after the wall impingement with the movie.

### **4. Validation of the Model with iso-Octane**

### 325 4.1 Wall film area

Table 1 details the conditions under which the wall film areas were compared in the measurement and calculations. A single component fuel, iso-octane (2,2,4trimethylpentane, iC<sub>8</sub>H<sub>18</sub>) was injected from the 6-hole nozzle with nozzle diameters of 0.13 mm into a constant volume vessel at room temperature and atmospheric pressure. The injection pressure,  $p_{inj}$  was changed as the variable.

Figure 6 shows the images of (a) the wall film photographed with the RIM method 331 from the rear of the frosted glass wall, and (b) the calculated wall film thickness, with the 332 injection pressure,  $p_{inj}$  of 13 MPa. In Fig.9 (a), the darkly colored areas represent regions 333 where the wall film formed, and the thick film near the location of the spray impingement 334 335 appear as white. In Fig.7 (b), the overall shape of the calculated wall film is very similar to the photograph, the calculated thicker region presented in red corresponds to the white 336 regions in the measured image. The thicker films formed at the location far from the spray 337 impingement points, and the film thickness other than the thicker region was in the order 338 339 of 10  $\mu$ m. These observations are in agreement with film thickness distributions of a 340 literature [36], in which the experimental conditions are similar to the present study.

Figure 7 shows profiles of the wall film area plotted for different injection pressures  $p_{inj}$ . Here, the film area in the calculations was defined as the sum of the areas where the film thickness was larger than 1  $\mu$ m, corresponding to the detectable level in the measurements. The measured results show that the wall film area increased with time until 5.5 ms, and then it maintained a nearly constant size. The higher injection pressure increased the wall film area. The calculations captured the changes in the initial spreading process of the film area, and the fact that the film area increased with increasing injection pressure, however the calculations underestimate the film area at the lower injection pressure. The reason for this discrepancy may be due to underestimation of the impinging droplet diameter at the lower injection pressures, and may be attributed to the droplet breakup model and the critical Weber number.

352 4.2 Heat flux between the film and wall

The heat flux between the film and wall,  $\dot{Q}_w$  would be an appropriate factor to validate the model as it plays an important role in the wall film vaporization as well as because accurate predictions of wall film formation and movement are required in the predictions.

Table 2 details the conditions under which the measured and calculated wall heat flux values were compared. A single component fuel, iso-octane was injected from an injector equipped with a 6-hole nozzle with nozzle diameters of 0.248 mm. The long injection period of 4 ms was adopted to measure the heat flux in a quasi-steady state. The heat flux was measured for one spray impinging on the wall as explained in Section 3.2, while the calculation assumed a single-hole nozzle with the same diameter. In the calculation, the heat flux between the film and wall,  $\dot{Q}_w$  was calculated as follows:

$$364 \qquad \dot{Q}_w = \lambda_l \frac{T_f - T_w}{\delta/2} \tag{16}$$

365 where 
$$\lambda_1$$
 is the liquid thermal conductivity.

Figure 8 shows photographs and calculated images of the wall film at 7 ms after the start of injection where the wall film is in the quasi-steady state. In Fig.8 (a), the photos were taken from the diagonally upward direction at an angle of 45° as shown in Fig.5 (a), making the scale of the picture longitudinally compressed. The calculated images in Fig.8 370 (b) superimposes dashed circles equivalent to the measured diameter of the wall film. Unlike the situation in Fig.7, the calculations overestimated the wall film spread. This 371372may be due to differences in the wall surface roughness, or due to differences between the effect of the oblique and orthogonal impingements. However, the calculations 373captured the experimental observation that the edge of the wall film was thicker than the 374central portion. There was boiling at the center of the wall film in both the (a) 375photographed and (b) calculated images at  $T_w$  of 100°C which is slightly higher than the 376 377 boiling point of iso-octane. Further, at the  $T_w$  of 120°C, the boiling was taking place over the whole of the wall film in the photograph (a), and the calculation shows less wall film 378in (b), indicating that actually most of the wall film had vaporized. 379

Figure 9 plots the profiles of the heat flux of the measurements and calculations, where 380 the wall temperature,  $T_w$  was set at 120°C. In the calculations, the heat flux was calculated 381 382for the region just below the nozzle, considering the area equivalent to the top surface of the thermocouple. The direction of the heat transfer toward the wall was defined as 383 positive. Since the temperature of the fuel spray is lower than the wall temperature, the 384heat transferred from the wall to the spray or wall film results the negative value. Both 385386 the measured and calculated heat fluxes decreased rapidly immediately after the spray 387 impingement, and they gradually increased from 4 ms after the start of injection when no spray reached impingement to the wall. Averaging the heat flux from 1 ms to 2.5 ms after 388 the start of injection, the measured value was  $-4.1 \text{ MW/m}^2$ , with the calculated value -3.5389  $MW/m^2$ , a difference of about 15%. 390

Figure 10 plots the change in the heat flux with the wall temperature  $T_w$  as measured and calculated. The heat flux decreased with the increase of the  $T_w$ . According to Schulz et al. who determined the transient wall temperature and heat flux at the spray impingement zone using an infrared thermography for an extensive range of influencing factors, the heat fluxes during the spray impact are -3 MW/m<sup>2</sup> at the  $T_w$  of 80°C and -4

396 MW/m<sup>2</sup> at the  $T_w$  of 120°C [37], which correspond to the heat flux measured in the present 397 study. There were the differences in the absolute values of the heat flux between the 398 measurements and calculations, but the decreases with  $T_w$  are practically identical, with 399 similar global gradients.

Figure 11 plots the change in the heat flux with the distance from the nozzle to the wall as measured and calculated. The heat flux increased with the increase of the distance. The trend corresponds to the results of Schulz et al. [37], but it has a limited impact on the heat fluxes measured and calculated within the range of the present study.

## 404 5. Formation and Vaporization of the Wall Film with a Gasoline Surrogate Fuel

# 405 5.1 Specification of the gasoline surrogate fuel

406 The composition of the gasoline surrogate fuel was determined to meet the octane number, aromatic content, and distillation curve of the regular gasoline available in Japan. 407 It was assumed that the RON (research octane number) can be expressed as a volume-408 averaged property, and the distillation curve was calculated following a calculation 409 410 method reported elsewhere [38]. It assumes an open system where the vaporized fuel is vented. The heat, Q is continuously supplied from outside the system to the liquid, and 411 consumed in increasing the temperature up to and vaporizing the liquid. Considering a 412vapor-liquid equilibrium (VLE), the composition in the liquid and vapor phases is 413414 calculated and renewed at every time step, via a VLE calculation with NIST 415SUPERTRAPP [39] which solves the Peng-Robinson equation of state [40].

Table 3 (a) details the components selected as the composition of the gasoline surrogate fuel, the properties, and the mixing fractions. The five components are needed to reproduce the desired distillation curve. Considering that the aromatics have higher boiling points than a range of other gasoline components [14], 1,2,4-trimethylbenzene 420 (C<sub>9</sub>H<sub>12</sub>) was chosen as the highest boiling point component, however, iso-butylbenzene 421 (C<sub>10</sub>H<sub>14</sub>) was used as a substitute in the calculations due to the lack of information on the 422 thermodynamic properties of 1,2,4-trimethylbenzene. Iso-pentane was chosen as the 423 lowest boiling point component since it exhibits low reactivity (high RON), and it is liquid 424 at the conditions involved here and is simple to handle. The medium boiling point 425 components: n-heptane, iso-octane, and toluene, function to adjust the RON and aromatic 426 content.

The properties and distillation curve of the gasoline surrogate fuel are shown in Table 3 (b) and Fig.12. The properties of the surrogate fuel are closely identical to the reference regular gasoline (commonly available in Japan). The distillation curve appears well matched, except for the disagreement at the distillation ratios from 40% to 80% and near the end point.

432 5.2 Formation and Vaporization of the Wall Film

In this section, first, the accuracy of the present model is evaluated by comparing the film area of the gasoline surrogate fuel as measured and calculated. Second, the vaporization process of a wall film of the gasoline surrogate fuel is discussed with the calculations.

The conditions under which the film area was evaluated are identical with Table 1, with the injector - wall arrangement, that in Fig.3 and 4, except for the wall temperature  $T_w$  of 60°C and the fuels tested. The fuel was injected with the pressure of 13 MPa into ambient air at atmospheric pressure.

Figure 13 shows the changes in the calculated film mass distributions of (a) the gasoline surrogate fuel and (b) the iso-octane. For the gasoline surrogate fuel there were no significant observable changes in the distributions of the wall film mass as shown in Fig.13 (a). The wall film vanished from the thinner film with (b) iso-octane since the heat flux inversely increased with the film thickness as expressed in Eq.(16). 446 Figure 14 plots (a) the measured and calculated area of the wall film and (b) the calculated film mass of the gasoline surrogate fuel and iso-octane at the wall temperature 447448  $T_w$  of 60°C. In Fig.14 (a), the measured film area of iso-octane (red open squares) decreased due to the vaporization noted from 5 ms after the start of injection. The wall 449 film of the gasoline surrogate fuel (blue open circles) show a wider film area than that of 450iso-octane, which decreased at a slow rate. This tendency matched with the experiment 451of Schulz [24]. The calculations underestimated the film area of the gasoline surrogate 452453fuel (solid blue line). This is because iso-pentane which is the lowest boiling point component may be assumed to form a vaporized layer on the wall immediately after the 454wall impingement and this layer reduces the heat flux from the wall to the film in the 455experiment, a process that was not incorporated in the calculations. Other than this 456inconsistency, the calculations demonstrate good agreement with the measurements and 457458capture the changes in the vaporization process from 5 ms after the start of injection. The changes in the calculated film mass in Fig.14 (b) reflect the results with the measured 459changes. 460

Figure 15 plots the calculated profiles of the mass fraction of the components present 461462in the wall film of the gasoline surrogate fuel. Compared with the original mass fractions 463 detailed in Table 3, it is clear that most of the iso-pentane (solid black plot) vaporized immediately after the wall impingement. For the medium boiling point components: iso-464octane (solid blue line), n-heptane (dashed black line), and toluene (solid gray line), the 465wall temperature  $T_w$  of 60°C is lower than their boiling points, and the vaporization was 466 467 at slower rates. At 20 ms after the start of injection, the highest boiling point component 468 iso-butylbenzene (dashed red line) formed the largest quantity of the wall film as little 469 had vaporized at the wall temperature here. Considering that the aromatic contents have higher boiling points among a range of gasoline components, they would present the 470possibility to yield soot, feeding the pool fires occurring in the warm-up operations of 47118

## 473 6. Conclusions

The present study developed a CFD model to predict the wall film formation and vaporization of multicomponent fuel sprays. The calculated results with the model were validated by a comparison with actual measurements. Finally, the model was used to understand details of the wall film behavior of a gasoline surrogate fuel. The conclusions may be summarized as follows:

- The calculations with the developed model reproduce the observed trend that the filmarea increases with increases in the fuel injection pressure.
- 2. The calculated film thickness at the edge of the wall film is thicker than at the centralportion, similar to the observation in the experiments.
- With iso-octane (boiling point 99.3°C), boiling occurs from the center of the wall film
  at the wall temperature of 100°C, and the whole wall film boils at the wall temperature
  of 120°C. The calculated results are consistent with these observations.
- 4864. The heat flux from the wall to the wall film increases with the increase in the wall487487 temperature, and the calculations also reproduce this change well.

488 5. At the wall temperature of 60°C, the wall film of the gasoline surrogate fuel exhibits
489 a very low vaporization rate, compared to that of pure iso-octane. This is because the

490 highest boiling point component in the surrogate fuel remains unevaporated in the

491 wall film. As aromatics are generally the higher boiling point components in gasoline,

they are potential sources of pool fires and soot in DISI gasoline engines.

493 In order to additionally validate the calculated film formation and evaporation processes,

494 at higher ambient pressure, further measurements should be planned.

## 496 Acknowledgements

This work was supported by Council for Science, Technology and Innovation (CSTI),
Cross-ministerial Strategic Innovation Promotion Program (SIP), "Innovative
combustion technology" (funding agency: JST).

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# 501 References

- 502 [1] Stevens, E. and Steeper, R., Piston Wetting in an Optical DISI Engine: Fuel Films,
   503 Pool Fires, and Soot Generation, SAE Technical Paper, No.2001-01-1203 (2001).
- 504 [2] Drake, M., Fansler, T., Solomon, A. and Szekely, G., Piston Fuel Films as a Source of
   505 Smoke and Hydrocarbon Emissions from a Wall-Controlled Spark-Ignited Direct 506 Injection Engine, SAE Technical Paper, No.2003-01-0547 (2003).
- 507 [3] Naber, J. D. and Reitz, R. D., Modeling Engine Spray/Wall Impingement, SAE
  508 Technical Paper, No. 880107 (1988).
- [4] Bai, C. and Gosman, A. D., Development of Methodology for Spray Impingement
   Simulation, SAE Technical Paper, No.950283 (1995).
- [5] Stanton, D. W. and Rutland, C. J., Modeling Fuel Film Formation and Wall Interaction
   in Diesel Engines, SAE Technical Paper, No.960628 (1996).
- [6] Mundo, C., Sommerfeld, M. and Tropea, C., Droplet-Wall Collisions: Experimental
  Studies of the Deformation and Breakup Process, Int. J. Multiphase Flow, Vol.21,
  No.2 (1995) 151-173.
- [7] Köpple, F., Jochmann, P., Hettinger, A. and Kufferath, A., A Novel CFD Approach for
  an Improved Prediction of Particulate Emissions in GDI Engines by Considering the
  Spray-Cooling on the Piston, SAE Technical Paper, No.2015-01-0385 (2015).
- [8] Kuhnke, D., Spray / Wall Interaction Modeling by Dimensionless Data Analysis, Ph D Thesis, University of Darmstadt (2004).
- [9] Zhang, Y., Jia, M., Liu, H. and Xie, M., Development of an Improved Liquid Film
  Model for Spray/Wall Interaction under Engine-Relevant Conditions, Int. J.
  Multiphase Flow, Vol.79 (2016) 74-87.
- [10] Senda, J., Kanda, T., Al-Roub, M., Farrell, P. V., Fukami, T. and Fujimoto, H.,
  Modeling Spray Impingement Considering Fuel Film Formation on the Wall, SAE
  Technical Paper, No. 970047 (1997).
- [11] Senda, J. and Fujimoto, H., Multidimensional Modeling of Impinging Sprays on the
  Wall in Diesel Engines, American Society of Mechanical Engineers, Applied
  Mechanical Review, Vol.52, No.4 (1999) 119-138.
- 530 [12] O'Rourke, P. J. and Amsden, A. A., A Particle Numerical Model for Wall Film
  531 Dynamics in Port-Injected Engines, SAE Technical Paper, No.961961 (1996).
- 532 [13] Jiao, Q. and Reitz, R. D., Modeling Soot Emissions from Wall Films in a Direct-
- 533 Injection Spray-Ignition Engine, International Journal of Engine Research, Vol.16,

534 Issue 8, (2014) 994-1013.

- 535 [14] Kalghatgi, G., Fuel/Engine Interactions, Chapter 2, SAE International (2014)
- [15] Jin, J. D. and Borman, G. L., A Model for Multicomponent Droplet Vaporization at
   High Ambient Pressures, SAE Technical Paper, No.850264 (1985).
- 538 [16] Ayoub, N. S. and Reitz, R. D., Multidimensional Computation of Multicomponent
   539 Spray Vaporization and Combustion, SAE Technical Paper, No.950285 (1995).
- [17] Lippert, A. M. and Reitz, R. D., Modeling of Multicomponent Fuels Using
  Continuous Distributions with Application to Droplet Evaporation and Sprays, SAE
  Technical Paper, No.972882 (1997).
- 543 [18] Miyagawa, H., Nagaoka, M., Akihama, K. and Fujikawa, T., Numerical Analysis on
  544 Multi-Component Fuel Behaviors in a Port-Injection Gasoline Engine, SAE Technical
  545 Paper, No.1999-01-3642 (1999).
- [19] Ra, Y. and Reitz, R. D., The application of a Multicomponent Droplet Vaporization
  Model to Gasoline Direct Injection Engines, International Journal of Engine Research,
  Vol.4, No.3 (2003) 193-218.
- [20] Kawano, D., Senda, J., Wada, Y., Fujimoto, H., Goto, Y., Odaka, M., Ishii, H. and
  Suzuki, H., Numerical Simulation of Multicomponent Fuel Spray, SAE Technical
  Paper, No.2003-01-1838 (2003).
- [21] Zhang, L. and Kong, S.-C., High-Pressure Vaporization Modeling of MultiComponent Petroleum-Biofuel Mixtures Under Engine Conditions, Combustion and
  Flame, Vol.158, Issue 9 (2011) 1705-1717.
- [22] Hosain, M. L., Fdhila, R. B. and Daneryd, A., Heat Transfer by Liquid Jets Impinging
  on a Hot Flat Surface, Applied Energy, Vol.164 (2016) 934-943.
- [23] Köpple, F., Jochmann, P., Kufferath, A. and Bargende, M., Investigation of the
  Parameters Influencing the Spray-Wall Interaction in a GDI Engine Prerequisite for
  the Prediction of Particulate Emissions by Numerical Simulation, SAE Int. J. Engines
  6 (2) (2013) 911-925.
- [24] Schulz, F. and Beyrau, F., Systematic Investigation of Fuel Film Evaporation, SAE
   Technical Paper, No.2018-01-0310 (2018).
- 563 [25] Mizobuchi, Y., Development of Automotive Engine Combustion Simulation
  564 Software "HINOCA", (written in Japanese) Journal of the Combustion Society of
  565 Japan, Vol.58, No.186 (2016) 191-196.
- [26] Ducros, F., Nicoud, F. and Poinsot, T., Wall-Adapting Local Eddy-Viscosity Models
   for Simulations in Complex Geometries, Proceedings of the Conference on Numerical
   Methods for Fluid Dynamics (1998) 293-299.
- [27] Beale, J. C. and Reitz, R. D., Modeling Spray Atomization with the KelvinHelmholtz/Rayleigh-Taylor Hybrid Model, Atomization and Sprays, Vol.9, Issue 6
  (1999) 623-650.

- [28] Tomoda, T., Kawauchi, M., Kubota, M., Nomura, Y. and Senda, J., Modeling of Wall
  Impinging Behavior with a Fan Shaped Spray, SAE Technical Paper, No.2003-011841 (2003).
- [29] Al-Roub, M., Farrell, P. V. and Senda, J., Near Wall Interaction in Spray Impingement,
   SAE Technical Paper, No.960863 (1996).
- [30] Ueda, T., Enomoto, T. and Kanematsu, M., Heat Transfer Characteristics and
  Dynamic Behavior of Saturated Droplets Impinging on a Heated Vertical Surface,
  Bulletin of the JSME, Vol.22, No.167 (1979) 724-732.
- [31] Cossali, G. E, Coghe, A. and Marengo, M., The Impact of a Single Drop on a Wetted
  Solid Surface, Experiments in Fluids, Vol.22, Issue 6 (1997) 463-472.
- [32] Mundo, C., Sommerfeld, M. and Tropea, C., Droplet-Wall Collisions: Experimental
  Studies of the Deformation and Breakup Process, International Journal of Multiphase
  Flow, Vol.21, No.2 (1995) 141-173.
- [33] Kalantari, D. and Tropea, C., Spray Impact onto Flat and Rigid Walls: Empirical
  Characterization and Modeling, International Journal of Multiphase Flow, Vol.33,
  Issue 5 (2007) 525-544.
- [34] Kobashi, Y., Kimoto, Y. and Kato, S., Experimental Validation of a Droplet
   Vaporization Model for Ethanol-Blended Fuels and its Application to Spray
   Simulation, SAE Technical Paper, No.2014-01-2733 (2014).
- [35] Enomoto, Y. and Furuhama, S., Study on Thin Film Thermocouple for Measuring
  Instantaneous Temperature on Surface of Combustion Chamber Wall in Internal
  Combustion Engine, Bulletin of JSME, Vol.28, No.235 (1985) 108-116.
- [36] Schulz, F. and Beyrau, F., The Effect of Operating Parameters on the Formation of
  Fuel Wall Films as a Basis for the Reduction of Engine Particulate Emissions, Fuel,
  Vol.238 (2019) 375-384.
- [37] Schulz, F., Schmidt, J., Kufferath, A. and Samenfink, W., Gasoline Wall Films and
  Spray/Wall Interaction Analyzed by Infrared Thermography, SAE Int. J. Engines 7(3)
  (2014) 1165-1177.
- [38] Senda, J., Higaki, T., Sagane, Y., Fujimoto, H., Takagi, Y. and Adachi, M., Modeling
  and Measurement on Evaporation Process of Multicomponent Fuels, Journal of
  Engines, Vol.109, Section 3 (2000) 347-358.
- [39] Friend, D. G. and Huber, M. L., Thermophysical Property Standard Reference Data
   from NIST, International Journal of Thermophysics, Vol.15, No.6 (1994) 1279-1288.
- [40] Peng, D.-Y. and Robinson, D. B., A New Two-constant Equation of State, Ind. Eng.
  Chem. Fundam., Vol.15, No.1 (1976) 59-64.
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1188	Table 1	Conditions for the film area r	neasurements and	l ca
1189				
1190	-			
1191		Ambient pressure	[MPa]	
1192	-	Ambient temperature	[°C]	
1193	-		[0]	
1194		Wall temperature, $T_{\mu}$	[°C]	
1195	-	Nozzle diameter	[mm]	
1196	-		[]	
1197		Injection pressure	[MPa]	
1199	-	Injection period	[ms]	
1200	-		[]	
1201		Fuel		
1202	_			
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alculations with iso-octane

1100			
1190 1191	Ambient pressure	[MPa]	0.10
1192	Ambient temperature	[ºC]	20
1193		[ 0]	20
1194	Wall temperature, $T_{}$	[°C]	20
1195	Nozzle diameter	[mm]	0.13
1196		[]	0.10
1197 1198	Injection pressure	[MPa]	5, 13, 20
1199	Injection period	[ms]	2.5
1200	Fuel		<b>.</b>
1201	Fuel		iso-octane
1202			(C <sub>8</sub> H <sub>18</sub> )
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Table 2Conditions used in evaluating the wall heat flux of iso-octane

28 29	Ambient pressure	[MPa]	0.10
30	Ambient temperature	[°C]	20
2	Wall temperature, $T_{w}$	[°C]	30, 60, 100, 120
	Nozzle diameter	[mm]	0.248
	Injection pressure	[MPa]	10
	Injection period	[ms]	4
	Impinging distance	[mm]	30, 40, 50
	Impinging angle	[° ]	90
	Total Injection quantity	[mg]	109
	Fuel		iso-octane
			$(C_{g}H_{1g})$

 $1266 \\ 1267$ 

- Table 3
   Gasoline surrogate fuel proposed in the present study
  - (a) boiling point and RON of single component fuels and their mixing fraction
    - (b) properties of gasoline surrogate fuel, compared with regular gasoline referenced

269			Boiling point [°C]	RON [-]	Volume fraction [vol.%]	Mass fraction [wt.%]
270		iso-pentane (C <sub>5</sub> H <sub>12</sub> )	28.0	96	45	39
271		n-heptane (C <sub>7</sub> H <sub>16</sub> )	98.4	0	10	10
272	(a)	iso-octane (C <sub>8</sub> H <sub>18</sub> )	99.3	100	20	20
273		Toluene (C <sub>7</sub> H <sub>8</sub> )	110.6	111	10	12
274		1,2,4-trimethylbenzene (C <sub>9</sub> H <sub>12</sub> )*	169.4	108	15	19
275						

 $^*$  replaced by iso-butylbenzene (C $_{10}H_{14}$ ) in the present study

(b)

Gasoline surrogate fuel	Reference regular gasoline		
90.5	90.8		
25.0	25.4		
711	730		
404	N/A		
	Gasoline surrogate fuel 90.5 25.0 711 404		